Lecture 2: Knowledge Graph Embedding Models

Relational Learning

İsmail İlkan Ceylan Advanced Topics in Machine Learning, University of Oxford 20.01.2021

Overview

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- A glimpse at embedding models

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- Translational models: TransE and RotatE

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- Summary

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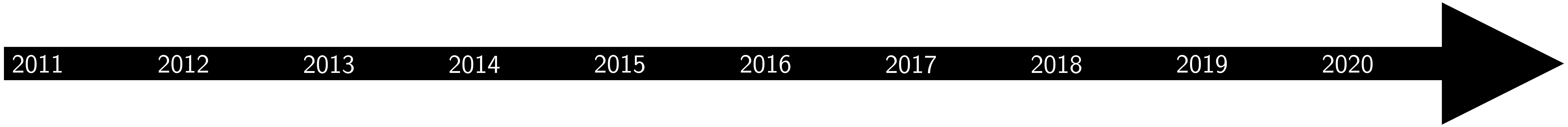

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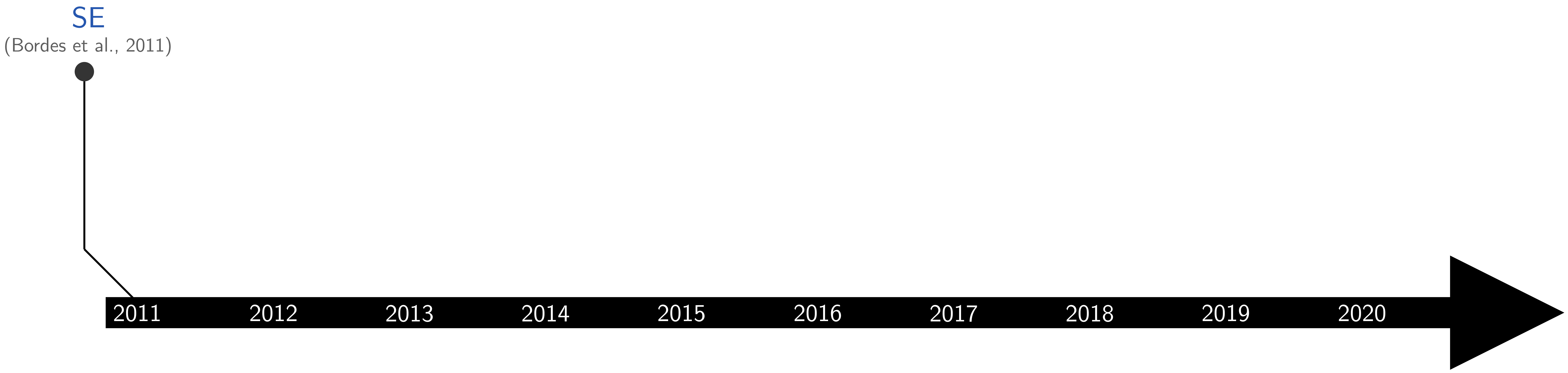

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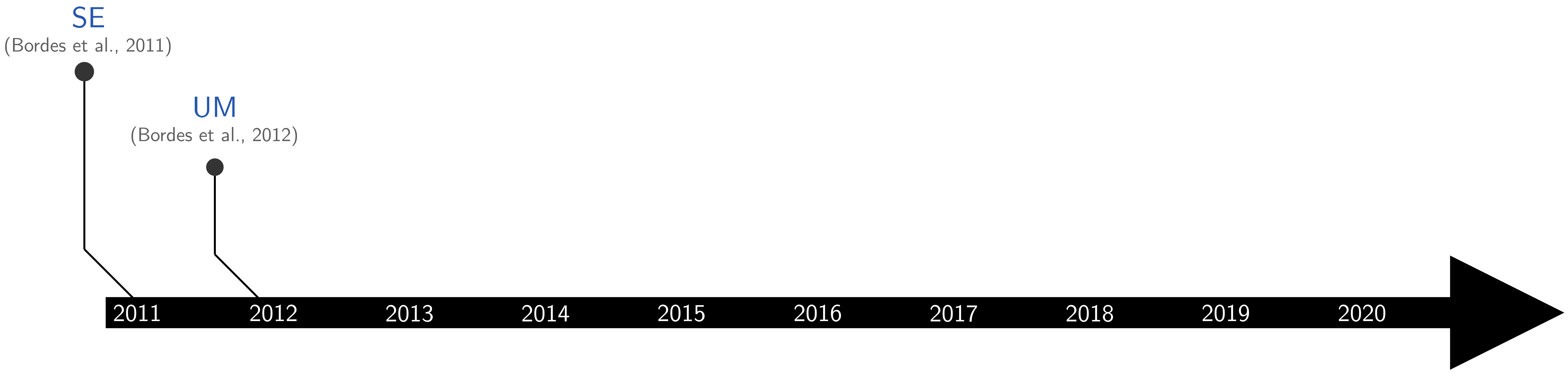

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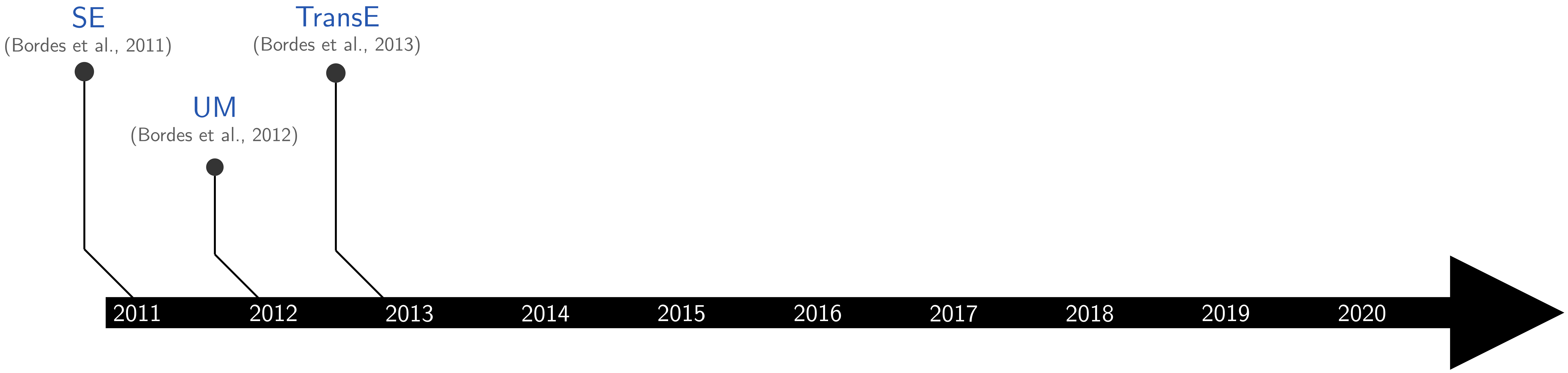

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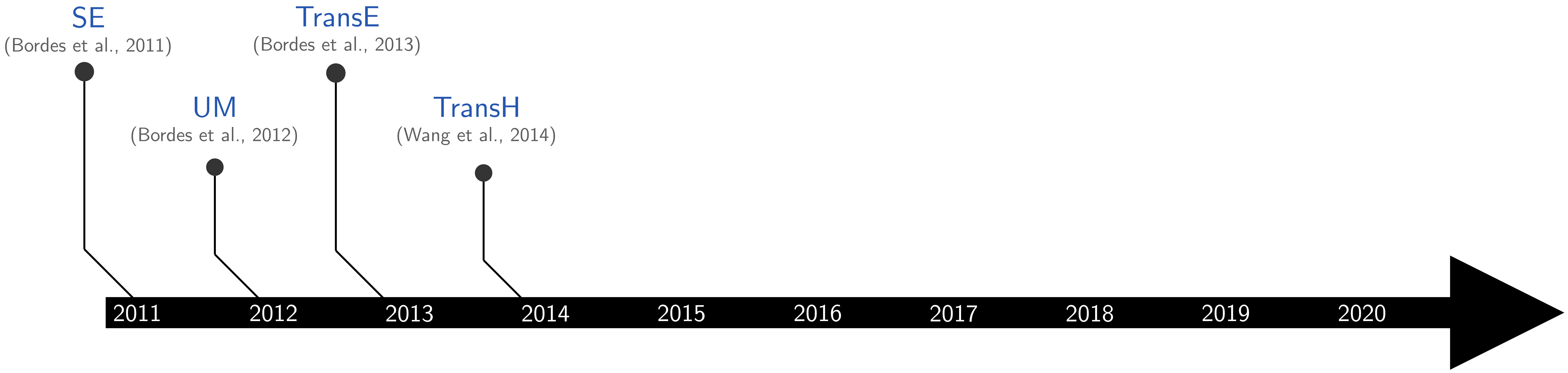

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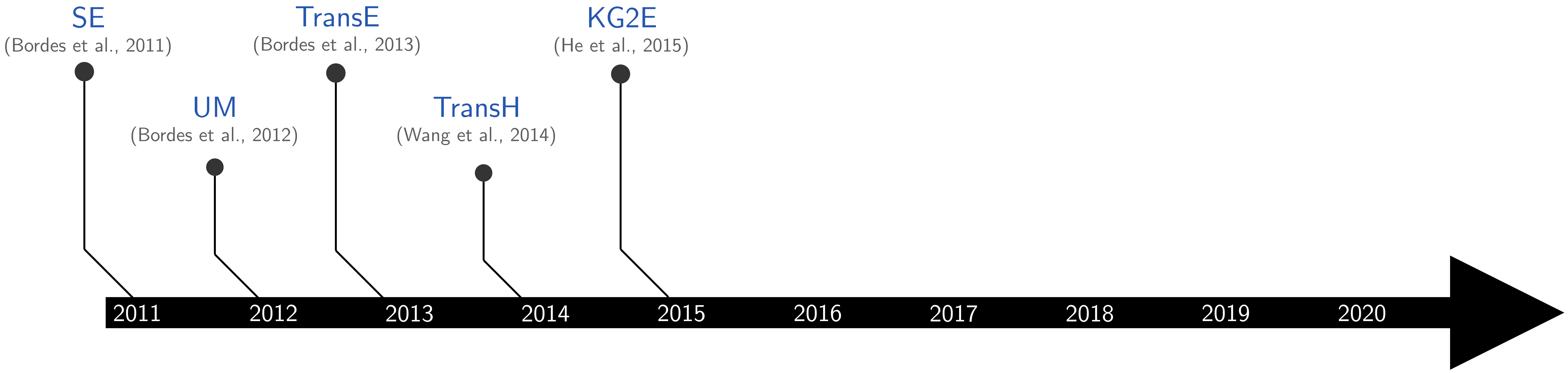

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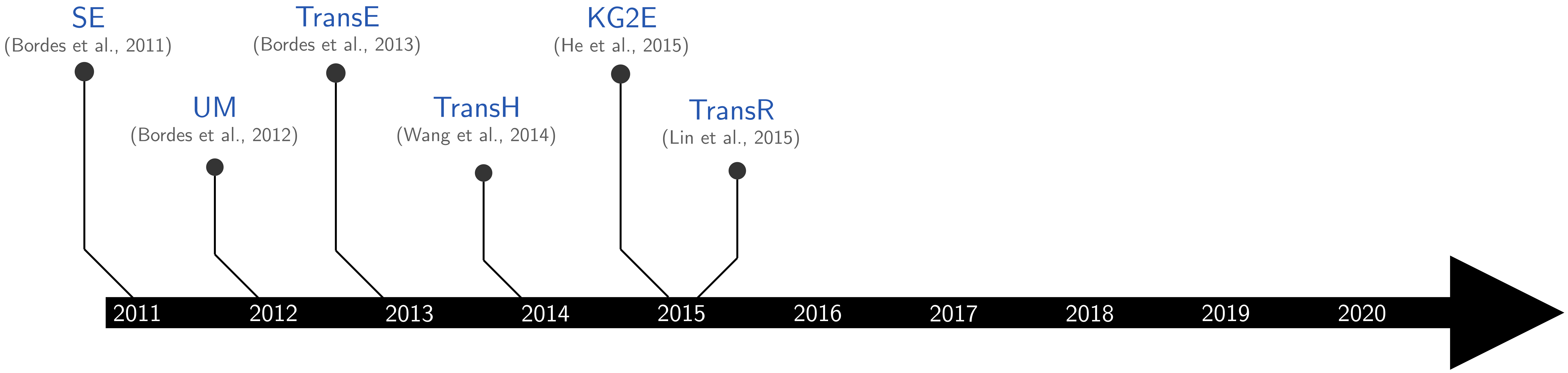

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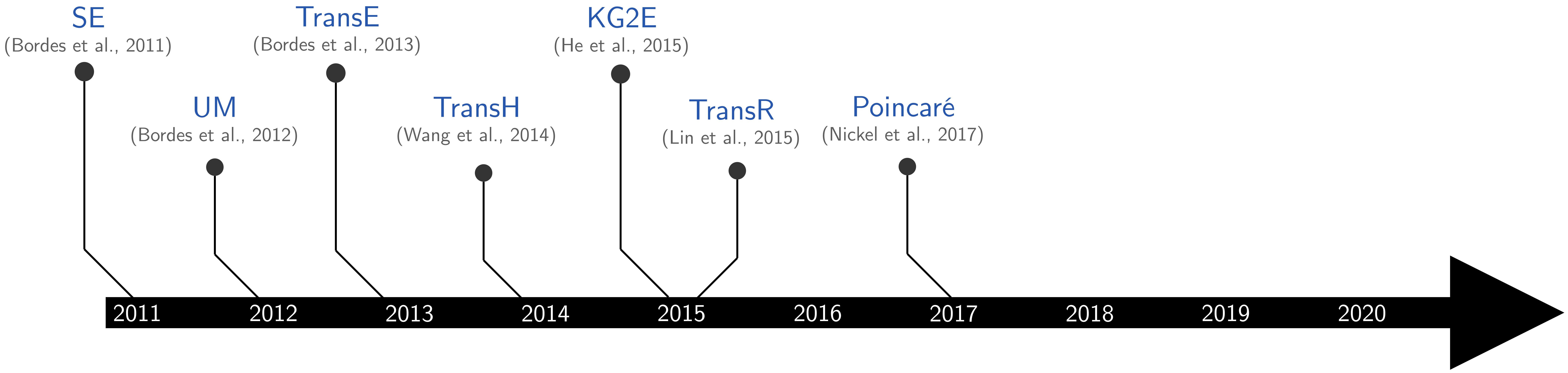

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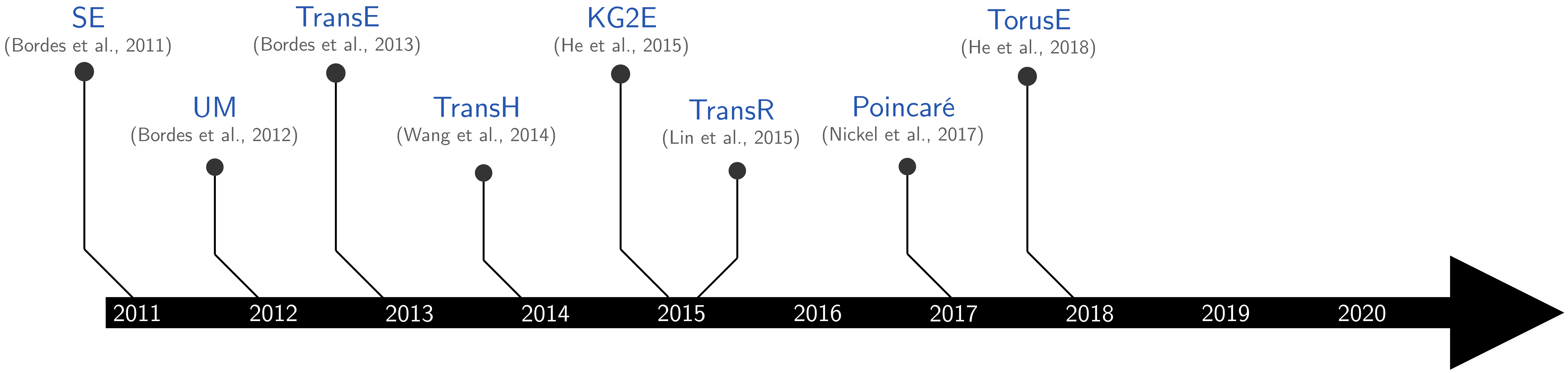

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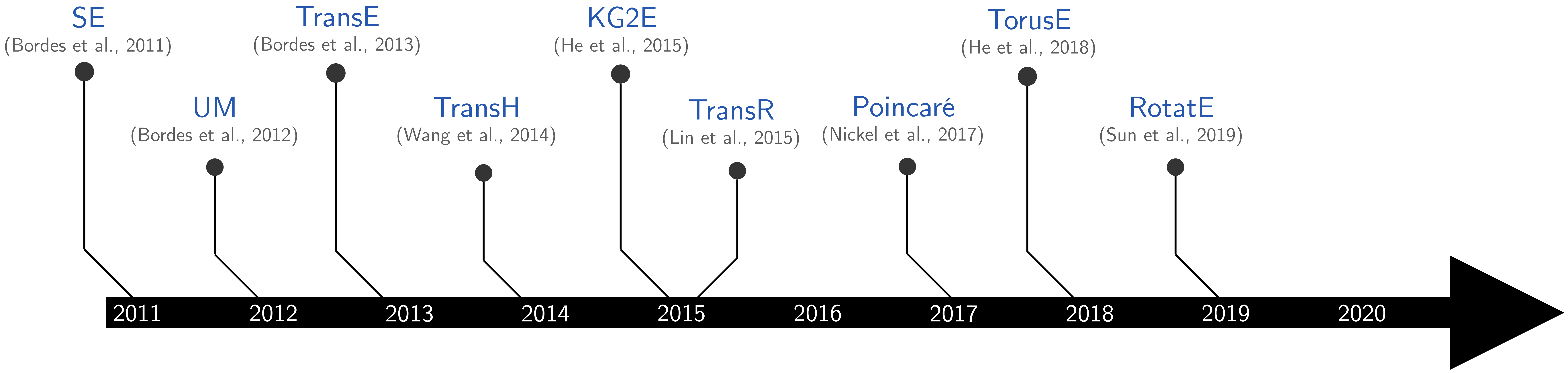

