

SpeedE: Euclidean Geometric Knowledge Graph Embedding Strikes Back

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Abstract

Geometric knowledge graph embedding models (gKGEs) have shown great potential for knowledge graph completion (KGC), i.e., automatically predicting missing triples. However, contemporary gKGEs require *high embedding dimensionalities* or *complex embedding spaces* for good KGC performance, drastically limiting their space and time efficiency. Facing these challenges, we propose SpeedE, a lightweight Euclidean gKGE that (1) provides strong inference capabilities, (2) is competitive with state-of-the-art gKGEs, even significantly outperforming them on YAGO3-10 and WN18RR, and (3) dramatically increases their efficiency, in particular, needing solely a fifth of the training time and a fourth of the parameters of the state-of-the-art ExpressivE model on WN18RR to reach the same KGC performance.

1 Introduction

Geometric knowledge graph embedding models (gKGEs) represent entities and relations of a *knowledge graph* (KG) as geometric shapes in the semantic vector space. gKGEs achieved promising performance on *knowledge graph completion* (KGC) and knowledge-driven applications (Wang et al., 2017; Broscheit et al., 2020); while allowing for an intuitive *geometric interpretation* of their captured patterns (Pavlović and Sallinger, 2023a,b).

Efficiency Problem. Recently, increasingly *more complex* embedding spaces were explored to boost the KGC performance of gKGEs (Sun et al., 2019; Zhang et al., 2019; Cao et al., 2021). However, more complex embedding spaces typically require more costly operations or more parameters, lowering their time and space efficiency compared to Euclidean gKGEs (Wang et al., 2021). Even more, most gKGEs require *high-dimensional embeddings* to reach good KGC performance, increasing their time and space requirements (Chami et al., 2020; Wang et al., 2021). Thus, the need for (1) complex

embedding spaces and (2) high-dimensional embeddings lowers the efficiency of gKGEs, hindering their application in resource-constrained environments, especially in mobile smart devices (Sun et al., 2019; Zhang et al., 2019; Wang et al., 2021).

Table 1: Dimensionality, MRR, convergence time, and number of parameters of SotA gKGE’s on WN18RR.

| 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 |

Challenge and Methodology. Although there has been much work on scalable gKGEs, any such work has focused exclusively on either reducing the embedding dimensionality (Balazevic et al., 2019a; Chami et al., 2020; Bai et al., 2021) or using simpler embedding spaces (Kazemi and Poole, 2018; Zhang et al., 2020; Pavlović and Sallinger, 2023b), thus addressing only one side of the efficiency problem. Facing these challenges, this work aims to design a *Euclidean* gKGE that performs well on KGC under *low-dimensional* conditions, reducing its storage space, inference, and training times. To reach this goal, we analyze ExpressivE (Pavlović and Sallinger, 2023b), a Euclidean gKGE that has shown promising performance on KGC under high-dimensional conditions.

Contribution. Based on ExpressivE, we propose the lightweight SpeedE model that (1) halves ExpressivE’s inference time and (2) enhances ExpressivE’s distance function, significantly improving its KGC performance. We evaluate SpeedE on the three standard KGC benchmarks, WN18RR, FB15k-237, and YAGO3-10, finding that it (3) is competitive with SotA gKGEs on FB15k-237 and even outperforms them significantly on WN18RR

and the large YAGO3-10 benchmark. Furthermore, we find that (4) SpeedE preserves ExpressivE’s KGC performance on WN18RR with much fewer parameters, in particular, requiring solely a fourth of the number of parameters of ExpressivE and solely a fifth of its training time to reach the same KGC performance (Table 1, also c.f. Section 6.3). In total, we propose the SpeedE model, which reaches strong KGC performance using low-dimensional embeddings while maintaining the low space and time requirements of Euclidean gKGEs.

Organization. Our paper is organized as follows: Section 2 introduces the KGC problem. Section 3 reviews related work. Section 4 discusses the ExpressivE model. Section 5 disassembles ExpressivE’s components to find a simpler model that still supports the core inference patterns (c.f. Section 2) and continues by building on these results to introduce the lightweight SpeedE model. Section 6 empirically evaluates SpeedE’s KGC performance and studies its space and time efficiency. Finally, Section 7 summarizes our results, and the appendix lists proofs, further experiments, and setup details.

2 Knowledge Graph Completion

This section discusses the KGC problem and its empirical evaluation (Abboud et al., 2020). First, we introduce the *triple vocabulary*, consisting of a finite set of *relations* \mathbf{R} and *entities* \mathbf{E} . We use this vocabulary to define triples, i.e., expressions of the form $r_j(e_h, e_t)$, where $r_j \in \mathbf{R}$, $e_h, e_t \in \mathbf{E}$, and where we call e_h the triple’s *head* and e_t its *tail*. A finite set of triples over the triple vocabulary is called a knowledge graph G . KGC describes the problem of predicting missing triples of G .

Empirical Evaluation. To experimentally evaluate gKGEs, a set of true and corrupted triples is required. True triples $r_i(e_h, e_t) \in G$ are corrupted by substituting either e_h or e_t with any $e_c \in \mathbf{E}$ such that the corrupted triple does not occur in G . To estimate a given triple’s truth, gKGEs define scores over triples and are optimized to score true triples higher than false ones. The KGC performance of a gKGE is measured with the *mean reciprocal rank* (MRR), the average of inverse ranks ($1/\text{rank}$), and H@k, the proportion of true triples within the predicted ones whose rank is at maximum k .

Theoretical Evaluation. A gKGE’s theoretical capabilities are commonly evaluated by studying the *inference patterns* it captures. An inference

pattern is a logical rule $\phi \Rightarrow \psi$, where ϕ is called its body and ψ its head. A rule $\phi \Rightarrow \psi$ is satisfied over a graph G iff if ϕ is satisfied in G , then ψ must be satisfied in G . A rule of the form $\phi \Rightarrow \perp$ states that the pattern ϕ is never satisfied in G . For instance, $r_1(X, Y) \wedge r_1(Y, X) \Rightarrow \perp$ represents that there is no pair of entities $X, Y \in \mathbf{E}$, such that both $r_1(X, Y) \in G$ and $r_1(Y, X) \in G$.

Intuition of Capturing. Following (Sun et al., 2019; Abboud et al., 2020; Pavlović and Sallinger, 2023b), a gKGE *captures* an inference pattern if there is an embedding instance such that the pattern is captured (1) exactly and (2) exclusively as formalized in the appendix. Capturing a pattern means, at an intuitive level, that there is an embedding instance such that (1) if the instance satisfies the pattern’s body, then it also satisfies its head, and (2) the instance does not capture any unwanted inference pattern.

Core Inference Patterns. Next, we briefly list important inference patterns that are commonly studied in the gKGE literature (Sun et al., 2019; Abboud et al., 2020; Pavlović and Sallinger, 2023b): (1) symmetry $r_1(X, Y) \Rightarrow r_1(Y, X)$, (2) anti-symmetry $r_1(X, Y) \wedge r_1(Y, X) \Rightarrow \perp$, (3) inversion $r_1(X, Y) \Leftrightarrow r_2(Y, X)$, (4) composition $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$, (5) hierarchy $r_1(X, Y) \Rightarrow r_2(X, Y)$, (6) intersection $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$, and (7) mutual exclusion $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$. We shall call these seven types of patterns *core inference patterns* henceforth.

3 Related Work

The main focus of our work lies on gKGEs, i.e., knowledge graph embedding models (KGEs) that allow for a geometric interpretation of their captured inference patterns. Thus, we have excluded neural KGEs as they are typically less interpretable (Dettmers et al., 2018; Socher et al., 2013; Nathani et al., 2019; Wang et al., 2021). gKGEs are commonly classified by how they embed relations:

Bilinear gKGEs embed relations as matrices, allowing them to factorize a graph’s adjacency matrix by computing the bilinear product of entity and relation embeddings. The pioneering bilinear model is RESCAL (Nickel et al., 2011), embedding relations with full-rank $d \times d$ matrices and entities with d -dimensional vectors. However, its parameter size grows quadratically with its dimensionality d , lim-

iting RESCAL’s scalability (Kazemi and Poole, 2018). Thus, more scalable bilinear gKGEs were proposed, such as DistMult (Yang et al., 2015), ComplEx (Trouillon et al., 2016), TuckER (Balazevic et al., 2019b), SimplE (Kazemi and Poole, 2018), QuatE (Zhang et al., 2019), and DualQuatE (Cao et al., 2021). Although these enhanced models could capture increasingly more inference patterns, none of them can capture composition patterns.

Spatial gKGEs embed relations as semantic regions within the embedding space. BoxE (Abboud et al., 2020) is the pioneering spatial gKGE, embedding relations with two bounded hyper-rectangles. This allows BoxE to capture most of the core inference patterns. However, purely spatial models cannot capture composition patterns.

Functional gKGEs embed relations as functions $f_{r_i} : \mathbb{K}^d \rightarrow \mathbb{K}^d$ and entities as high-dimensional points $e_j \in \mathbb{K}^d$ over some field \mathbb{K} . The pioneering functional model is TransE (Bordes et al., 2013), which embeds relations as translations from head to tail entity embeddings. However, representing relations as translations limits TransE from capturing inference patterns, such as symmetry or hierarchy. Thus, many extensions were proposed, solving some of these limitations, such as RotatE (Sun et al., 2019), MuRP (Balazevic et al., 2019a), RotH (Chami et al., 2020), HAKE (Zhang et al., 2020) and ConE (Bai et al., 2021). However, none of these models can capture hierarchy patterns.

Spatio-Functional gKGEs. Recently, Pavlović and Sallinger (2023b) proposed ExpressivE, a *spatio-functional gKGE* that combines the advantages of both spatial and functional models by embedding relations as hyper-parallelograms. Thereby, it can capture all core inference patterns simultaneously.