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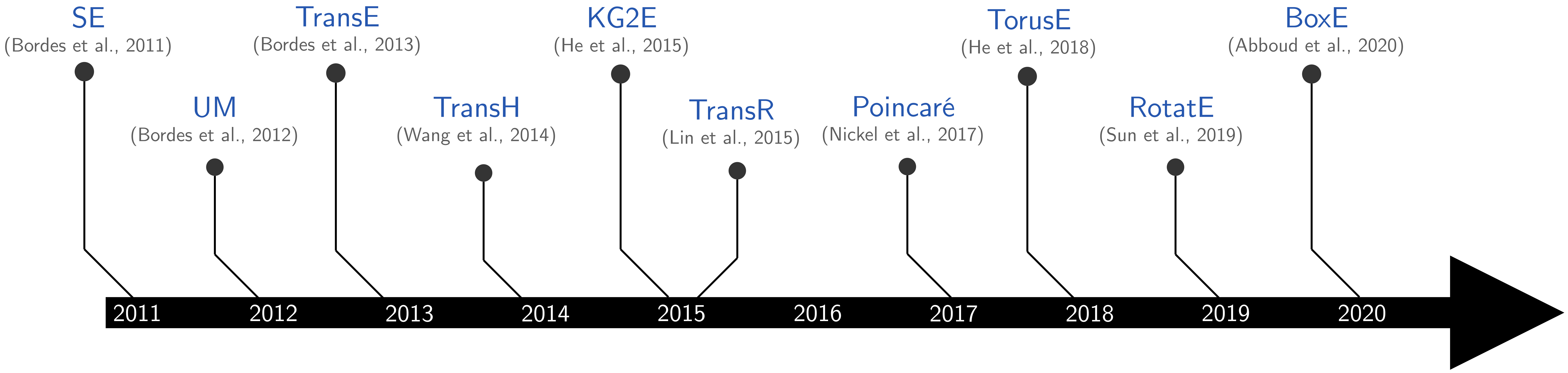

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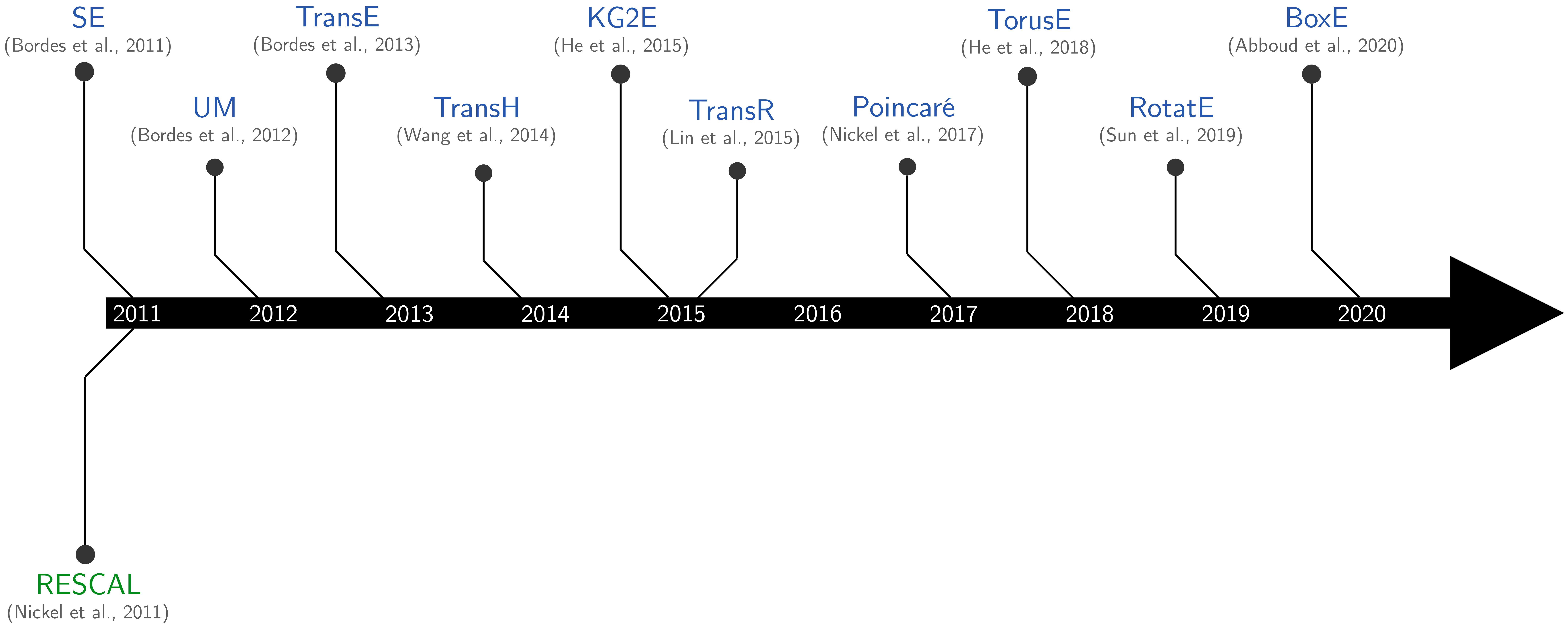

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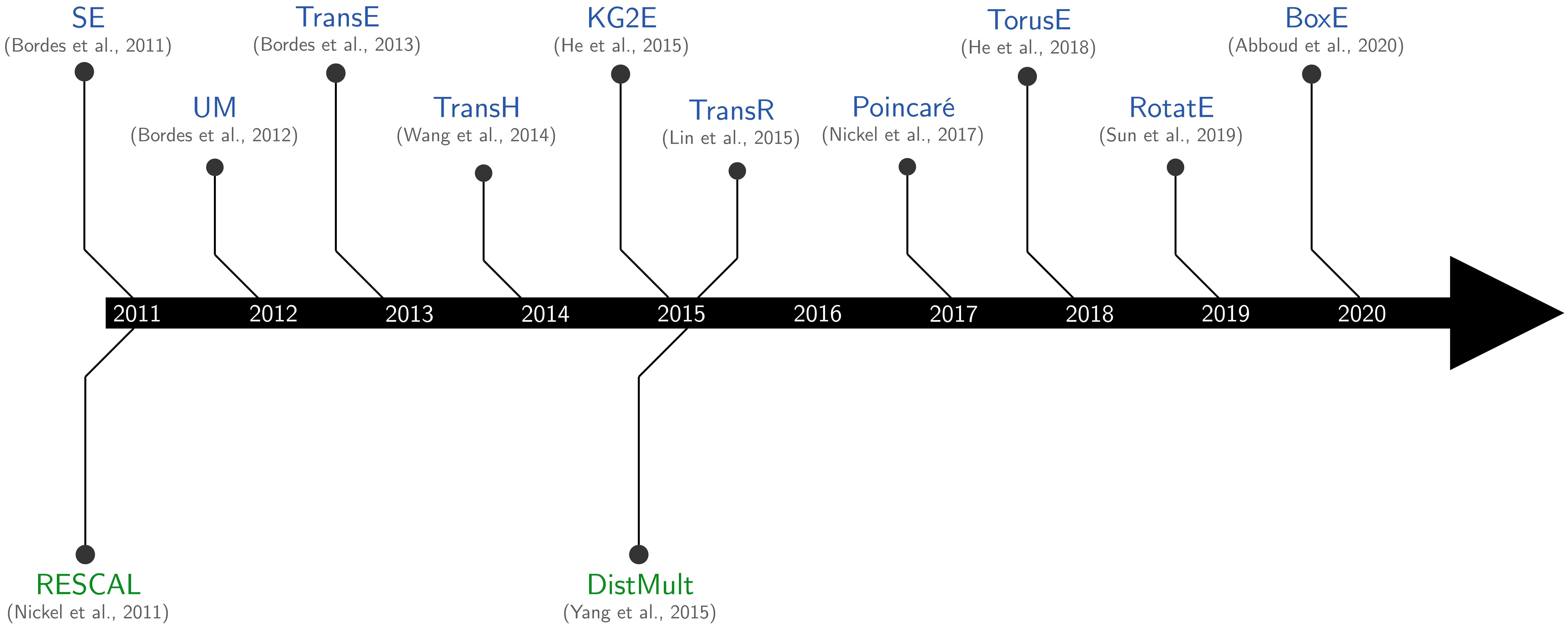

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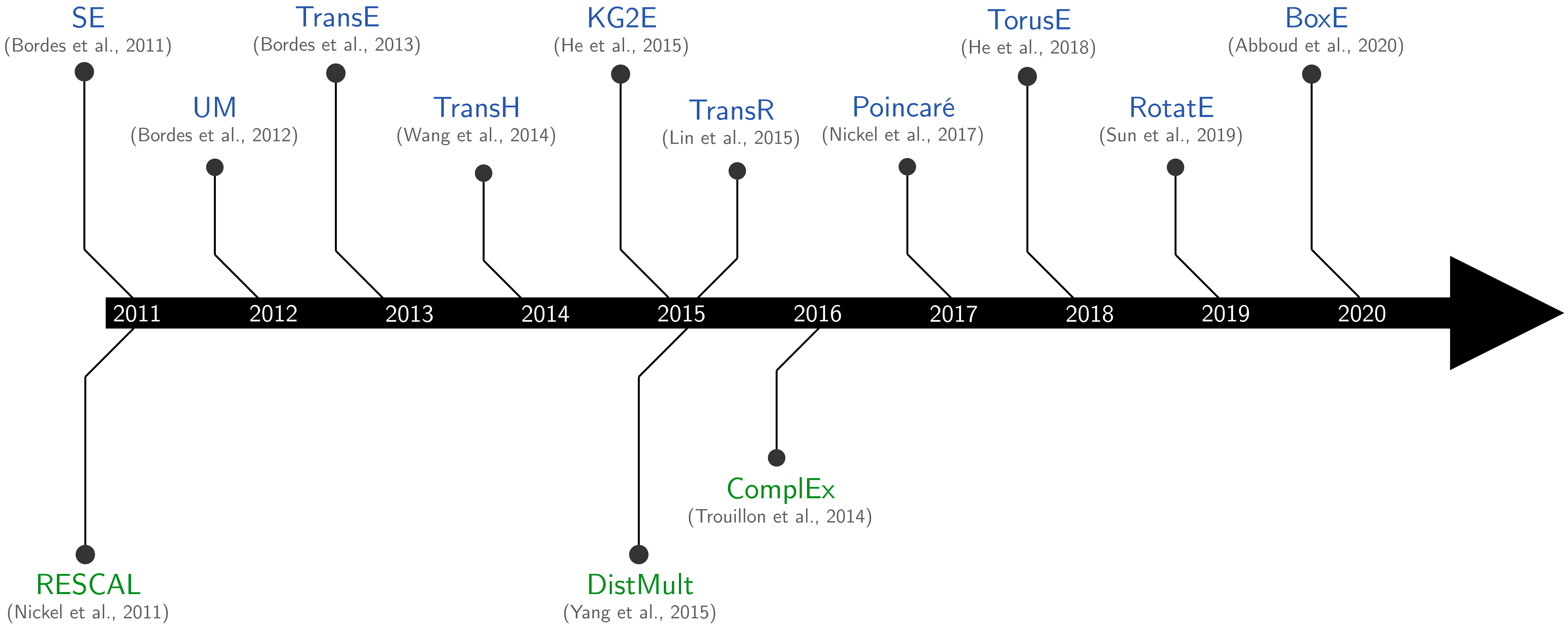

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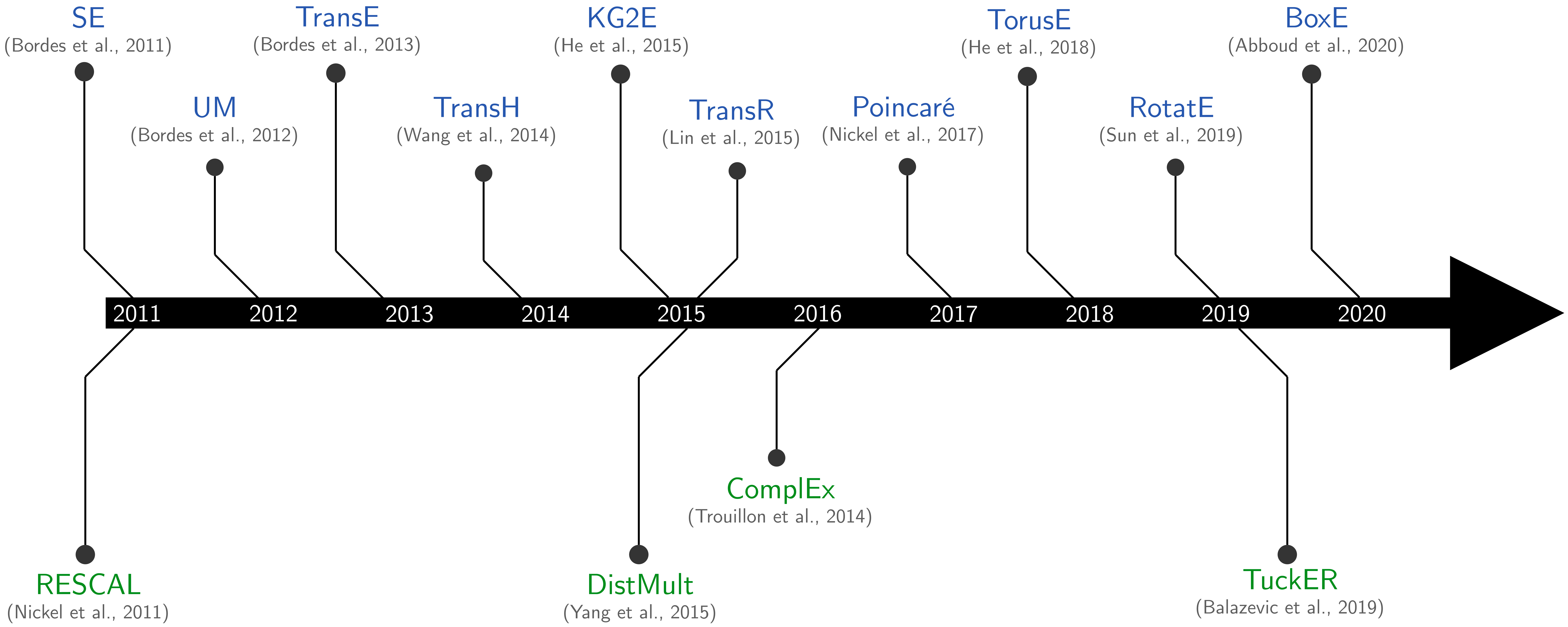

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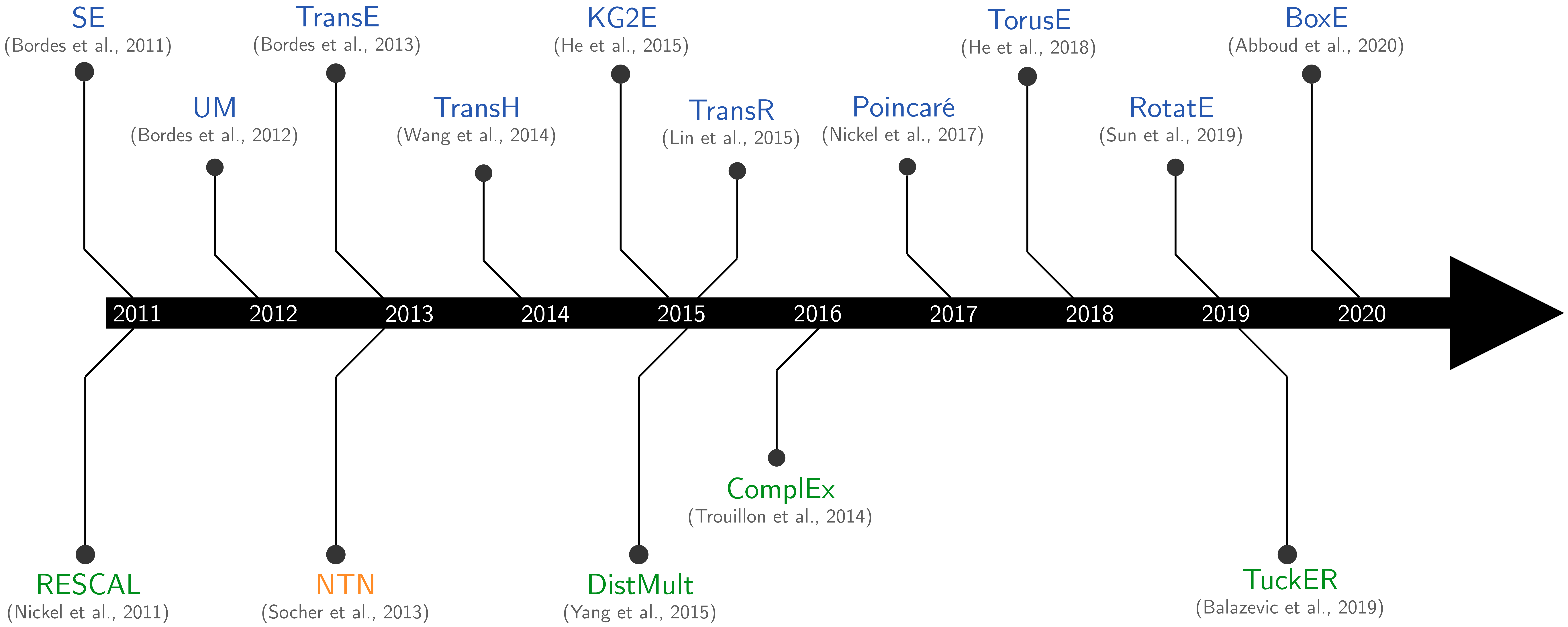

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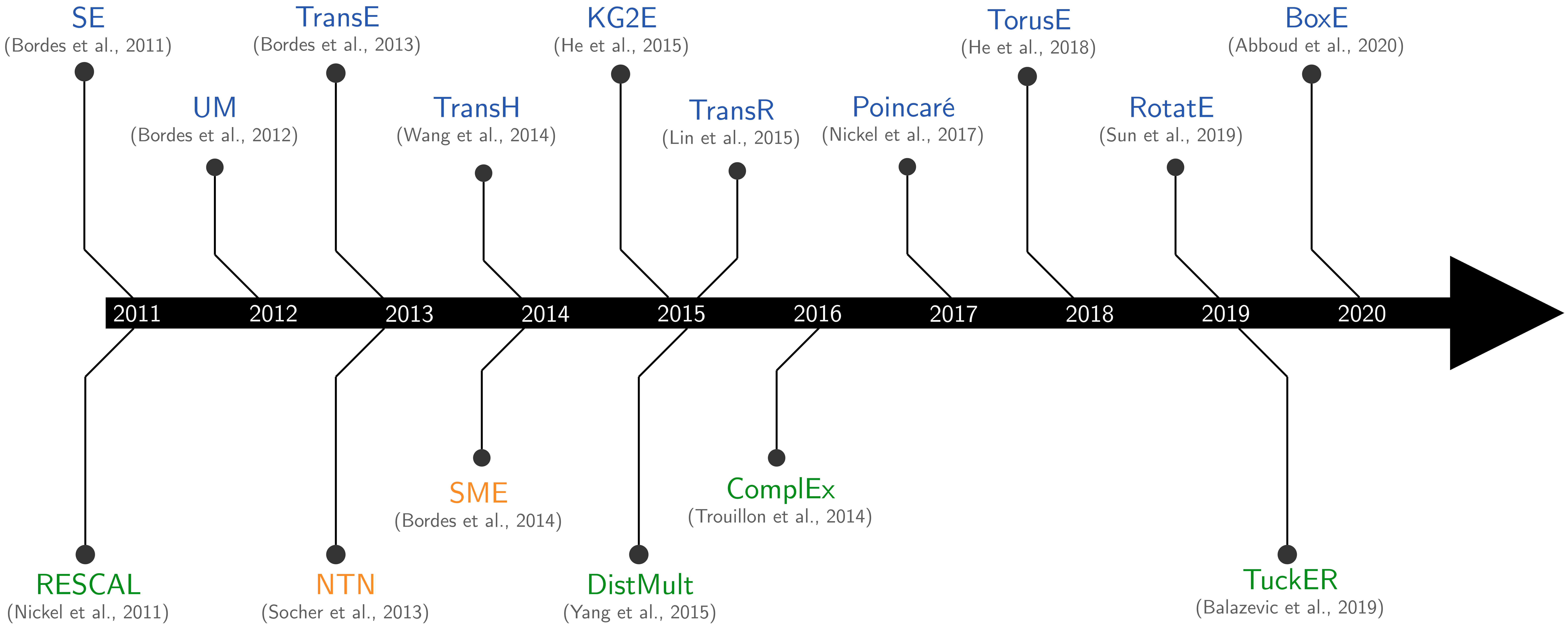

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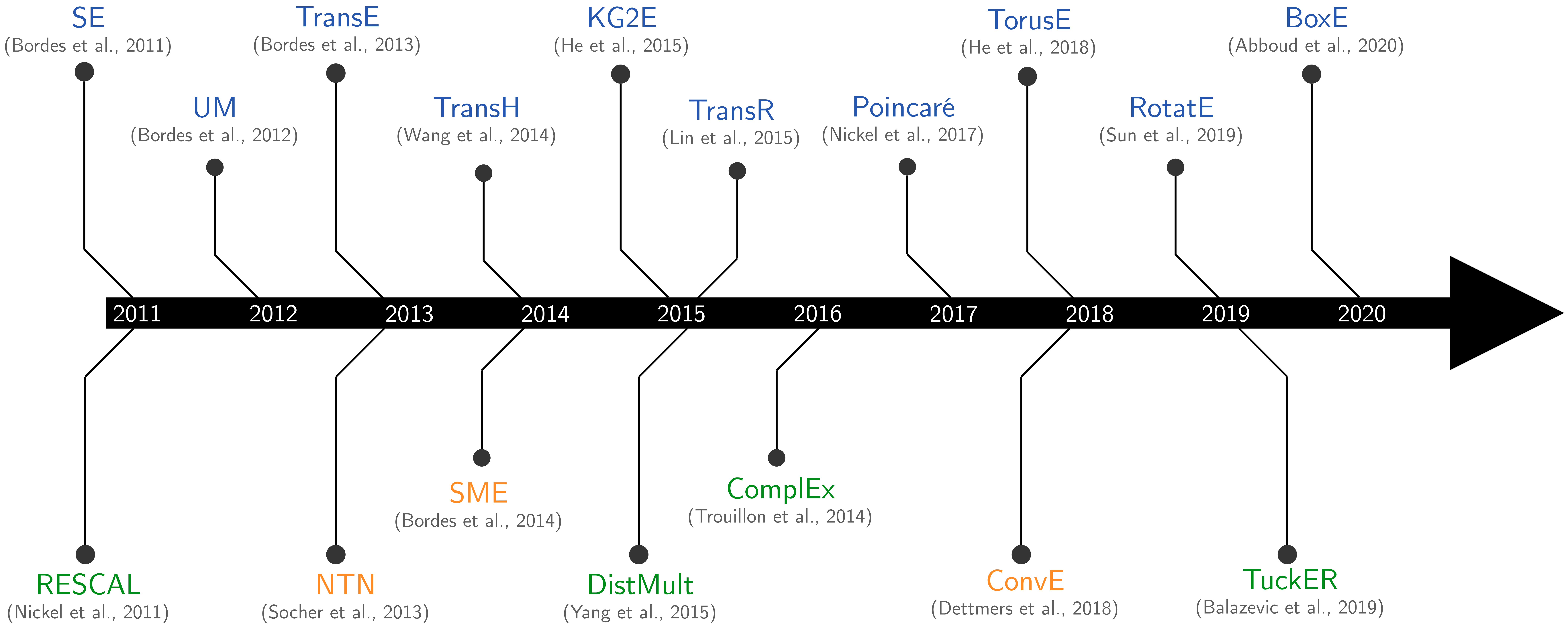

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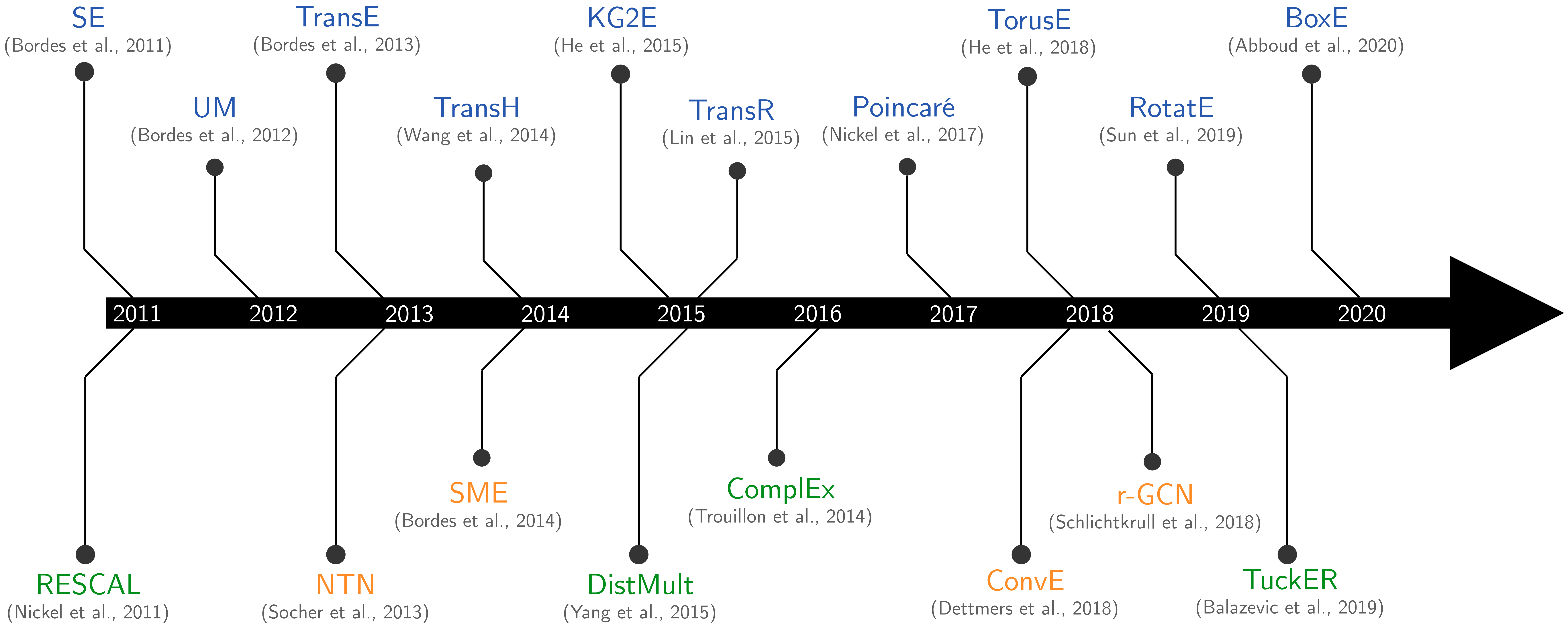

Translational Models

TransE: Representation

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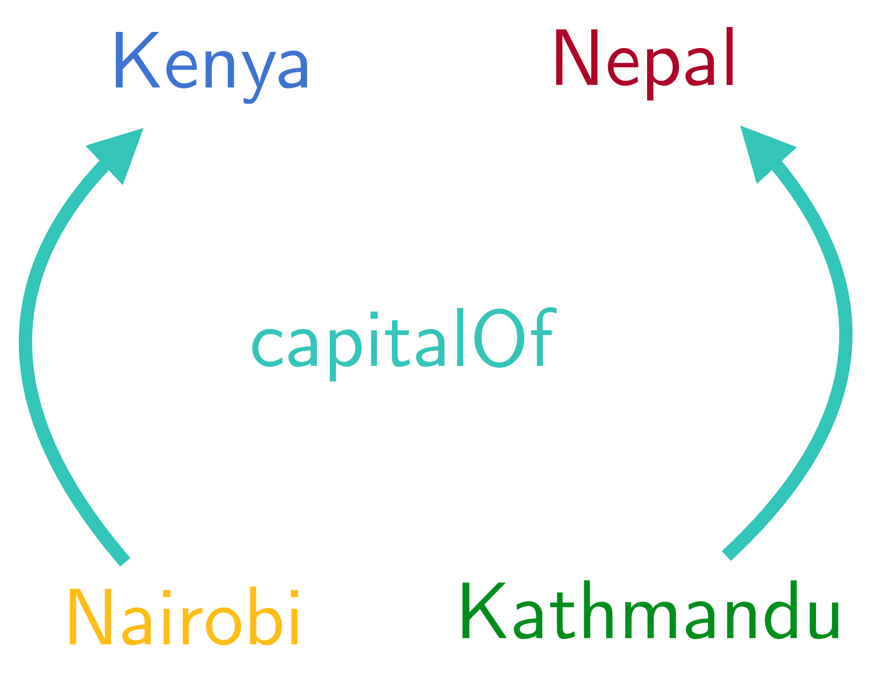

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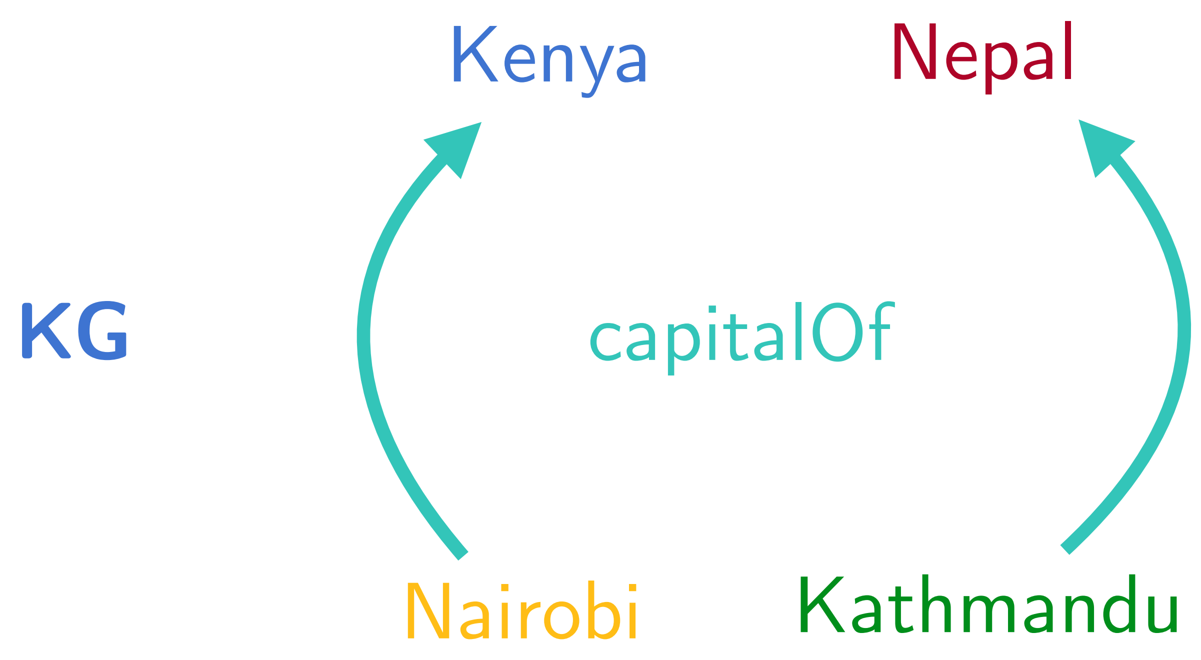

- TransE encodes entities $h, t \in E$ and relations $r \in R$, through d-dimensional vectors $\mathbf{h}, \mathbf{t}, \mathbf{r} \in \mathbb{R}^d$.

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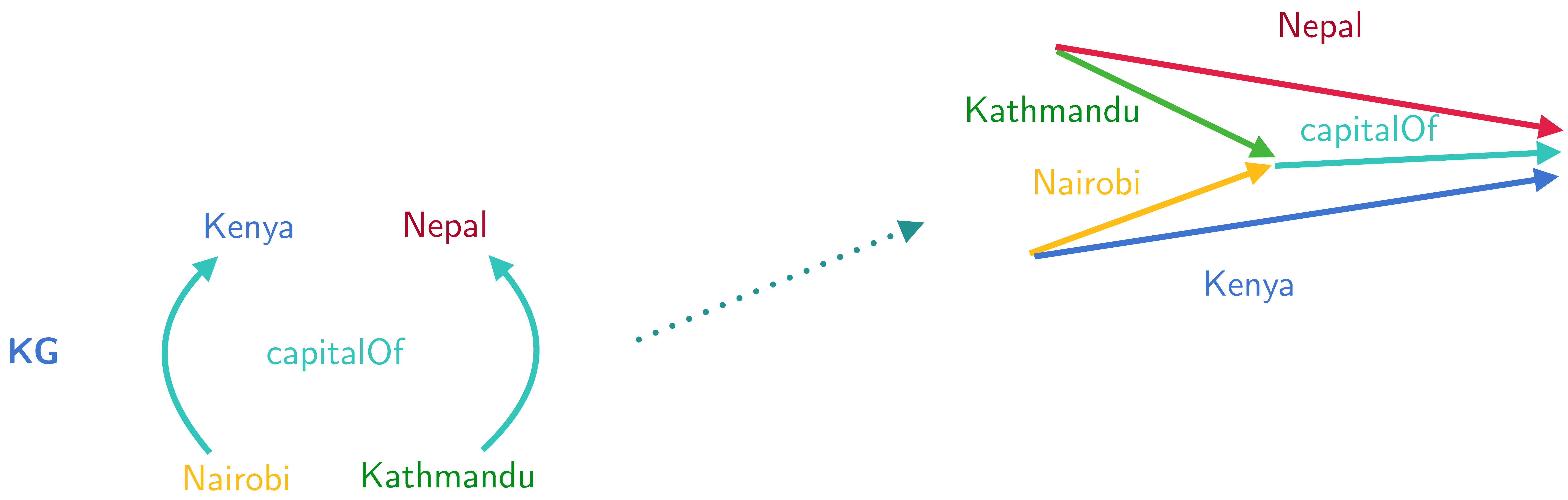

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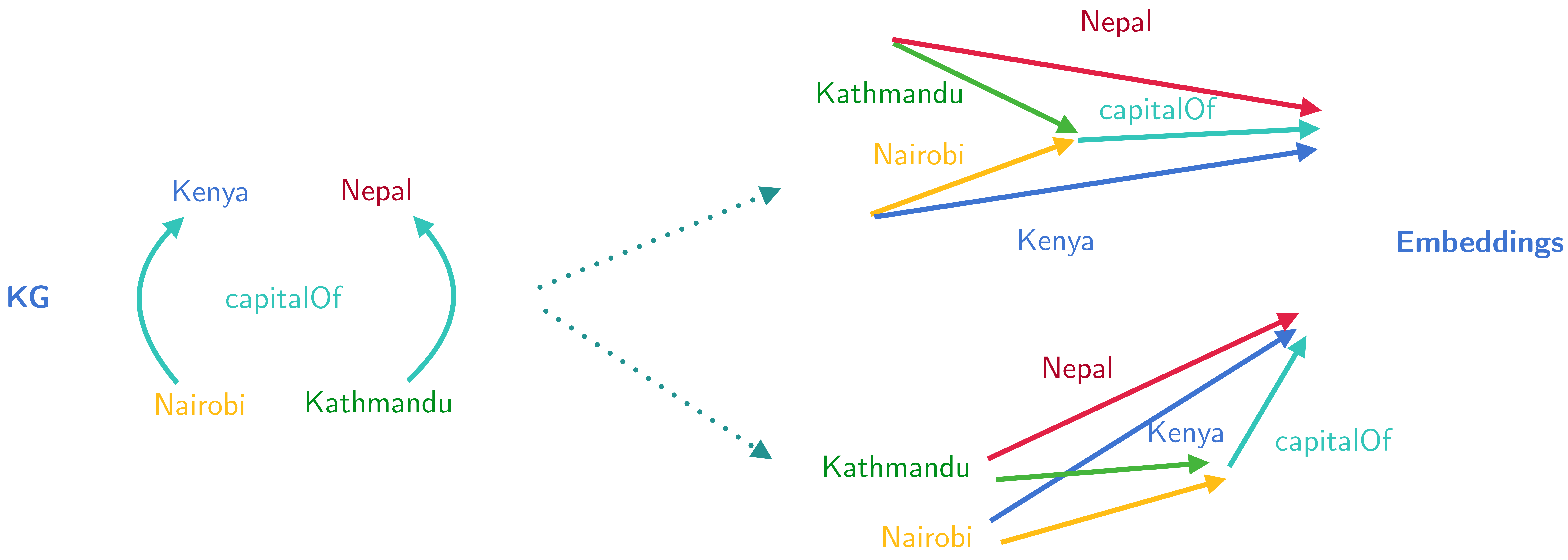

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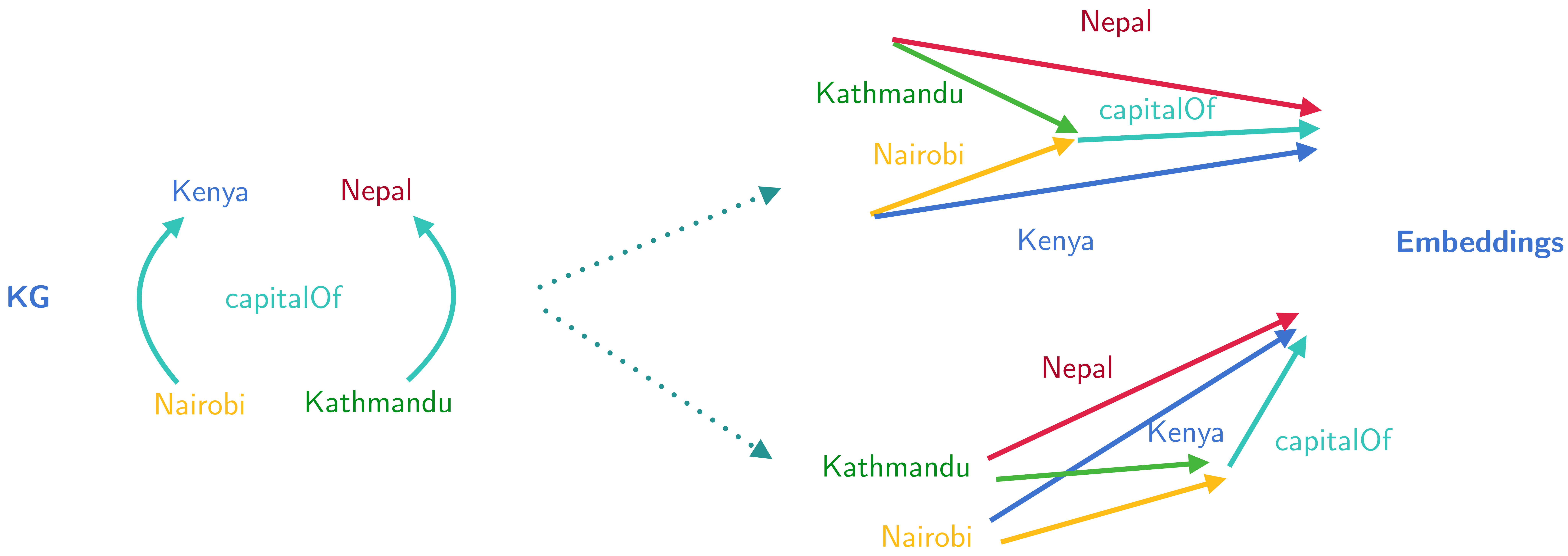