Embedding Space Problem. Although these model families are vastly different, many contemporary gKGEs overcome the limitations of former ones by exploring increasingly *more complex* spaces. For example, while (a) RESCAL and DistMult use the Euclidean space \mathbb{R} , (b) ComplEx uses the complex space, extending \mathbb{R} by one imaginary unit, (c) QuatE uses the quaternion space, extending \mathbb{R} by three imaginary units, and (d) DualQuatE uses the dual-quaternion space, extending \mathbb{R} by seven imaginary units. Thus, a d -dimensional entity embedding of (a) RESCAL and DISTMULT requires d , (b) ComplEx requires $2d$, (c) QuatE

requires $4d$, and (d) DualQuatE requires even $8d$ real-valued parameters. Therefore, gKGEs based in more complex embedding spaces typically require more parameters, lowering their efficiency compared to Euclidean gKGEs (Wang et al., 2021).

High-Dimensionality Problem. Even more, most gKGEs require *high-dimensional* embeddings to reach good KGC performance (Chami et al., 2020; Wang et al., 2021). Yet, high embedding dimensionalities of 200, 500, or 1000 (Sun et al., 2019; Zhang et al., 2019) increase the time and space requirements of gKGEs, limiting their efficiency and application to resource-constrained environments, especially mobile smart devices (Wang et al., 2021).

Hyperbolic gKGEs such as RotH and AttH (Chami et al., 2020) embed entities and relations in the hyperbolic space, which allows for high-fidelity and parsimonious representations of *hierarchical relations* (Balazevic et al., 2019a; Chami et al., 2020), i.e., relations that describe hierarchies between entities, such as *part_of*. This allowed them to reach promising KGC performance using low-dimensional embeddings, addressing the high-dimensionality problem (Chami et al., 2020). Yet, most hyperbolic gKGEs were limited to expressing a single global entity hierarchy per relation. ConE (Bai et al., 2021) solves this problem by embedding entities as hyperbolic cones and relations as transformations between these cones. However, hyperbolic gKGEs typically cannot directly employ Euclidean addition and scalar multiplication but require far more costly hyperbolic versions of these operations, termed Möbius Addition and Multiplication. Thus, they fail to address the embedding space problem, which results in high time requirements for hyperbolic gKGEs (Wang et al., 2021).

Euclidean gKGEs have recently shown strong representation, inference, and KGC capabilities under high-dimensional conditions. On the one hand, HAKE (Zhang et al., 2020) achieved promising results for representing hierarchical relations on which hyperbolic gKGEs are typically most effective. On the other hand, ExpressivE (Pavlović and Sallinger, 2023b) managed to capture all core inference patterns. Although Euclidean gKGEs address the embedding space problem, their reported KGC results under low dimensionalities are dramatically lower than those of hyperbolic gKGEs (Chami et al., 2020). Thus, they currently fail to address the high-dimensionality problem.

Our work is inspired by (1) the gap of gKGEs addressing both sides of the efficiency problem, i.e., the use of (a) complex embedding spaces and (b) high-dimensional embeddings (Wang et al., 2021), and (2) the promising results of Euclidean gKGEs under high embedding dimensionalities (Pavlović and Sallinger, 2023b). In contrast to prior work, our paper *jointly* focuses on both sides of the efficiency problem to design a highly resource-efficient gKGE.

4 The ExpressivE Model

This section reviews ExpressivE (Pavlović and Sallinger, 2023b), a Euclidean gKGE with strong KGC performance under high dimensionalities.

Representation. ExpressivE embeds entities $e_h \in \mathbf{E}$ via vectors $e_h \in \mathbb{R}^d$ and relations $r_j \in \mathbf{R}$ via hyper-parallellograms in \mathbb{R}^{2d} . The hyper-parallellogram of a relation r_j is parameterized via the following three vectors: (1) a *slope vector* $s_j \in \mathbb{R}^{2d}$ representing the slopes of its boundaries, (2) a *center vector* $c_j \in \mathbb{R}^{2d}$ representing its center, and (3) a *width vector* $w_j \in (\mathbb{R}_{\geq 0})^{2d}$ representing its width. At an intuitive level, a triple $r_j(e_h, e_t)$ is captured to be *true* by an ExpressivE embedding if the concatenation of its head and tail embedding is within r_j 's hyper-parallellogram. Formally, this means that a triple $r_j(e_h, e_t)$ is true if the following inequality is satisfied:

$$(e_{ht} - c_j - s_j \odot e_{th})^{|\cdot|} \preceq w_j \quad (1)$$

Where $e_{xy} := (e_x || e_y) \in \mathbb{R}^{2d}$ with $||$ representing concatenation and $e_x, e_y \in \mathbf{E}$. Furthermore, the inequality uses the following operators: the element-wise less or equal operator \preceq , the element-wise absolute value $x^{|\cdot|}$ of a vector x , and the element-wise (i.e., Hadamard) product \odot .

Scoring. ExpressivE employs the typical distance function $D : \mathbf{E} \times \mathbf{R} \times \mathbf{E} \rightarrow \mathbb{R}^{2d}$ of spatial gKGEs (Abboud et al., 2020; Pavlović and Sallinger, 2023b), which is defined as follows:

$$D(h, r_j, t) = \begin{cases} \tau_{r_j(h,t)} \odot m_j, & \text{if } \tau_{r_j(h,t)} \preceq w_j \\ \tau_{r_j(h,t)} \odot m_j - k_j, & \text{otherwise} \end{cases} \quad (2)$$

Where \odot denotes the element-wise division operator, $\tau_{r_j(h,t)} := (e_{ht} - c_j - s_j \odot e_{th})^{|\cdot|}$ denotes the triple embedding, $m_j := \mathbf{2} \odot w_j + \mathbf{1}$ represents the distance function's slopes, and $k_j := \mathbf{0.5} \odot (m_j - \mathbf{1}) \odot (m_j - \mathbf{1} \odot m_j)$.

Based on this distance function $D(h, r_j, t)$, we define ExpressivE's scoring function for quantifying the plausibility of a given triple $r_j(h, t)$ as follows:

$$s(h, r_j, t) = -||D(h, r_j, t)||_2 \quad (3)$$

5 The Methodology

Our goal is to design a gKGE that addresses the efficiency problems raised by the use of (1) complex embedding spaces and (2) high-dimensional embeddings while (3) allowing for a geometric interpretation of its embeddings (Abboud et al., 2020; Pavlović and Sallinger, 2023b). We reach this goal by designing a KGC model that (1) is based in the Euclidean space, (2) reaches high KGC performance under low-dimensional conditions while at the same time supports the *core inference patterns* (Section 2), and (3) is a gKGE.

Toward our goal, Section 5.1 analyzes the SotA ExpressivE model, finding that it uses redundant parameters that negatively affect its inference time. By redundant parameters, we mean parameters that can be removed while preserving the support of the core inference patterns (Section 2). Facing this problem, we propose the lightweight Min_SpeedE model that removes these redundancies, halving ExpressivE's inference time (Section 5.1).

However, Min_SpeedE loses the ability to adjust its distance function, which is essential for representing hierarchical relations (as empirically verified in Section 6). Thus, Section 5.2 introduces SpeedE, a model that enhances Min_SpeedE by adding carefully designed parameters for flexibly adjusting the distance function while preserving Min_SpeedE's low inference times.

5.1 Min_SpeedE

To design Min_SpeedE, let us first analyze ExpressivE's parameters, particularly its width vector. Adjusting ExpressivE's width vector w_j has two competing effects: (1) it alters the distance function's slopes (by m_j in Inequality 2), and (2) it changes which entity pairs are inside the relation hyper-parallellogram (by w_j in Inequality 1). To increase ExpressivE's time efficiency substantially, we introduce Min_SpeedE, a constrained version of ExpressivE that replaces the relation-wise width vectors $w_j \in (\mathbb{R}_{\geq 0})^{2d}$ by a constant value $w \in \mathbb{R}_{> 0}$ - that is shared across all relations $r_j \in \mathbf{R}$. The following paragraphs theoretically analyze Min_SpeedE's inference capabilities and time efficiency.

Inference Capabilities. We find that Min_SpeedE surprisingly still captures the core inference patterns (given in Section 2) and prove this in Theorem 5.1. We give the full proof in the appendix and discuss one of the most interesting parts here, namely, hierarchy patterns.

Theorem 5.1. *Min_SpeedE captures the core inference patterns, i.e., symmetry, anti-symmetry, inversion, composition, hierarchy, intersection, and mutual exclusion.*

Hierarchy Patterns. According to Pavlović and Sallinger (2023b), an ExpressivE model captures a hierarchy pattern $r_1(X, Y) \Rightarrow r_2(X, Y)$ iff r_1 's hyper-parallellogram is a proper subset of r_2 's. Thus, one would expect that ExpressivE's ability to capture hierarchy patterns is lost in Min_SpeedE, as the width parameter $w \in \mathbb{R}_{>0}$ (responsible for adjusting a hyper-parallellogram's size) is shared across all hyper-parallellograms. However, the actual size of a hyper-parallellogram does not solely depend on its width but also on its slope parameter $s_j \in \mathbb{R}^{2d}$, allowing one hyper-parallellogram H_1 to properly subsume another H_2 even when they share the same width parameter w . We have visualized two hyper-parallellograms $H_2 \subset H_1$ with the same width parameter w in Figure 1.

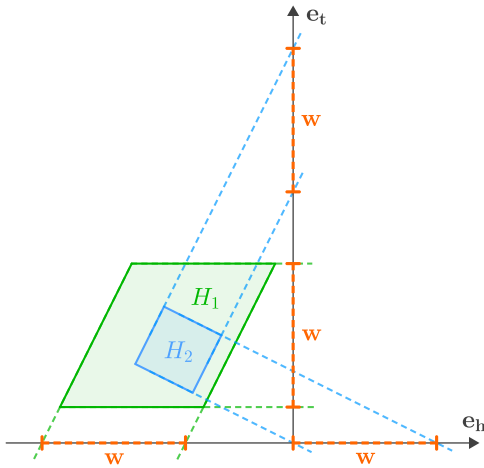


Figure 1: Representation of the two-dimensional relation hyper-parallellograms H_1 and H_2 , such that H_1 subsumes H_2 and such that they share the same width parameter w in each dimension.