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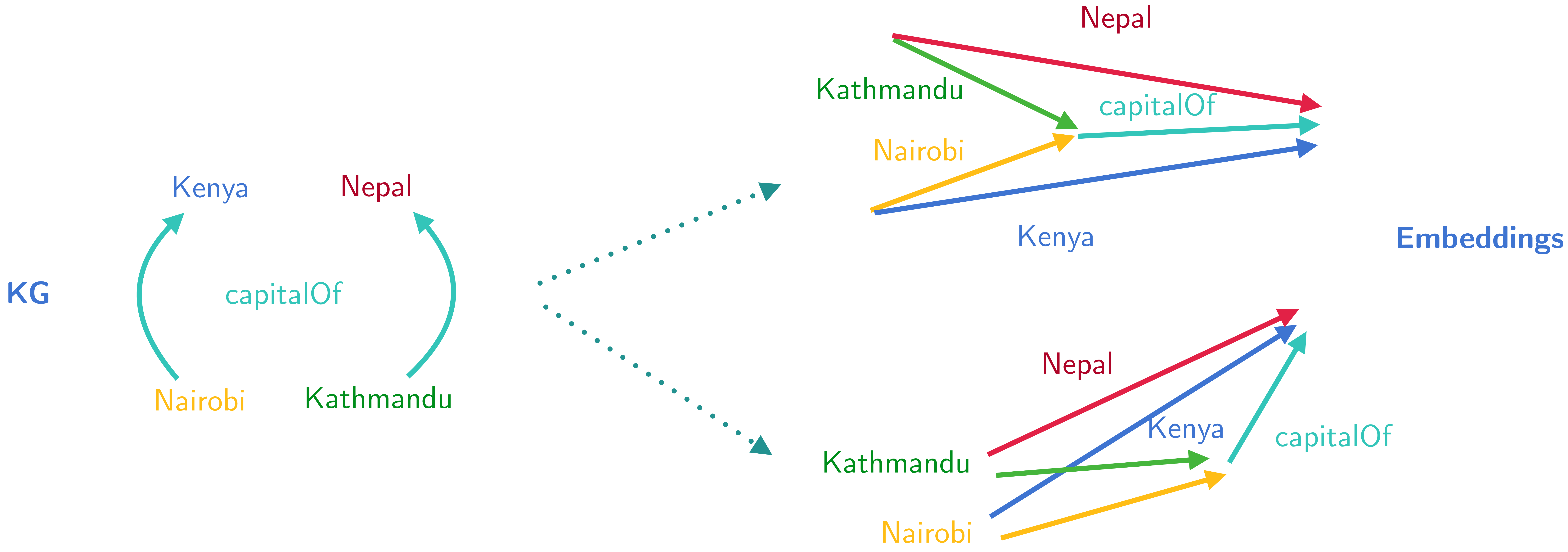

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- TransE is optimised to minimise (resp., maximise) the dissimilarity of true facts (resp., negative facts).

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Scoring: Consider a dissimilarity measure d, such as L_1 or L_2 norm, where $d(\mathbf{h} + \mathbf{r}, \mathbf{t})$ represents how dissimilar $\mathbf{h} + \mathbf{r}$, and $\mathbf{t}$ are, e.g., $d(\mathbf{h} + \mathbf{r}, \mathbf{t}) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|$.

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$$\mathscr{L} = \gamma + d(\mathbf{h}+\mathbf{r},\mathbf{t}) + \sum_{r(h',t')\in N^{r(h,t)}} - d(\mathbf{h}'+\mathbf{r},\mathbf{t}') - \gamma \ ,$$

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Optimisation: The optimisation is carried out by stochastic gradient descent, where all embeddings for entities and relationships are first initialised 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.

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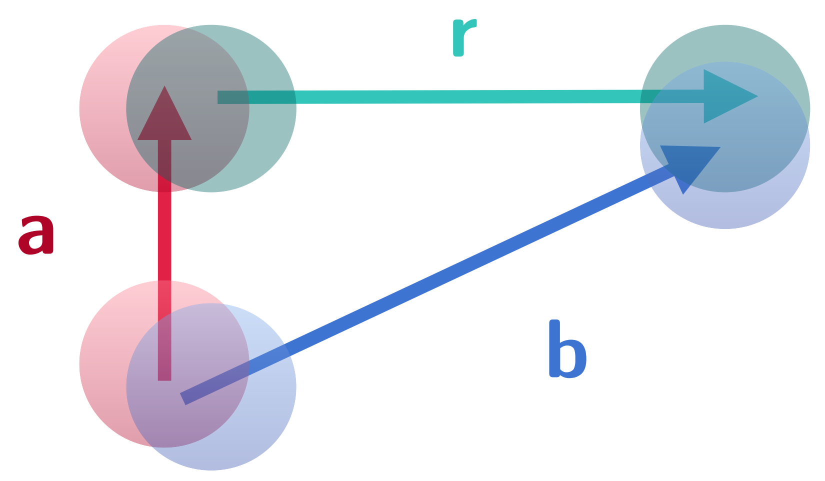

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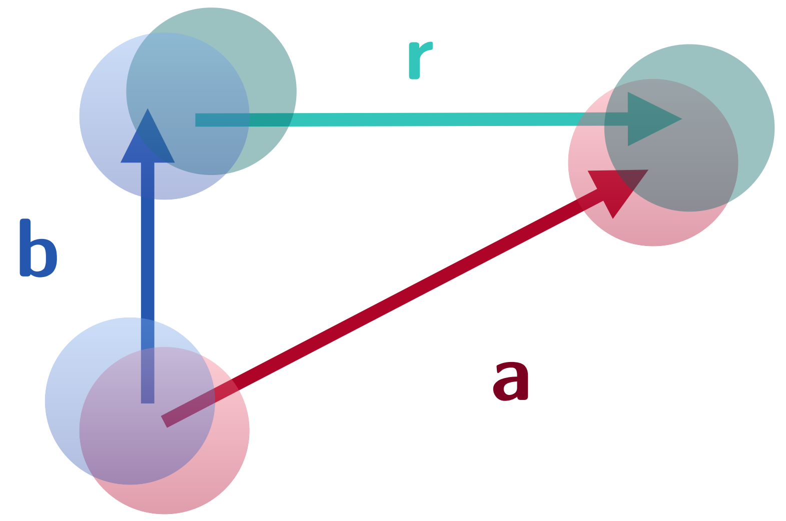

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To realise these facts jointly, we need $r = 0$, as shown in (iii), but then, the facts $\{r(a,a), r(b,b)\}$, are necessarily classified as true facts, although these could well be false facts.

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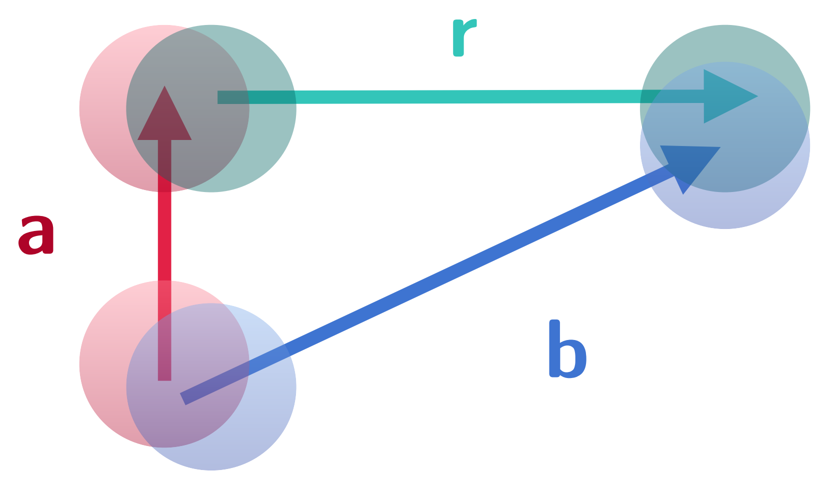

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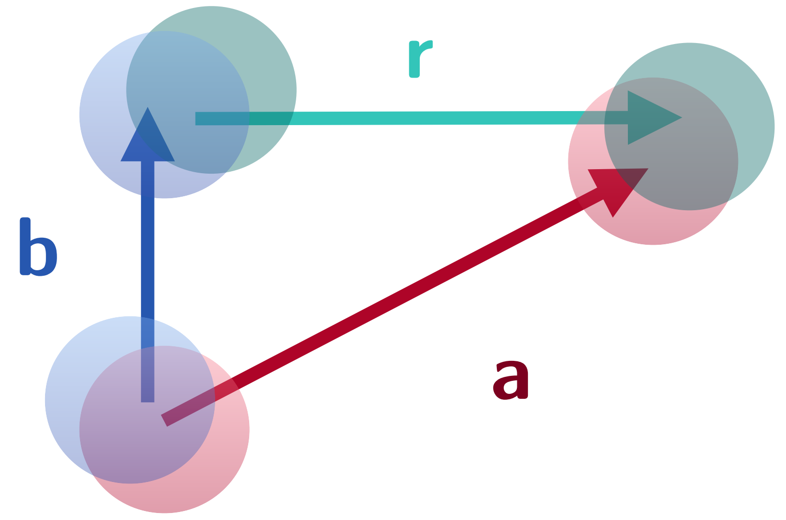
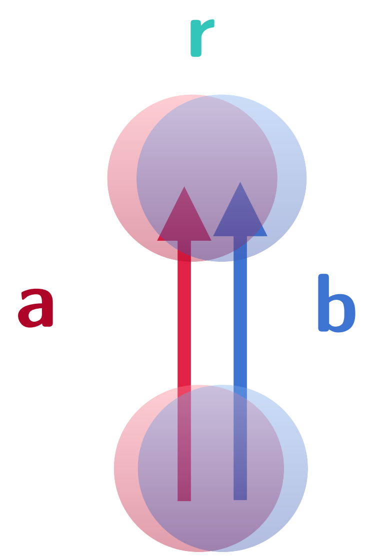


(iii) $r(a,b)$ & $r(b,a)$



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This also means that 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, as it cannot encode the set of true facts $\{r(a,b), r(b,a)\}$ and the set of false facts $\{r(a,a), r(b,b)\}$ simultaneously.

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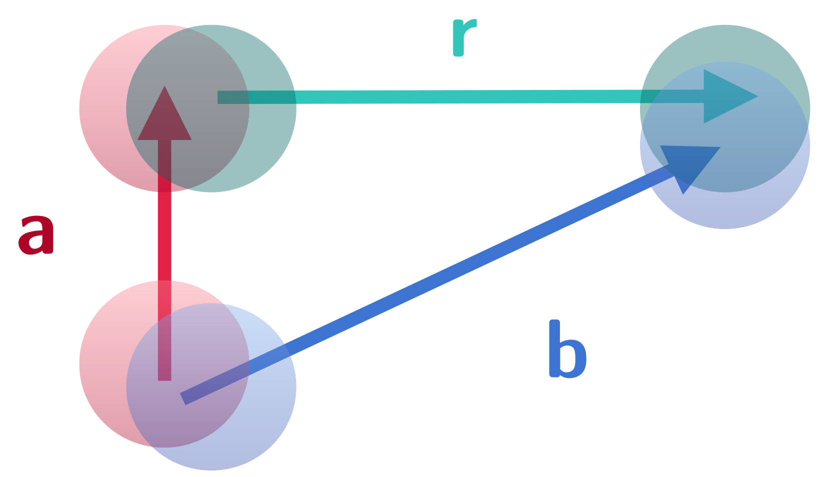

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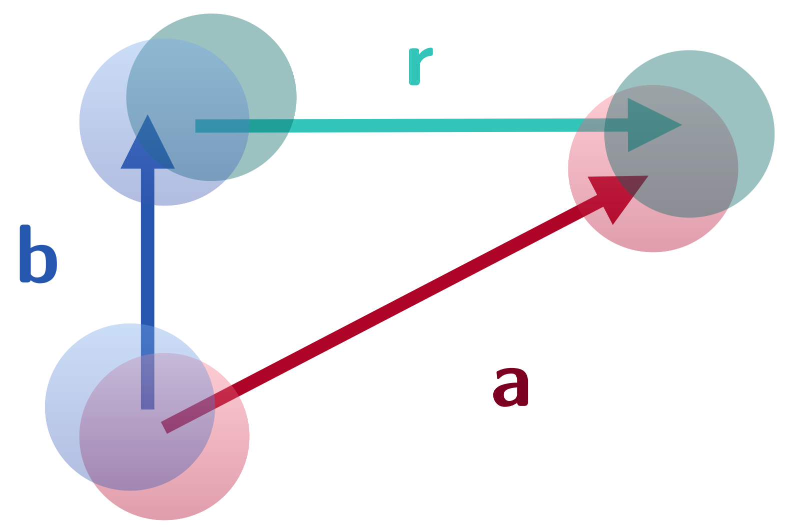

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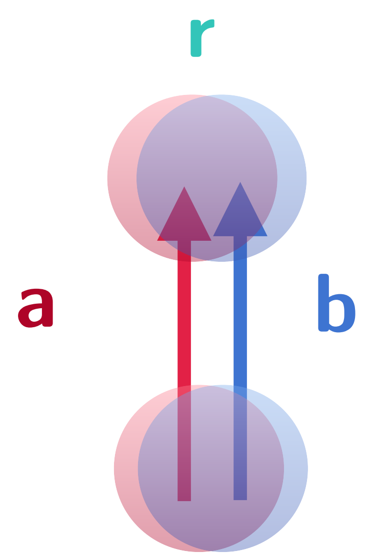

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Consider a relation such as cousinOf with entities alice, bob to see a problematic example. TransE is limited in various other ways, as we shall see later.

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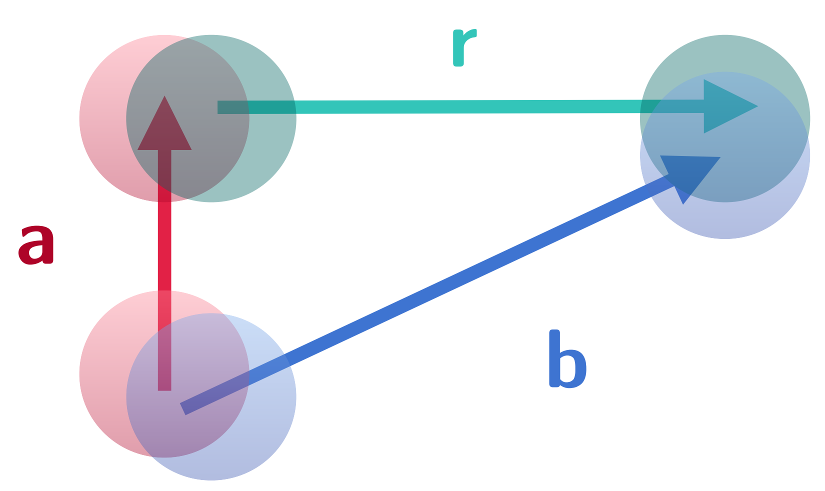

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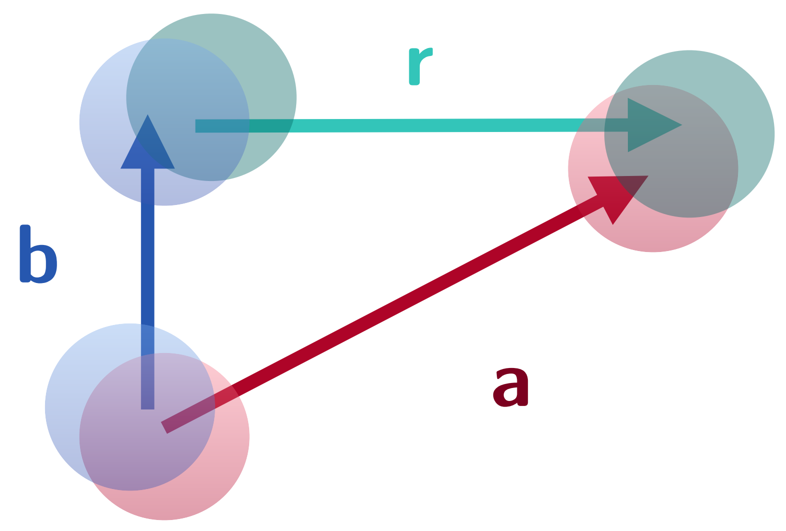

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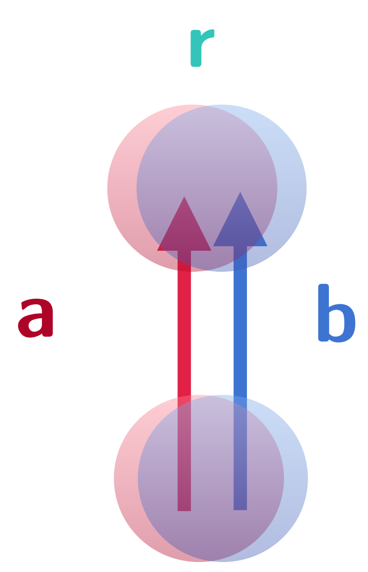