Intuition. Min_SpeedE can capture $H_2 \subset H_1$ as w (depicted with orange dotted lines) represents the intersection of the bands (depicted with blue and green dotted lines), expanded from

the hyper-parallellogram, and the axis of the band's corresponding dimension. Thus, a hyper-parallellogram's actual size can be adapted by solely changing its slopes, removing the need for a learnable width parameter per dimension and relation.

Inference Time. The most costly operations during inference are operations on vectors. Thus, we can estimate ExpressivE's and Min_SpeedE's inference time by counting the number of vector operations necessary for computing a triple's score: By reducing the width vector to a scalar, many operations reduce from a vector to a scalar operation. In particular, the calculation of m_j and k_j uses solely scalars in Min_SpeedE instead of vectors. Thus, ExpressivE needs 15, whereas Min_SpeedE needs solely 8 vector operations to compute a triple's score. This corresponds to Min_SpeedE using approximately half the number of vector operations of ExpressivE for computing a triple's score, thus roughly halving ExpressivE's inference time, which aligns with Section 6.3's empirical results.

Key Insights. Fixing the width to a constant value w stops Min_SpeedE from adjusting the distance function's slopes. As we will empirically see in Section 6, the effect of this is a severely degraded KGC performance on hierarchical relations. Introducing independent parameters for adjusting the distance function's slopes solves this problem. However, these parameters must be designed carefully to (1) preserve ExpressivE's geometric interpretation and (2) retain the reduced inference time provided by Min_SpeedE. Each of these aspects will be covered in detail in the next section.

5.2 SpeedE

SpeedE further enhances Min_SpeedE by adding the following two carefully designed scalar parameters to each relation embedding: (1) the inside distance slope $s_j^i \in [0, 1]$ and (2) the outside distance slope s_j^o with $s_j^i \leq s_j^o$. Let $m_j^i := 2s_j^i w + 1$, $m_j^o := 2s_j^o w + 1$, and $k_j := m_j^o(m_j^o - 1)/2 - (m_j^i - 1)/(2m_j^i)$, then SpeedE defines the following distance function:

$$D(h, r_j, t) = \begin{cases} \tau_{r_j(h,t)} \odot m_j^i, & \text{if } \tau_{r_j(h,t)} \preceq w \\ \tau_{r_j(h,t)} \odot m_j^o - k_j, & \text{otherwise} \end{cases} \quad (4)$$

Again, the distance function is separated into two piece-wise linear functions: (1) the inside distance $D_i(h, r_j, t) = \tau_{r_j(h,t)} \odot m_j^i$ for triples that are captured to be true (i.e., $\tau_{r_j(h,t)} \preceq w$) and (2) the outside distance $D_o(h, r_j, t) = \tau_{r_j(h,t)} \odot m_j^o - k_j$

for triples that are captured to be false (i.e., $\tau_{r_j}(h, t) \succ w$). Based on this function, SpeedE defines the score as $s(h, r_j, t) = -\|D(h, r_j, t)\|_2$.

Geometric Interpretation. The intuition of s_j^i and s_j^o is that they control the slopes of the respective linear inside and outside distance functions. However, without any constraints on s_j^i and s_j^o , SpeedE would lose ExpressivE’s intuitive geometric interpretation (Pavlović and Sallinger, 2023b) as s_j^i and s_j^o could be chosen in such a way that distances of embeddings within the hyper-parallelogram are larger than those outside. By constraining these parameters to $s_j^i \in [0, 1]$ and $s_j^i \leq s_j^o$, we preserve lower distances within hyper-parallelograms than outside and, thereby, the intuitive geometric interpretation of our embeddings.

Inference Time. The additional introduction of two scalar distance slope parameters $s_j^i, s_j^o \in \mathbb{R}$ per relation r_j does not change the number of vector operations necessary for computing a triple’s score and, thus, does not significantly affect SpeedE’s inference time. Thus, we expect that SpeedE retains the time efficiency of Min_SpeedE, as empirically validated in Section 6.3.

With this, we have finished our introduction and theoretical analysis of SpeedE. What remains to be shown is its empirical performance, which we shall evaluate next.

6 Experiments

This section empirically evaluates SpeedE: Section 6.1 describes the experimental setup. Section 6.2 studies SpeedE’s KGC performance, finding that it is competitive with SotA gKGEs on FB15k-237 and even significantly outperforms them on YAGO3-10 and WN18RR. Section 6.3 studies SpeedE’s space and time efficiency, finding that on WN18RR, SpeedE needs a quarter of ExpressivE’s parameters to reach the same KGC performance while training five times faster than it.