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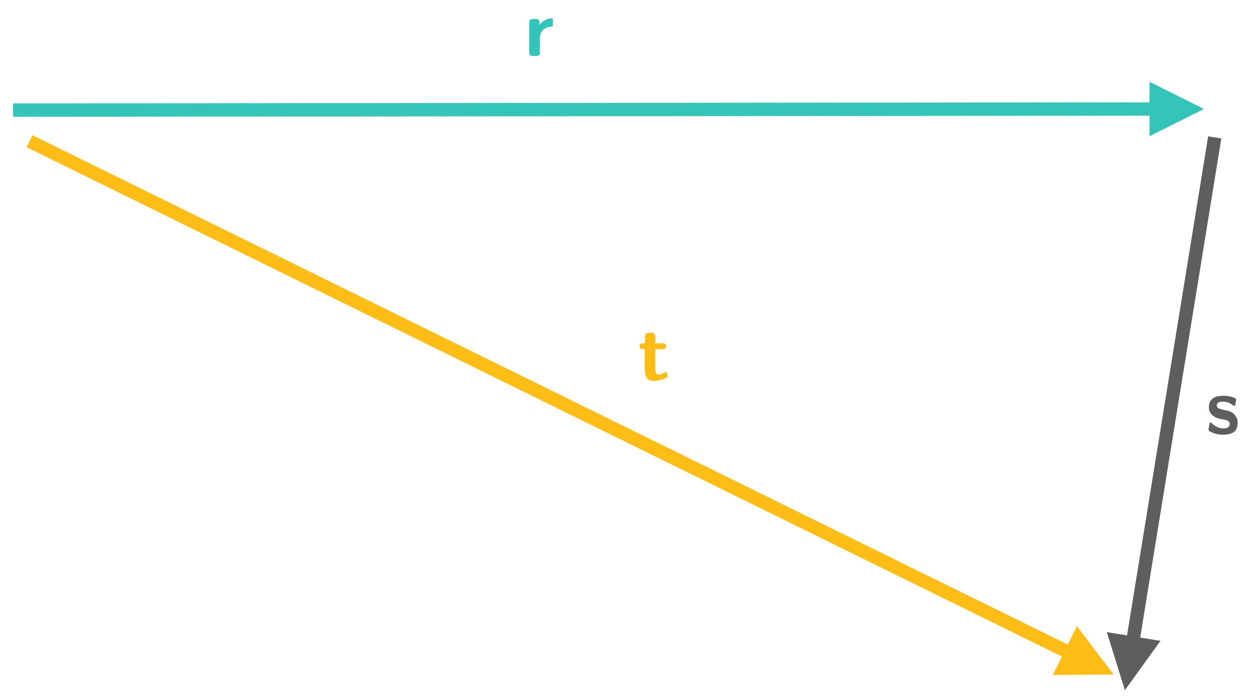

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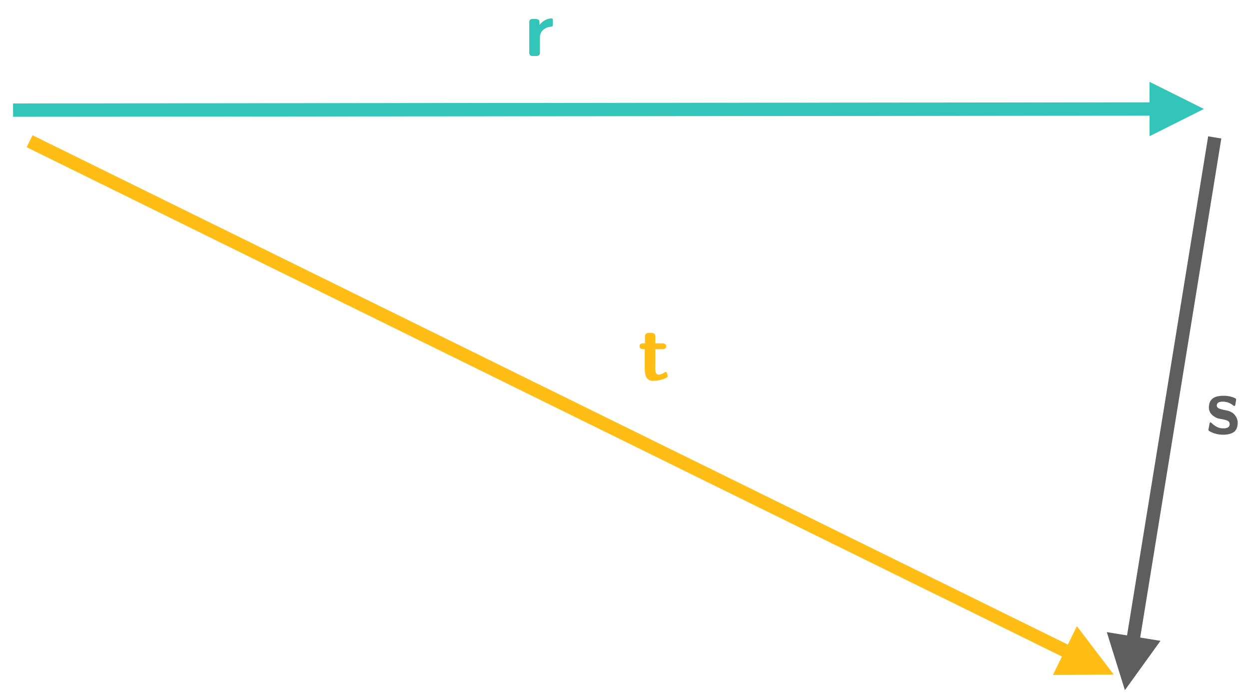

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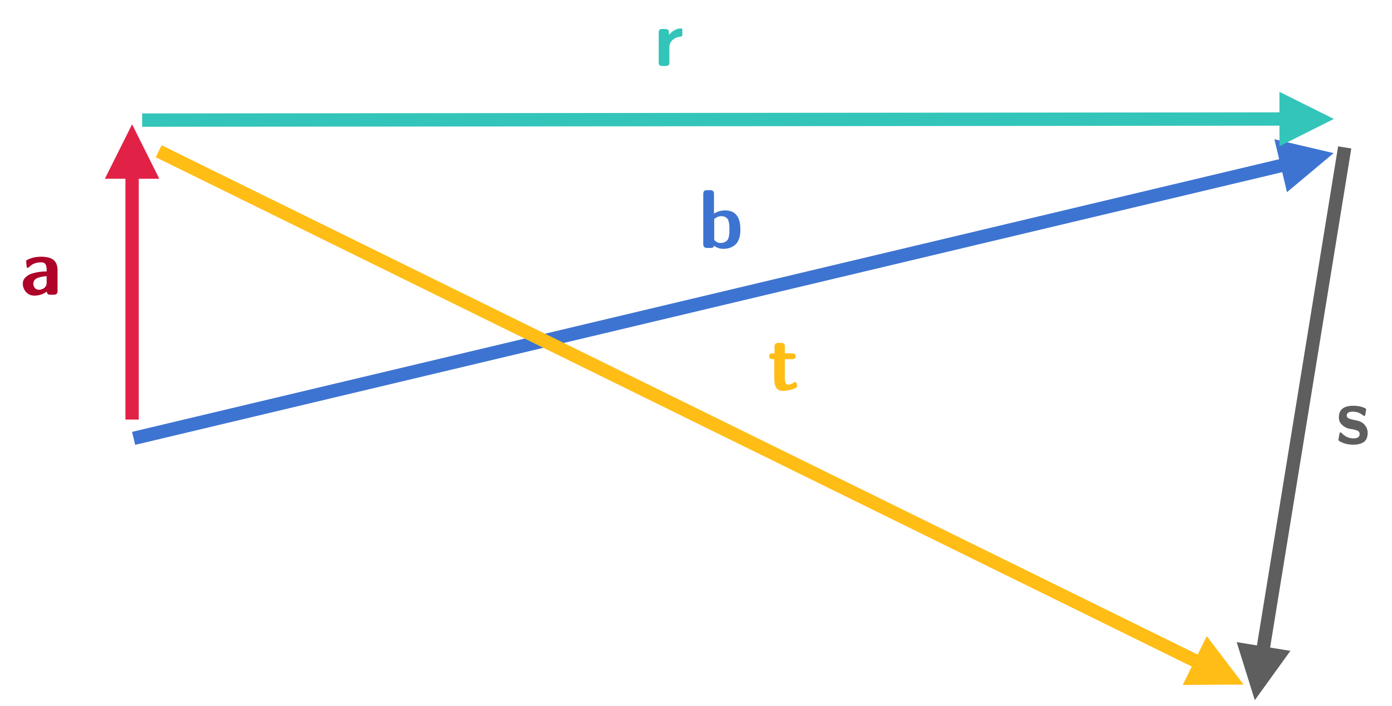

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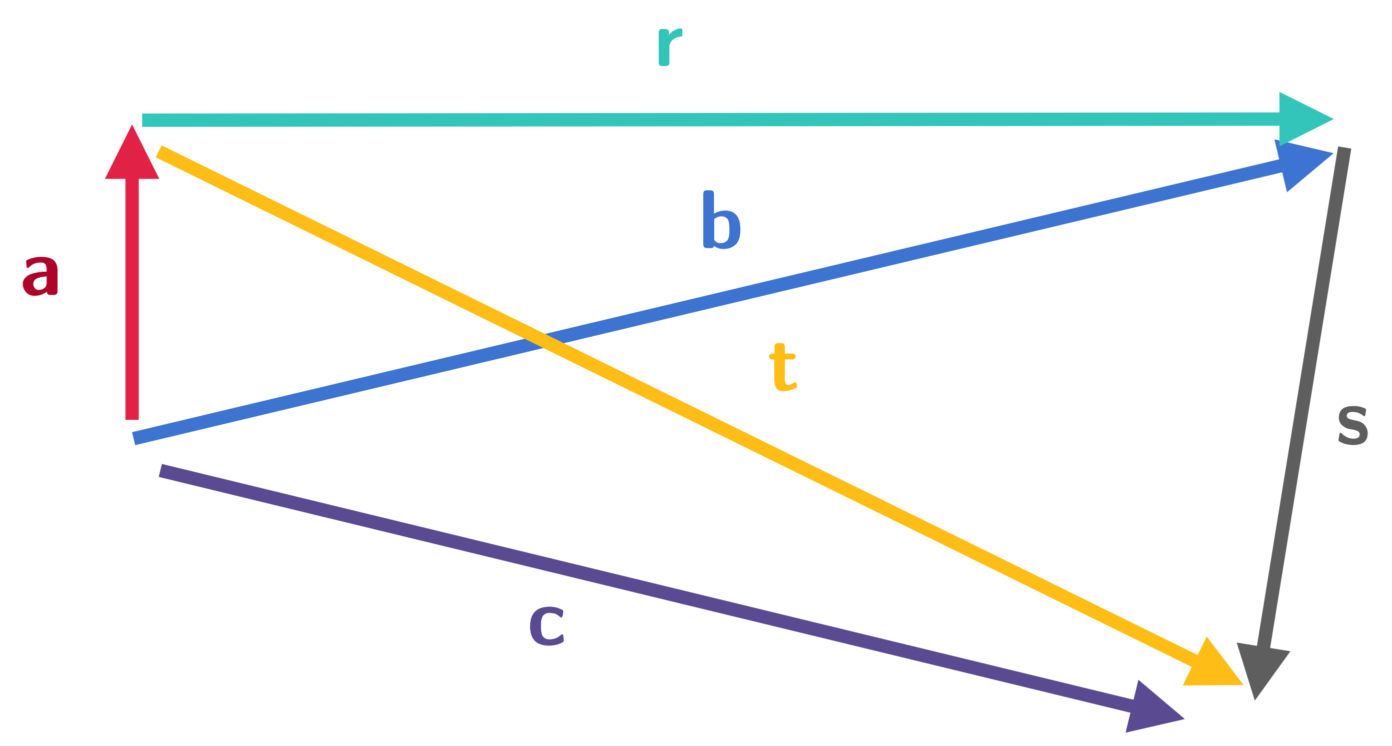

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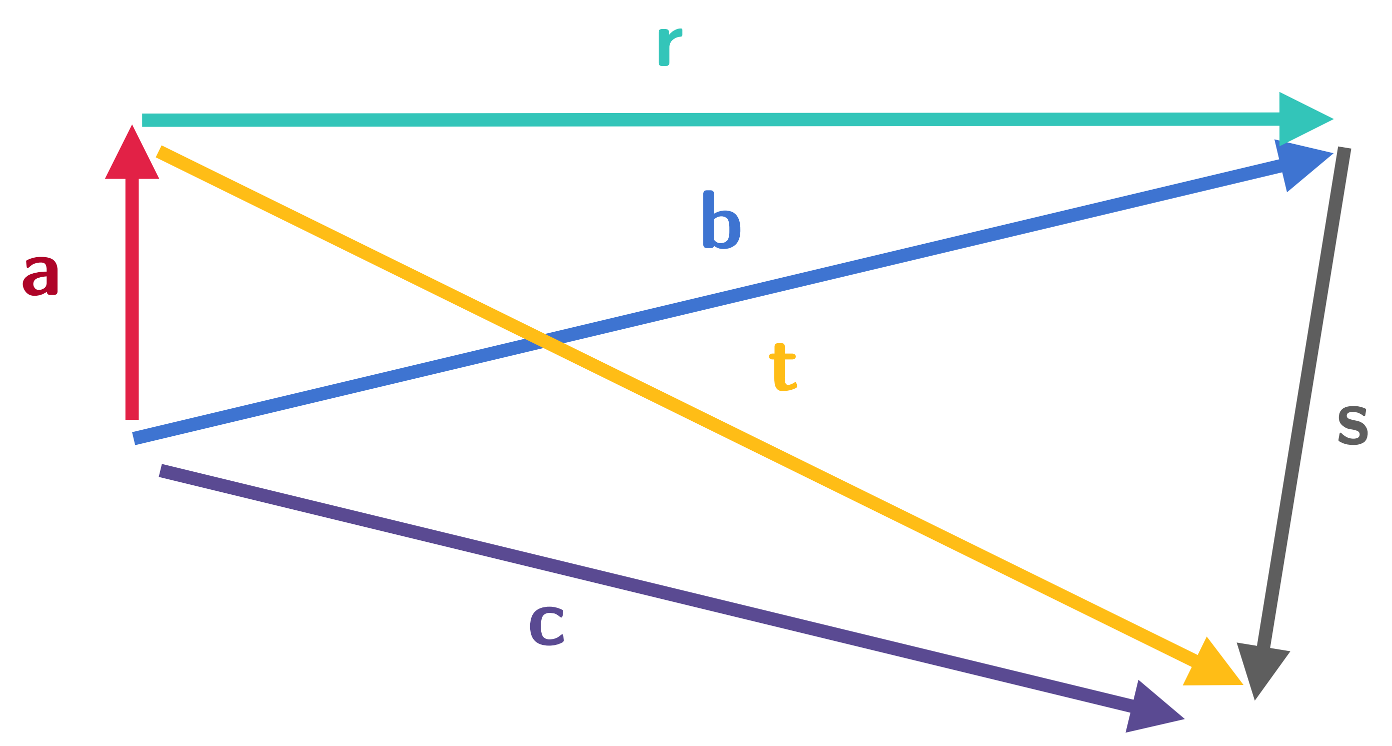

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Hence, TransE can capture the composition pattern.

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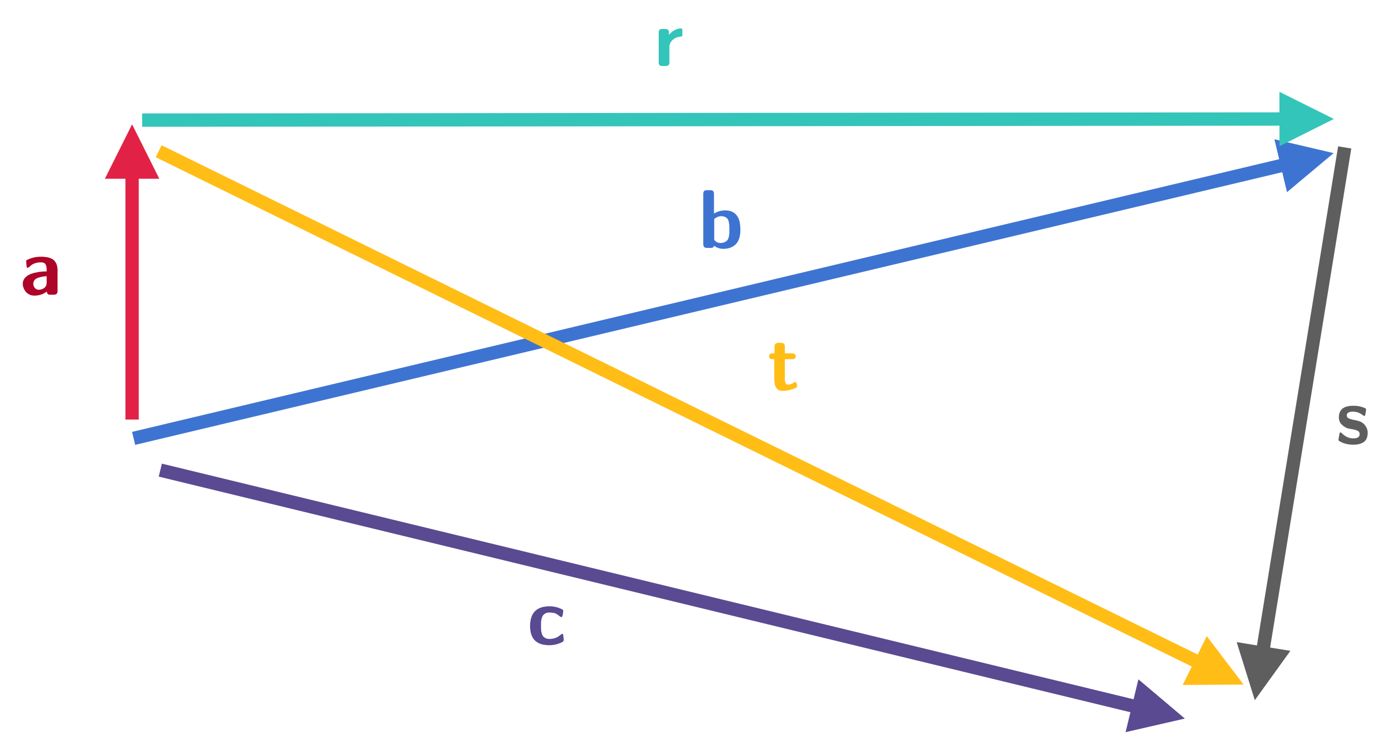