6.1 Experimental Setup

Datasets. We empirically evaluate SpeedE on the three standard KGC benchmarks, WN18RR (Bordes et al., 2013; Dettmers et al., 2018), FB15k-237 (Bordes et al., 2013; Toutanova and Chen, 2015), and YAGO3-10 (Mahdisoltani et al., 2015). We provide detailed information about these benchmarks, including their languages, licenses, and number of triples in Appendix I.2.

Characteristics. Table 2 displays the following characteristics of the benchmarks: their number of entities $|E|$ and relations $|R|$, their curvature C_G (taken from Chami et al. (2020)), and the Krackhardt scores κ (taken from Bai et al. (2021)), consisting of the four metrics: (*connectedness, hierarchy, efficiency, LUBedness*). Both C_G and κ state how tree-like a benchmark is and, thus, how hierarchical its relations are. Following the procedure of Chami et al. (2020), we employ the standard augmentation protocol (Lacroix et al., 2018), adding inverse relations to the benchmarks.

Table 2: Benchmark dataset characteristics. Curvature C_G is from (Chami et al., 2020); the lower, the more hierarchical the data. Krackhardt scores κ are from (Bai et al., 2021); the higher, the more hierarchical the data.

| Dataset | $ E $ | $ R $ | C_G | κ |
|-----------|---------|-------|-------|--------------------------|
| FB15k-237 | 14,541 | 237 | -0.65 | (1.00, 0.18, 0.36, 0.06) |
| WN18RR | 40,943 | 11 | -2.54 | (1.00, 0.61, 0.99, 0.50) |
| YAGO3-10 | 123,143 | 37 | -0.54 | - |

Setup. We compare our SpeedE model to (1) the Euclidean gKGEs ExpressivE (Pavlović and Sallinger, 2023b), HAKE (Zhang et al., 2020), TuckER (Balazevic et al., 2019b), MuRE (Balazevic et al., 2019a), and RefE, RotE, and AttE (Chami et al., 2020), (2) the complex gKGEs ComplEx-N3 (Lacroix et al., 2018) and RotatE (Sun et al., 2019), and (3) the hyperbolic gKGEs ConE (Bai et al., 2021), MuRP (Balazevic et al., 2019a), and RefH, RotH, and AttH (Chami et al., 2020). Following Pavlović and Sallinger (2023b), we train SpeedE and ExpressivE for up to 1000 epochs using gradient descent and the Adam optimizer (Kingma and Ba, 2015) and stop the training if the validation H@10 score does not increase by minimally 0.5% for WN18RR, YAGO3-10, and 1% for FB15k-237 after 100 epochs. We average the experimental results over three runs on each benchmark to handle marginal performance fluctuations. Furthermore, as in (Chami et al., 2020), we evaluate SpeedE and ExpressivE in the low-dimensional setting using an embedding dimensionality of 32.

Reproducibility. We list further details on our experimental setup, hardware, hyperparameters, libraries (Ali et al., 2021), and definitions of metrics in the appendix. To facilitate the reproducibility of our results, we provide SpeedE’s source code in a public GitHub repository¹.

¹<https://github.com/AleksVap/SpeedE>

Table 3: Low-dimensional ($d = 32$) KGC performance of SpeedE, Min_SpeedE, ExpressivE, and SotA gKGEs on WN18RR, FB15k-237, and YAGO3-10 split by embedding space. The results of: SpeedE, Min_SpeedE, and ExpressivE were obtained by us; ConE are from (Bai et al., 2021), HAKE and RotatE are from (Zheng et al., 2022), TuckER are from (Wang et al., 2021), and any other gKGE are from (Chami et al., 2020).

| | Model | WN18RR | | FB15k-237 | | YAGO3-10 | |
|-----------------|---------------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | | MRR | H@1 | MRR | H@1 | MRR | H@1 |
| Euclidean Space | SpeedE | .493 | .446 | .320 | .227 | .413 | .332 |
| | Min_SpeedE | .485 | .442 | .319 | .226 | .410 | .328 |
| | ExpressivE | .485 | .442 | .298 | .208 | .333 | .257 |
| | TuckER | .428 | .401 | .306 | .223 | - | - |
| | MuRE | .458 | .421 | .313 | .226 | .283 | .187 |
| | RefE | .455 | .419 | .302 | .216 | .370 | .289 |
| | RotE | .463 | .426 | .307 | .220 | .381 | .295 |
| | AttE | .456 | .419 | .311 | .223 | .374 | .290 |
| | HAKE | .416 | .389 | .296 | .212 | .253 | .164 |
| | Non-Euclidean Space | RotatE | .387 | .330 | .290 | .208 | .235 |
| ComplEx-N3 | | .420 | .390 | .294 | .211 | .336 | .259 |
| MuRP | | .465 | .420 | .323 | .235 | .230 | .150 |
| RefH | | .447 | .408 | .312 | .224 | .381 | .302 |
| RotH | | .472 | .428 | .314 | .223 | .393 | .307 |
| AttH | | .466 | .419 | .324 | .236 | .397 | .310 |
| ConE | | .471 | .436 | - | - | - | - |

6.2 Knowledge Graph Completion

This section evaluates the KGC performance of SpeedE and SotA gKGEs. Furthermore, we study how well these models represent hierarchical relations, on which hyperbolic gKGEs are typically most effective (Balazevic et al., 2019a; Chami et al., 2020). Finally, we analyze the effect of embedding dimensionality on SpeedE’s KGC performance.