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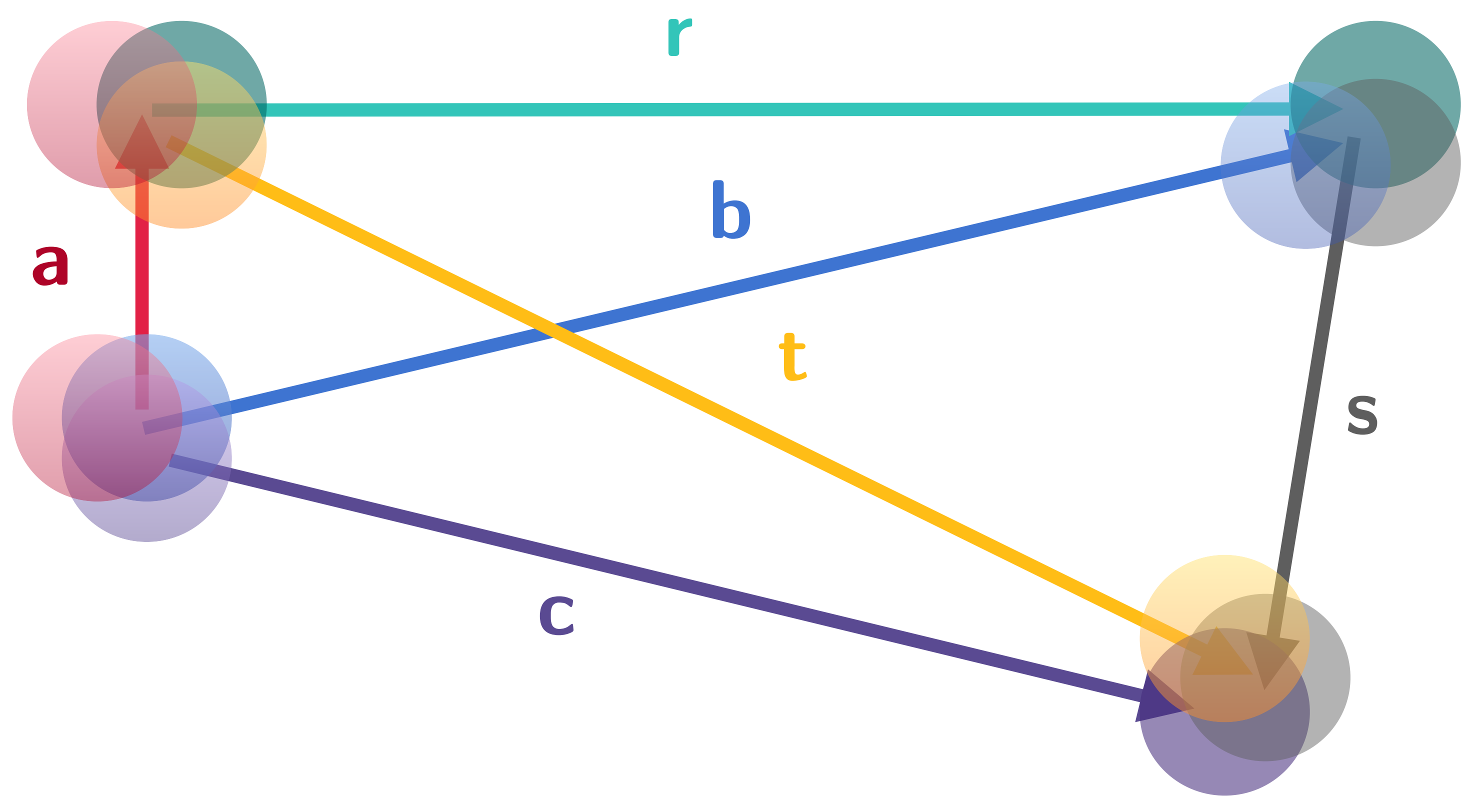

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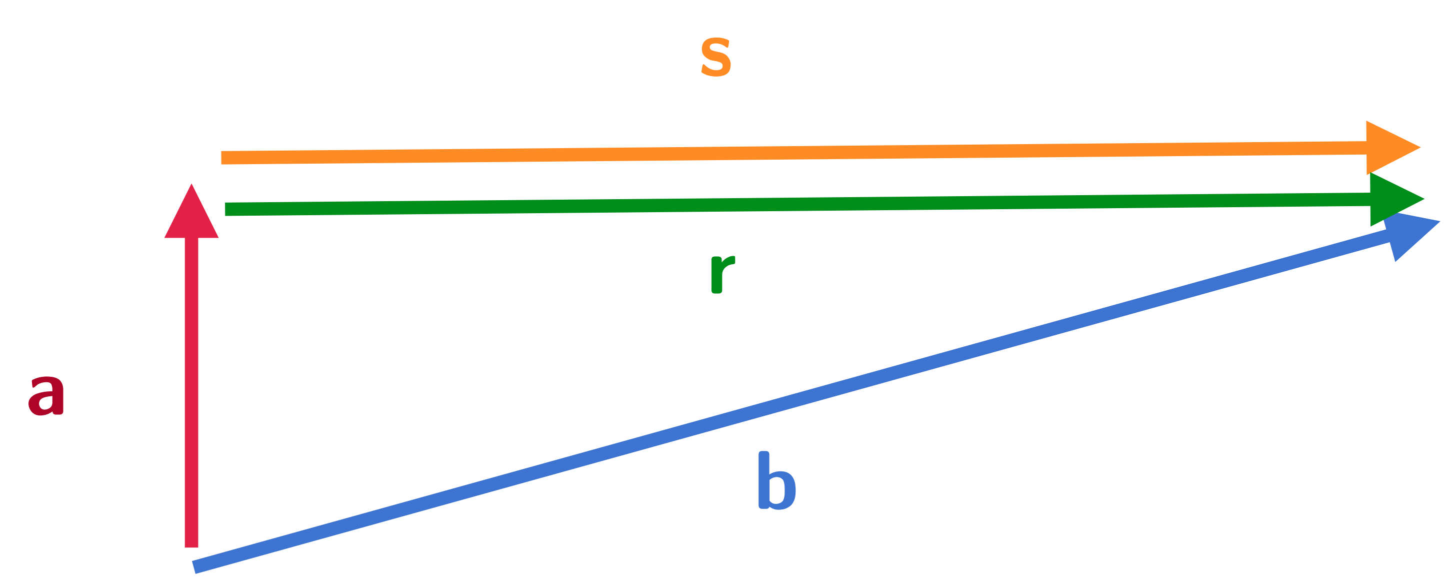

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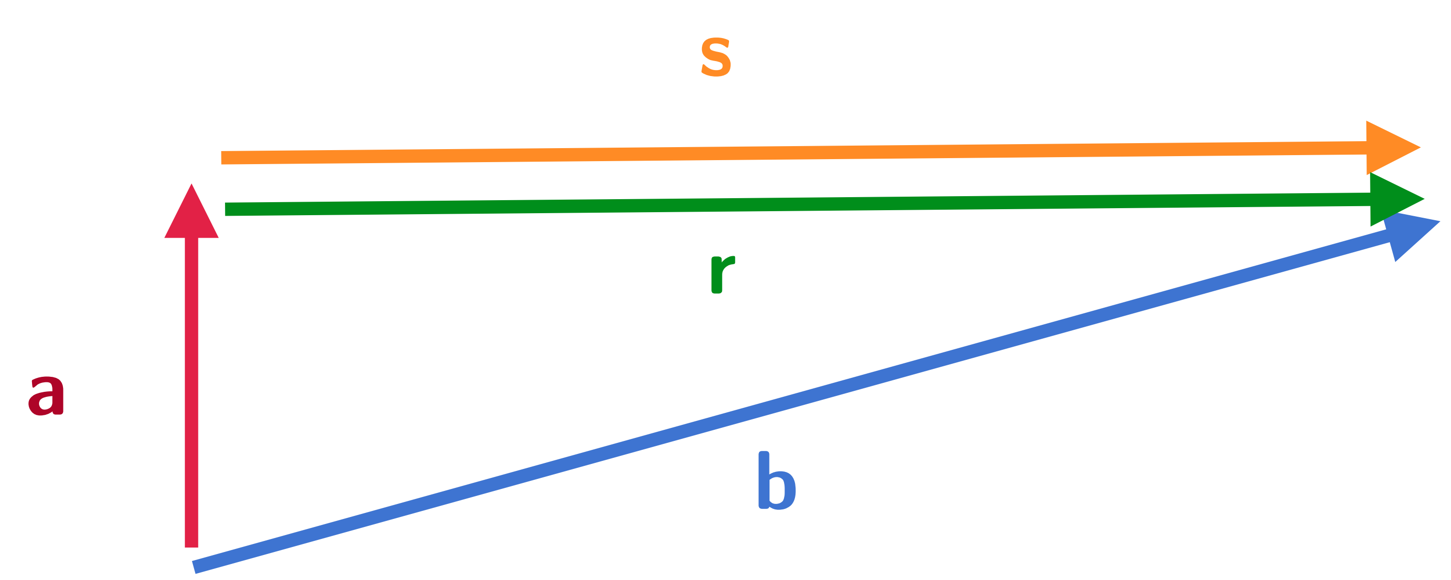

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Similarly to the symmetry pattern, the lack of ability to capture the hierarchy pattern is a serious limitation, as it is also prevalent in datasets (e.g., the relation capitalOf implies the relation cityIn).

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

RotatE

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

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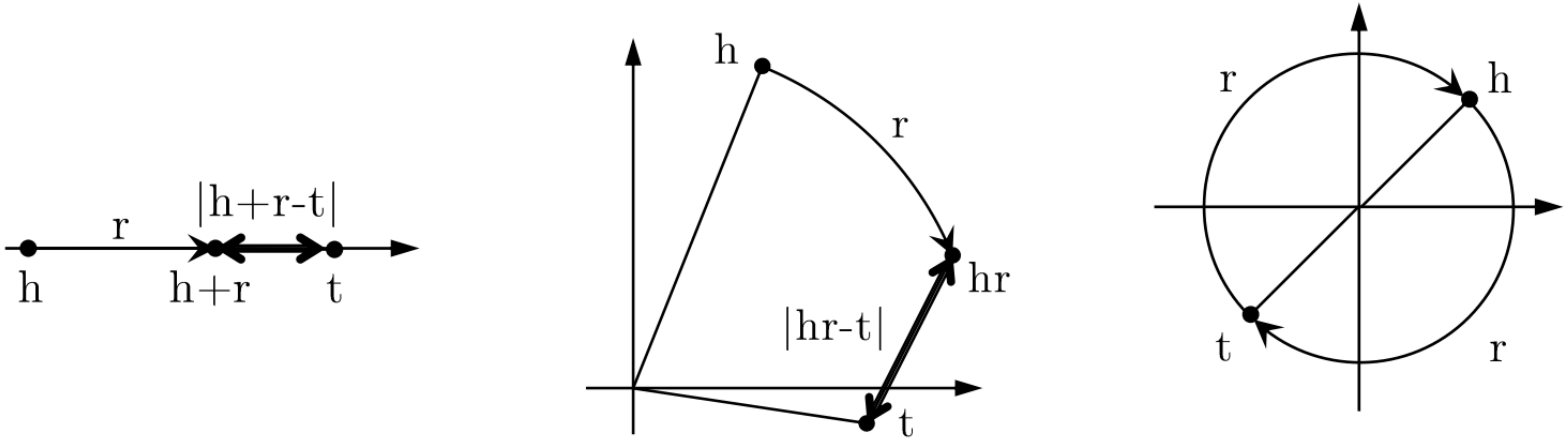

(a) TransE models **r** as translation in real line.

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(c) RotatE: an example of modeling symmetric relations **r** with $r_i = -1$

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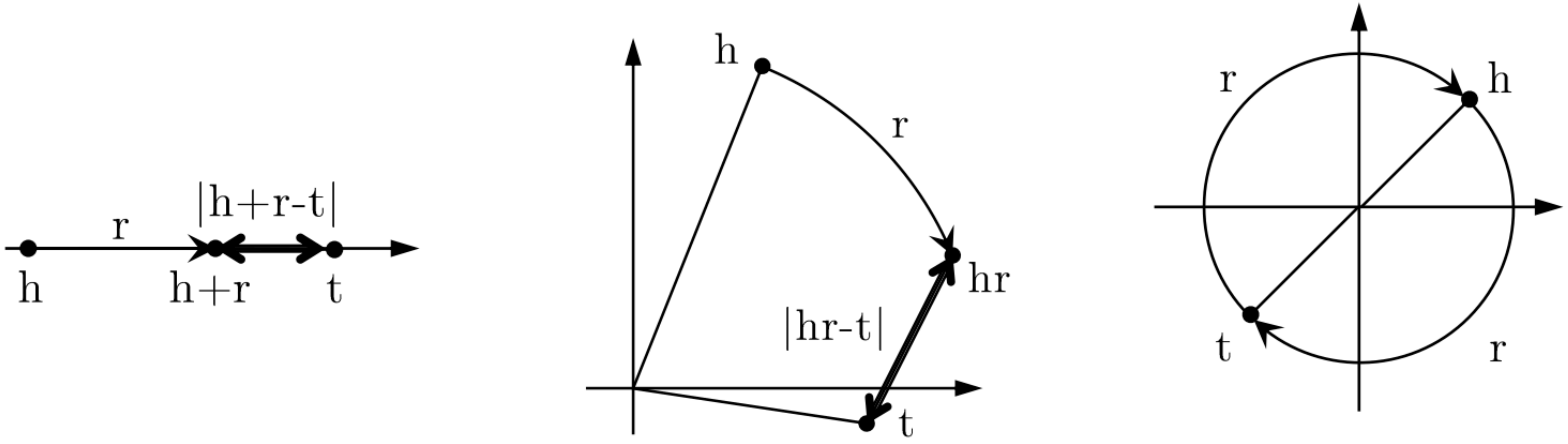

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Question: Does RotatE capture TransE as a special case?

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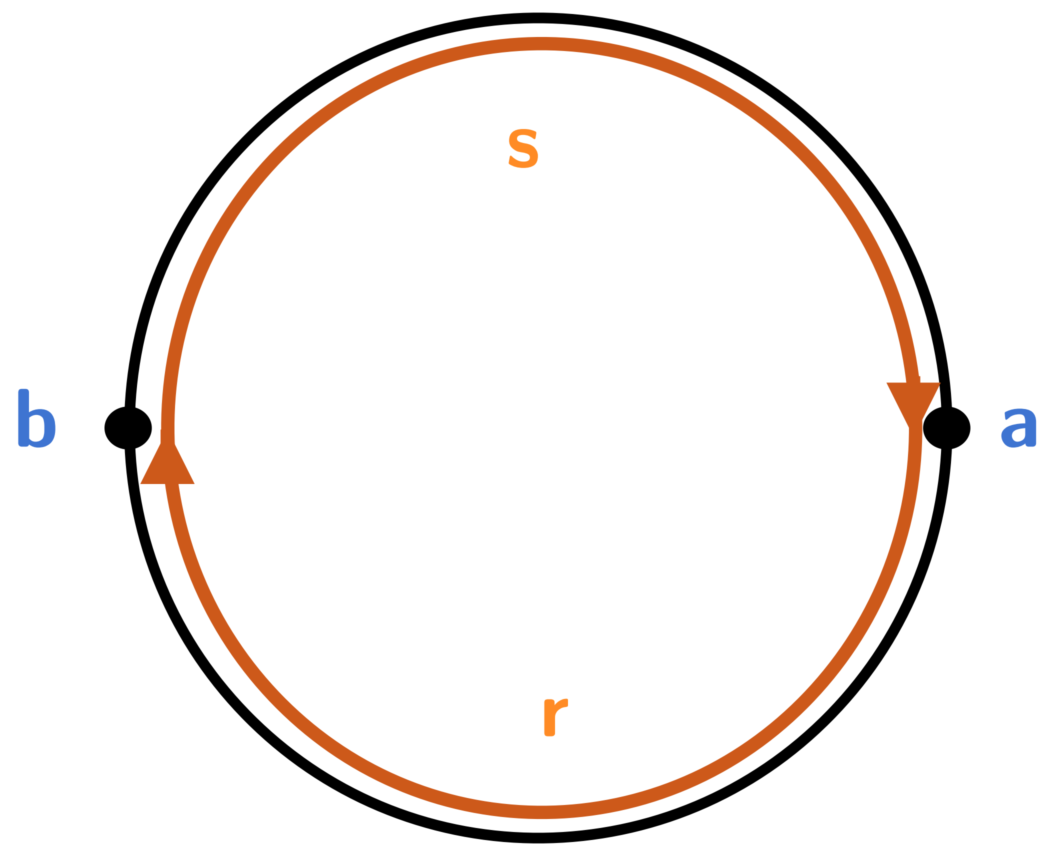

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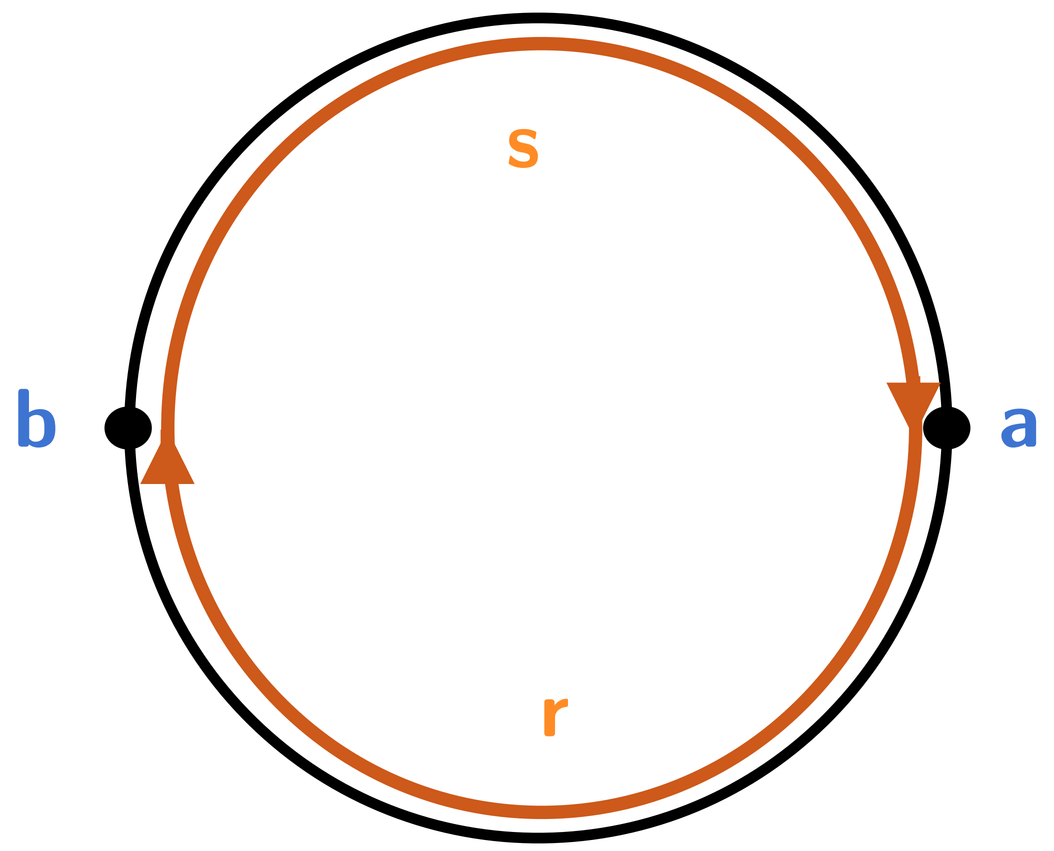

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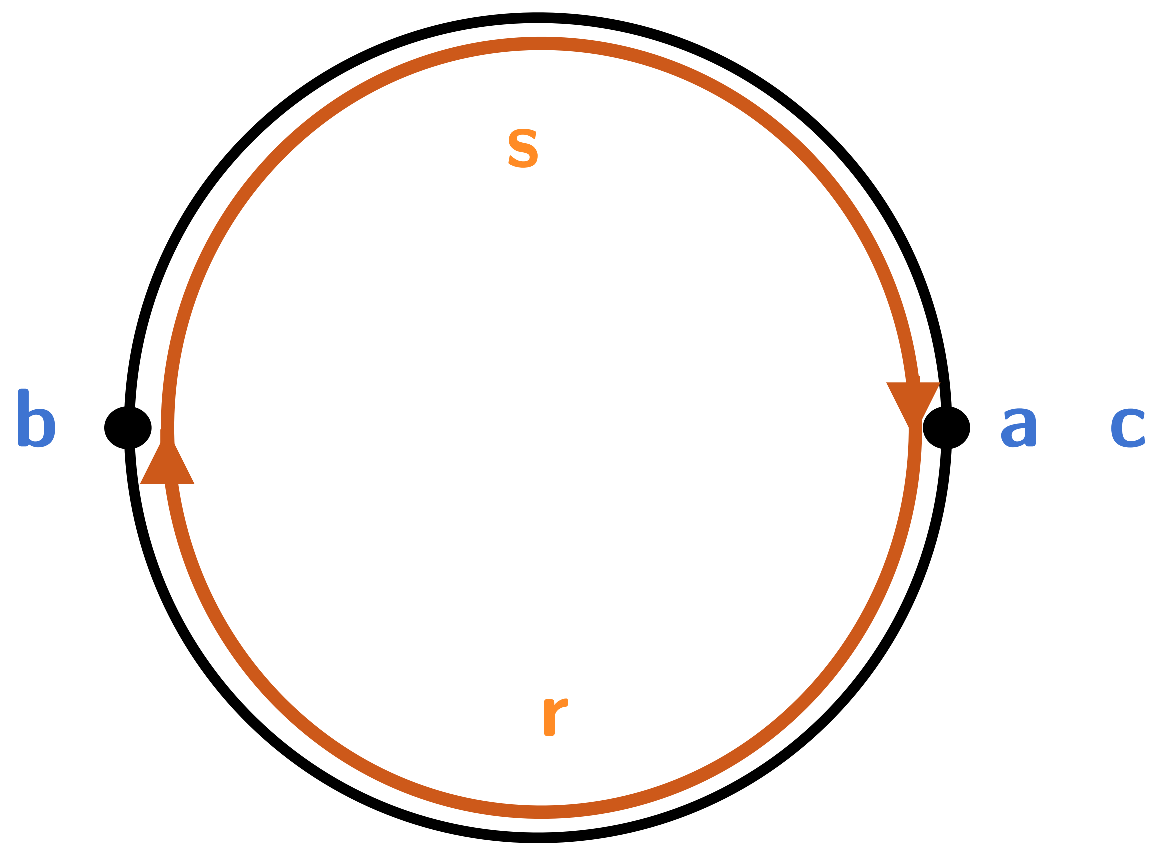

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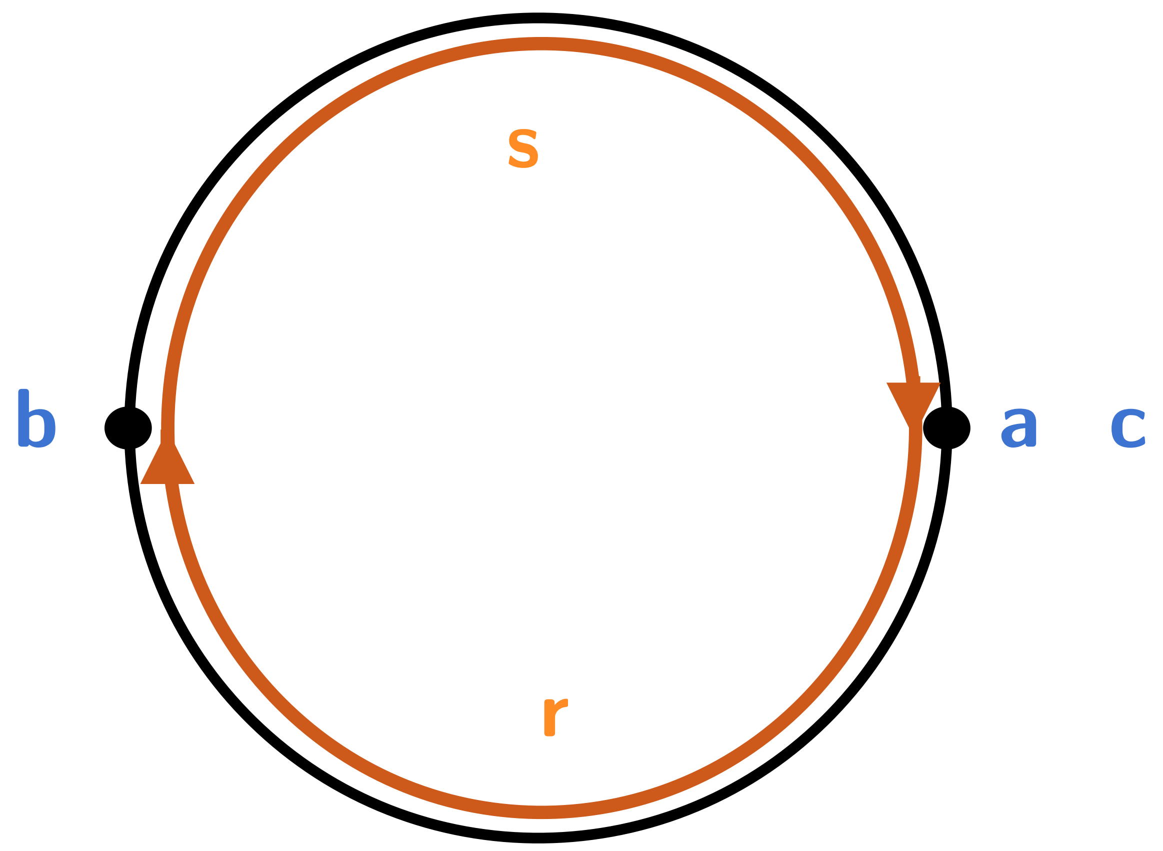

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This observation is not limited to this configuration: RotatE sets $\mathbf{r}$ and $\mathbf{s}$ symmetric to capture the initial two facts, though the relations need not be symmetric. If we consider the set $F = \{r(c,b)\}$ as the set of false facts, and then it is easy to see that RotatE cannot fit these facts simultaneously.

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To capture facts of the form $r(a, b), s(a, b), \ldots$ we need the rotations from a to b need to be similar, i.e., $\mathbf{r} \approx \mathbf{s}$, effectively enforcing relation equivalence.

Bilinear models

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Differently from translational models, bilinear models typically use a multiplicative approach, i.e., a bilinear product, to represent the relationships, hence the name "bilinear".

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Though expressive, 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.

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DistMult cannot differentiate between head entity and tail entity since $\mathbf{h}^\top \mathbf{D}_r \mathbf{t} = \mathbf{t}^\top \mathbf{D}_r \mathbf{h}$. This means that all relations are modelled as symmetric regardless, i.e., even anti-symmetric relations will be represented as symmetric.

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DistMult cannot differentiate between head entity and tail entity since $\mathbf{h}^\top \mathbf{D}_r \mathbf{t} = \mathbf{t}^\top \mathbf{D}_r \mathbf{h}$. This means that all relations are modelled as symmetric regardless, i.e., even anti-symmetric relations will be represented as symmetric.

Expressiveness: DistMult is not fully expressive, i.e., clearly underfitting any dataset with facts from an asymmetric relation.

DistMult

DistMult is a bilinear model that restricts RESCAL to a diagonal matrix instead of a full rank matrix.

Representation: 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 $\mathbf{D}_r$.

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

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ComplEx is an interesting trade-off, as it generalises 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, simply define the relation r as a scalar multiplication of a relation s, e.g., for $\lambda > 1$, set $s = \lambda r$. Then, any $\mathbf{h}^\top \mathbf{D_r t}$ implies $\mathbf{h}^\top \mathbf{D_s t}$, and and hence $\forall x, y \; r(x, y) \Rightarrow s(x, y)$. The argument for ComplEx is analogous.

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Note that this does not mean that bilinear models can capture relational hierarchies, i.e., it only means that one instance of such rule can be captured. Hierarchies captured in bilinear models are inherently linear, and this is an important limitation as we shall see later.

Box embedding models

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Basic Idea: Every concept (i.e., unary relation) and entity in a KG are represented by a box. In this setup, entity class membership, as well as relation similarity, is captured by means of box intersection in the lattice representation space. For instance, Oxford being a City is captured by 2 boxes, one for the Oxford entity and another for the city class, such that the Oxford box fits entirely into the City box.

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Can box embeddings be used for knowledge graph completion?

BoxE: Model Representation

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Representation: BoxE encodes each entity $h, t \in E$ in terms of two d-dimensional vectors $\mathbf{h}, \mathbf{b_h} \in \mathbb{R}^d$ and $\mathbf{t}, \mathbf{b_t} \in \mathbb{R}^d$, respectively. 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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The final embedding of a head entity h relative to a fact $r(h, t)$ is given by: $\mathbf{h}^{\mathbf{r(h,t)}} = \mathbf{h} + \mathbf{b_t}$. Similarly, the final embedding of a tail entity t relative to a fact $r(h, t)$ is given by: $\mathbf{t}^{\mathbf{r(h,t)}} = \mathbf{t} + \mathbf{b_h}$.

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In BoxE, a (binary) relation $r \in R$, is represented 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.

BoxE: Scoring and Spatial Properties

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Scoring: BoxE defines a distance function that determines how close a head entity is to a head box, and similarly, how close a tail entity is to a tail box. BoxE scores a fact $r(h,t)$ as the sum of the L-x norms of such function:

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

where dist is a distance function that grows slowly if a point is in the box (relative to the centre of the box), but grows rapidly if the point is outside of the box, so as to drive points more effectively into their target boxes and ensure they are minimally changed, and can remain there once inside.

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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. Hence, BoxE can be seen as a hybrid spatio-translational model.

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. Expressive!

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Intuitively, head and tail boxes define regions, such that 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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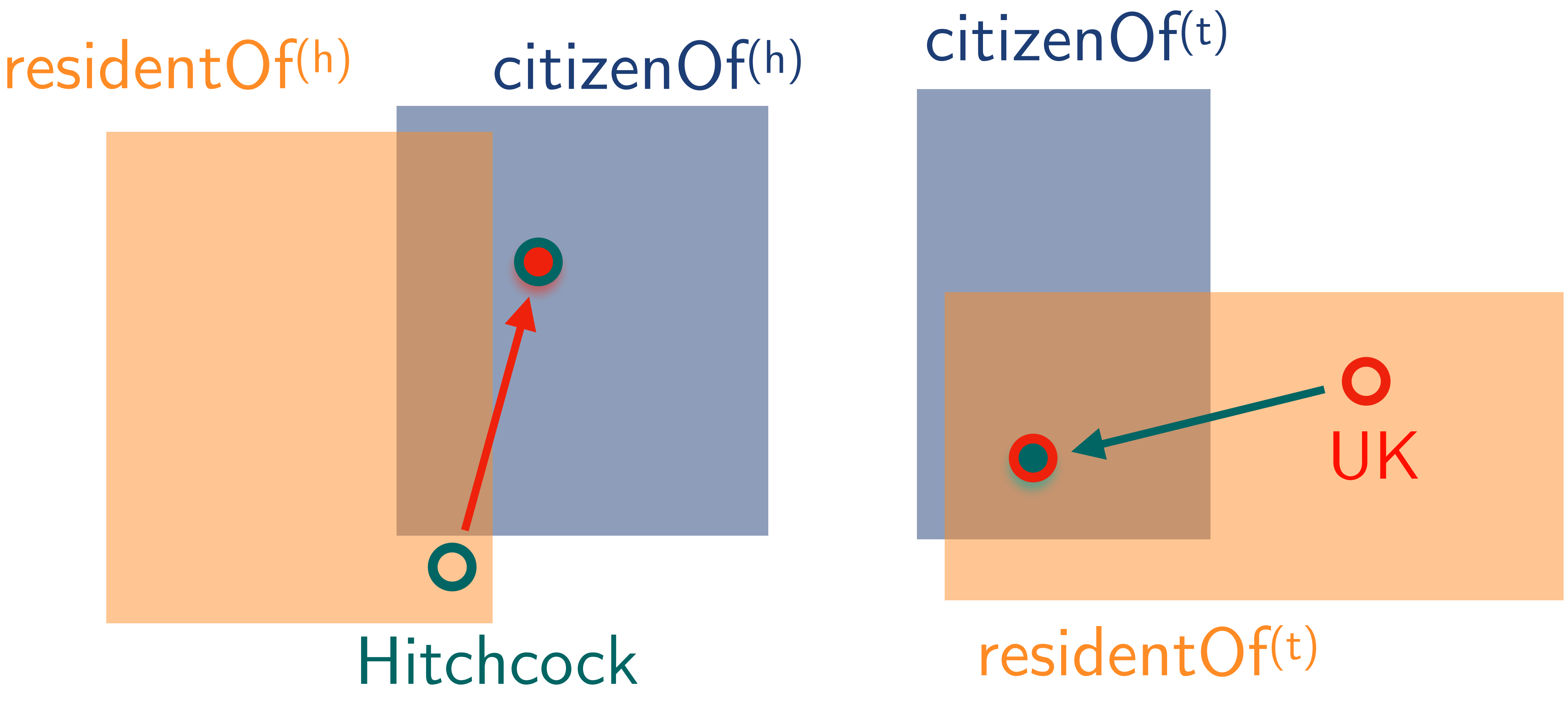

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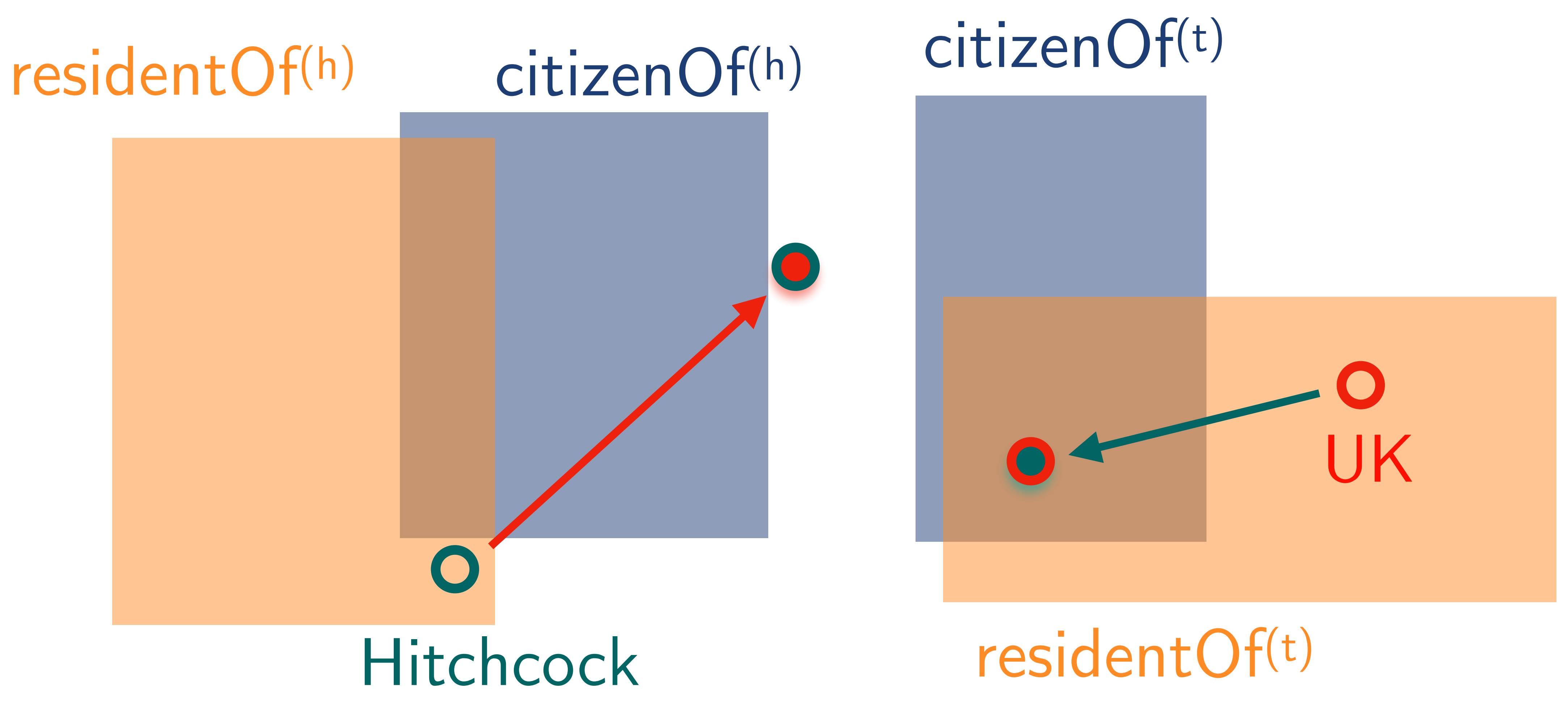