Low-Dimensional KGC. Following the evaluation protocol of Chami et al. (2020), we evaluate each gKGE’s performance under $d = 32$. We report the MRR and H@1 in Table 3 and provide the complete results in the appendix. Table 3 reveals that on YAGO3-10 — the largest benchmark, containing over a million triples — SpeedE outperforms any SotA gKGE by a relative difference of 7% on H@1, providing strong evidence for SpeedE’s scalability to large KGs. Furthermore, it shows that our enhanced SpeedE model is competitive with SotA gKGEs on FB15k-237 and even outperforms any competing gKGE on WN18RR by a large margin. Furthermore, SpeedE’s performance gain over Min_SpeedE on the highly hierarchical dataset WN18RR (see Table 2) provides strong empirical evidence for the effectiveness of the distance slope parameters for representing hierarchical relations under low-dimensional conditions. SpeedE’s performance on the more hierarchical WN18RR al-

ready questions the necessity of hyperbolic gKGEs for representing hierarchical relations, which will be further investigated in the following.

Hierarchical Relations (Chami et al., 2020; Zhang et al., 2020) describe hierarchies between entities, such as *part_of*. Hyperbolic gKGEs have shown great potential for representing hierarchical relations, outperforming Euclidean gKGEs under low-dimensional conditions and thereby justifying the increased model complexity added by the hyperbolic space (Chami et al., 2020). To study SpeedE’s performance on hierarchical relations, we evaluate SpeedE on the triples of any hierarchical relation of WN18RR following the methodology of Bai et al. (2021). Table 4 presents the results of this study. It reveals that SpeedE significantly improves over ExpressivE on most relations and outperforms RotH on five out of the seven hierarchical ones. Most notably, SpeedE improves over RotH by a relative difference of 23% on H@10 on the hierarchical relation *_member_of_domain_usage*, providing empirical evidence for SpeedE’s promising potential for representing hierarchical relations even under low-dimensional settings. The performance gain on hierarchical relations is likely due to the added distance slope parameters, which allow for independently adjusting the distance function’s slopes.

Table 4: H@10 of ExpressivE, RotH, and SpeedE on hierarchical relations (Bai et al., 2021) of WN18RR.

| Relation | ExpressivE | RotH | SpeedE |
|---------------------------------|--------------|--------------|--------------|
| <i>_member_meronym</i> | 0.362 | 0.399 | <u>0.379</u> |
| <i>_hypernym</i> | <u>0.276</u> | <u>0.276</u> | 0.301 |
| <i>_has_part</i> | 0.308 | 0.346 | <u>0.330</u> |
| <i>_instance_hypernym</i> | 0.509 | <u>0.520</u> | 0.543 |
| <i>_member_of_domain_region</i> | <u>0.365</u> | <u>0.365</u> | 0.397 |
| <i>_member_of_domain_usage</i> | 0.545 | 0.438 | <u>0.538</u> |
| <i>_synset_domain_topic_of</i> | <u>0.468</u> | 0.447 | 0.502 |

Dimensionality Study. To analyze the effect of the embedding dimensionality on the KGC performance, we evaluate state-of-the-art gKGEs on WN18RR under varied dimensionalities. Figure 2 visualizes the results of this study, displaying error bars for our SpeedE model with average MRR and standard deviation computed over three runs. The figure reveals that, surprisingly, ExpressivE significantly outperforms RotH, especially under low-dimensional conditions, and that the enhanced SpeedE model achieves an additional performance improvement over ExpressivE. This result provides further evidence for the great potential of Euclidean

gKGEs under low-dimensional conditions.

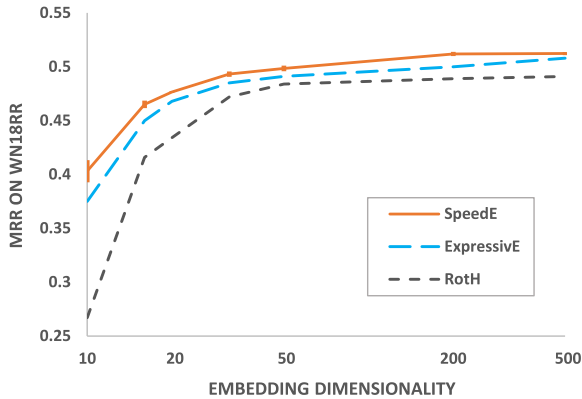


Figure 2: MRR of SotA gKGEs on WN18RR using $d \in \{10, 16, 20, 32, 50, 200, 500\}$.