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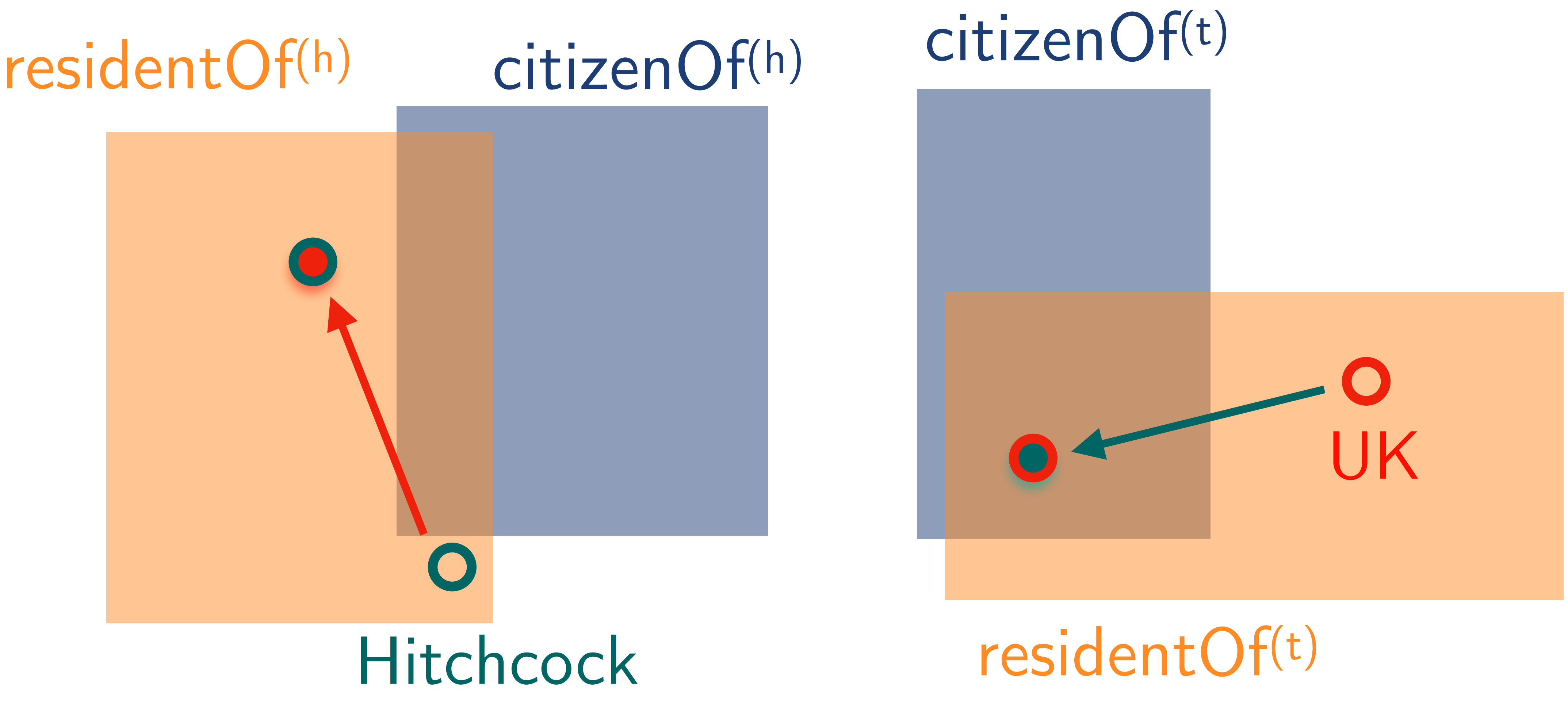

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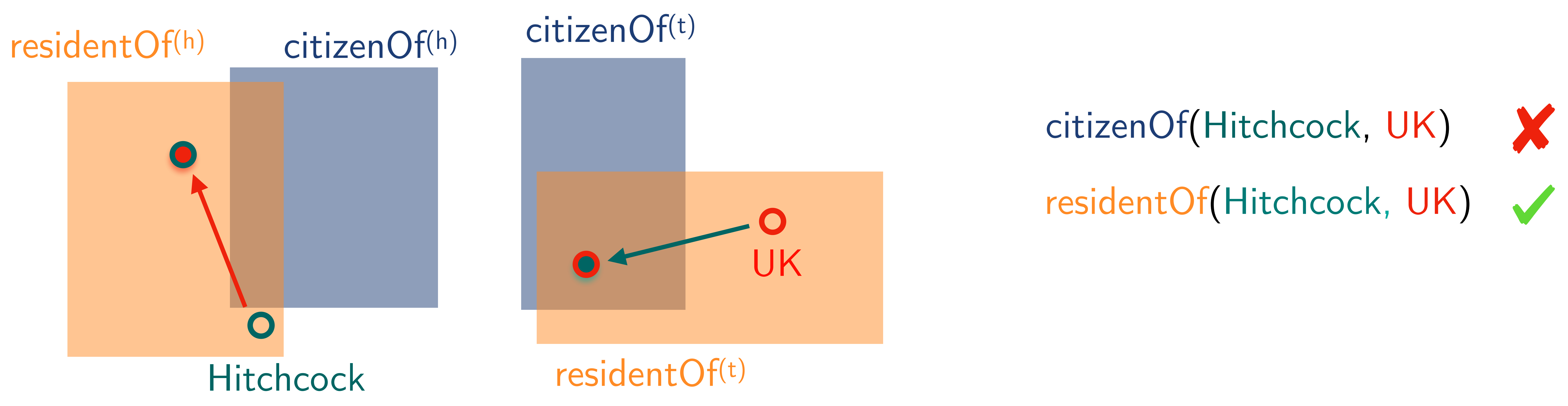

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Expressiveness: BoxE is indeed fully expressive. Any fact $r(h, t)$ can be made false in the model, by defining a bump vector for, e.g., the head entity h such that the tail entity t is pushed outside of the tail box of r in a single dimension. This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

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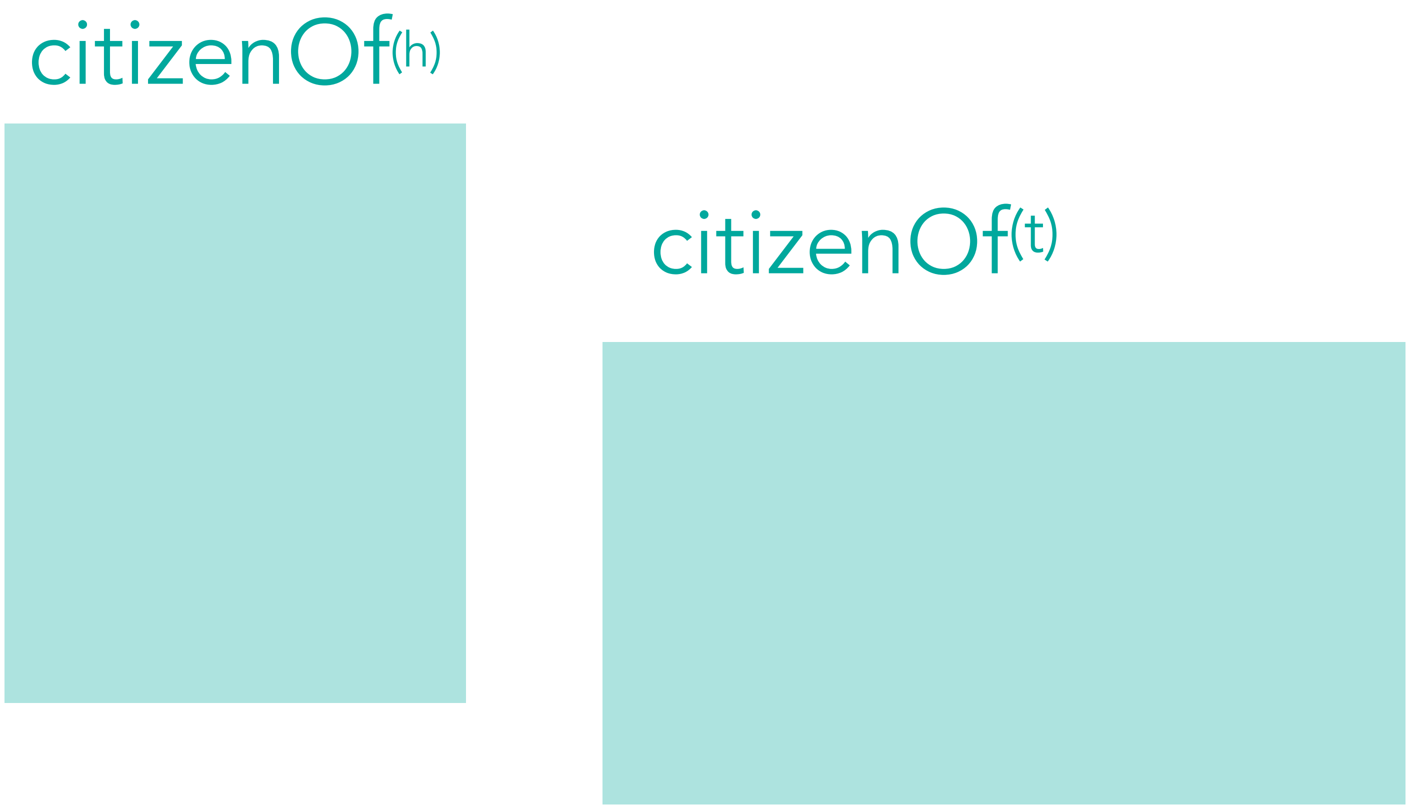

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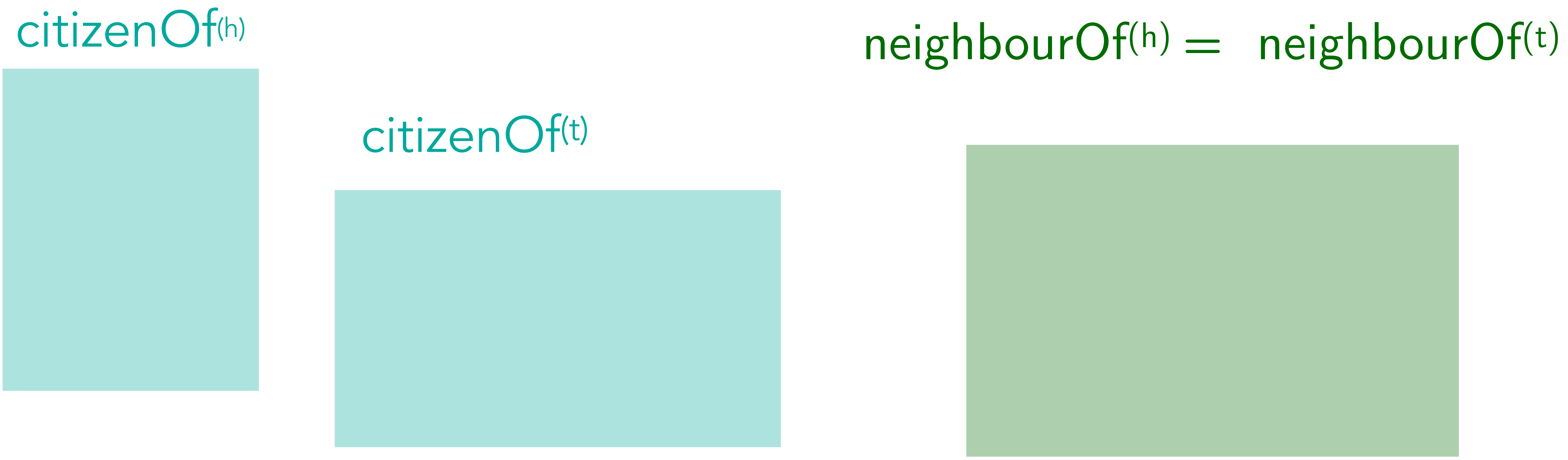

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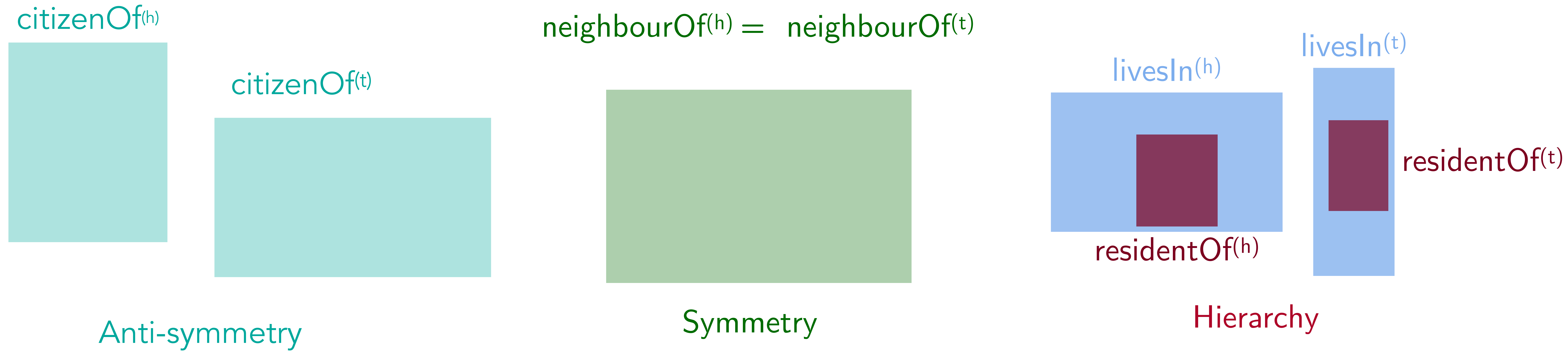

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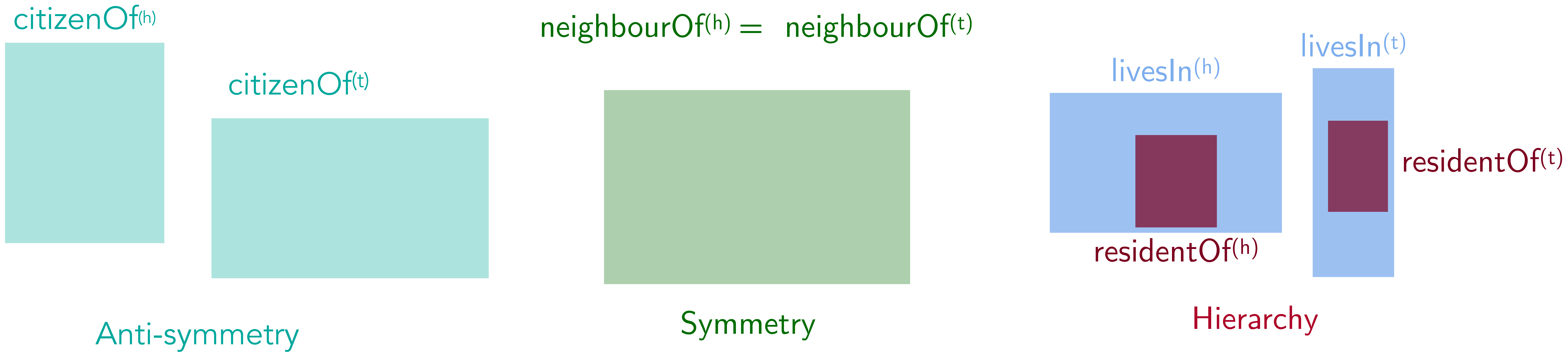

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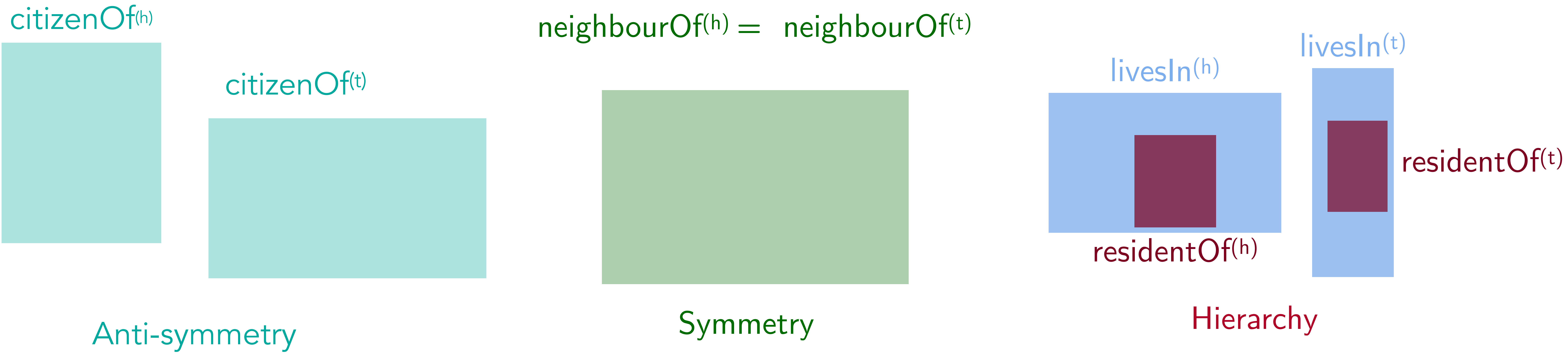

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This approach does not work for the composition pattern: $\forall x, y, z \; r(x, y) \wedge s(y, z) \Rightarrow t(x, z)$! In fact, BoxE cannot capture composition as an inference pattern.

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For example, TransE or RotatE can separately capture the composition rules:

$$\forall x, y, z \; r_1(x, y) \wedge r_4(y, z) \Rightarrow r_3(x, z) \text{ and } \forall x, y, z \; r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z),$$

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This means that even 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.

Overview of Embedding Models

Embedding Models: Representation and Scoring

Model	Entity representation	Relation representation	Scoring function
TransE	$\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$d(\mathbf{h} + \mathbf{r}, \mathbf{t}) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|$
RotatE	$\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$	$\mathbf{r} \in \mathbb{C}^d$	$d(\mathbf{h} \odot \mathbf{r}, \mathbf{t}) = \|\mathbf{h} \odot \mathbf{r} - \mathbf{t}\|$
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 $\mathbf{r}^{\mathbf{h}}, \mathbf{r}^{\mathbf{t}} \in \mathbb{R}^d$	$\left\| \mathrm{dist}(\mathbf{h}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r}^{(\mathbf{h})}) \right\|_x + \left\| \mathrm{dist}(\mathbf{t}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r}^{(\mathbf{t})}) \right\|_x$

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RotatE	$\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$	$\mathbf{r} \in \mathbb{C}^d$	$d(\mathbf{h}\odot\mathbf{r}, \mathbf{t}) = \Vert\mathbf{h}\odot\mathbf{r}-\mathbf{t}\Vert$
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	$\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$	$\mathbf{D}_r \in \mathbb{C}^d \times \mathbb{C}^d$	$\text{Re}(\mathbf{h}^\top \mathbf{D}_r \bar{\mathbf{t}})$
BoxE	$\mathbf{h}, \mathbf{t}, \mathbf{b}_\mathbf{h}, \mathbf{b}_\mathbf{t} \in \mathbb{R}^d$	Hyper-rect's $\mathbf{r}^\mathbf{h}, \mathbf{r}^\mathbf{t} \in \mathbb{R}^d$	$\Big\Vert \text{dist}(\mathbf{h}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r}^{(\mathbf{h})}) \Big\Vert_x + \Big\Vert \text{dist}(\mathbf{t}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r}^{(\mathbf{t})}) \Big\Vert_x$

A summary of the models covered in the lecture: Entity representations $h, t \in E$ and relation representations $r \in R$ are given, and the scoring function is given for an arbitrary fact $r(h, t)$.

Embedding Models: Representation and Scoring

Model	Entity representation	Relation representation	Scoring function
TransE	$\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$d(\mathbf{h}+\mathbf{r}, \mathbf{t}) = \Vert\mathbf{h}+\mathbf{r}-\mathbf{t}\Vert$
RotatE	$\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$	$\mathbf{r} \in \mathbb{C}^d$	$d(\mathbf{h}\odot\mathbf{r}, \mathbf{t}) = \Vert\mathbf{h}\odot\mathbf{r}-\mathbf{t}\Vert$
RESCAL	$\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$	$\mathbf{M}_r \in \mathbb{R}^d \times \mathbb{R}^d$	$\mathbf{h}^\top \mathbf{M}_r \mathbf{t}$
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Model specific representation constraints are excluded from the Table, and so are regularisation constraints. Please refer to the respective original work 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 / generalised 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.

Outlook and Discussions

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We will briefly revisit knowledge graph completion in the context of graph neural networks, later in the course.

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

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