High-Dimensional KGC. The KGC performance of SotA gKGEs under high-dimensional conditions (i.e., $d \geq 200$) is listed in the appendix. It reveals that on FB15k-237, SpeedE achieves highly competitive KGC performance compared to gKGEs of its own family while dramatically outperforming any competing gKGE on WN18RR.

6.3 Space and Time Efficiency

This section empirically analyzes SpeedE’s space and time efficiency compared to SotA gKGEs.

Time per Epoch. Following the methodology of Wang et al. (2021), Table 5 displays the training time per epoch of SpeedE and SotA gKGEs for WN18RR, FB15k-237, and YAGO3-10 with embedding dimensionality $d = 32$, negative sampling size $n = 500$, and batch size $b = 500$. The times per epoch were recorded on a GeForce RTX 2080 Ti GPU of our internal cluster. The empirical results of the table align with the theoretical results of Sections 5.1 and 5.2, stating that SpeedE approximately halves ExpressivE’s inference time and, thus, also its time per epoch. Furthermore, the results emphasize SpeedE’s efficiency benefits over SotA gKGEs, as they reveal that under the same configurations, SpeedE solely requires about a sixth of RotH’s and AttH’s time per epoch.

Next, to provide a fair comparison of each gKGE’s space and time efficiency, we measure the convergence time of gKGEs with approximately equal KGC performance. Specifically, we observe that SpeedE with dimensionality $d = 50$ achieves comparable or slightly better KGC performance on WN18RR to ExpressivE with $d = 200$ and the best-published results of RotH, HAKE, and ConE

Table 5: Time per epoch of SpeedE, ExpressivE, RotH, and AttH.

| 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 |

with $d = 500$. In particular, the results are summarized in Table 1 (provided in Section 1).

Hypotheses. Since (1) the dimensionality of SpeedE embeddings is much smaller in comparison to RotH’s, HAKE’s, ConE’s, and ExpressivE’s dimensionality, while (2) SpeedE achieves comparable or even slightly better KGC performance, we expect a considerable improvement in SpeedE’s space and time efficiency at comparable KGC performance. Next, based on Table 1’s results, we analyze how strongly SpeedE reduces the model size and convergence time of competing gKGEs.

Model Size Analysis. Since $|\mathbf{R}| \ll |\mathbf{E}|$ in most graphs, (WN18RR: $|\mathbf{R}|/|\mathbf{E}| = 0.00012$) and since SpeedE, ExpressivE, ConE, and RotH embed each entity with a single real-valued vector, SpeedE ($d = 50$) needs solely a quarter of ExpressivE’s ($d = 200$) and a tenth of ConE’s and RotH’s ($d = 500$) number of parameters, while preserving their KGC performance on WN18RR (Table 1). As HAKE requires two real-valued vectors per entity, SpeedE ($d = 50$) solely needs a twentieth of HAKE’s ($d = 500$) parameters to achieve a slightly better KGC performance. Table 1 lists the number of parameters of a trained SpeedE model and SotA gKGEs, empirically confirming that SpeedE significantly reduces the size of competing gKGEs.

Convergence Time Analysis. To quantify the convergence time, we measure for each gKGE the time to reach a validation MRR score of 0.490, i.e., approximately 1% less than the worst reported MRR score of Table 1. As outlined in the table, SpeedE converges already after 6min. Thus, while keeping strong KGC performance on WN18RR, SpeedE speeds up ExpressivE’s convergence time by a factor of 5, HAKE’s by a factor of 9, ConE’s by a factor of 15, and RotH’s by a factor of 20.

Discussion. These results show that SpeedE is not only competitive with SotA gKGEs on FB15k-237 and significantly outperforms them on YAGO3-10

and WN18RR but even preserves their KGC performance on WN18RR with much fewer parameters and a dramatically shorter convergence time, in particular speeding up the convergence time of the SotA ExpressivE model by a factor of 5, while using solely a fourth of its number of parameters.

7 Conclusion

Although there has been much work on resource-efficient gKGEs, any such work has focused exclusively on reducing the embedding dimensionality (Balazevic et al., 2019a; Chami et al., 2020; Bai et al., 2021) or using simpler embedding spaces (Kazemi and Poole, 2018; Zhang et al., 2020; Pavlović and Sallinger, 2023b), thus addressing only one side of the efficiency problem.

In this work, we address the embedding space and dimensionality side jointly by introducing SpeedE, a lightweight gKGE that (1) provides strong inference capabilities, (2) is competitive with SotA gKGEs, even significantly outperforming them on YAGO3-10 and WN18RR, and (3) dramatically increases the efficiency of current gKGEs, needing solely a fifth of the training time and a fourth of the number of parameters of the SotA ExpressivE model on WN18RR to reach the same KGC performance.

8 Limitations and Future Work

SpeedE and ExpressivE use one d -dimensional vector to embed entities and four, respectively, six d -dimensional vectors to embed relations. Thus, ExpressivE and SpeedE have the same space complexity, which is linear in the number of relations and entities (i.e., $O(d|E| + d|R|)$). A critical limitation of both models is that they use the same dimensionality d for relations and entities. Being able to decouple the relation and entity embedding dimensionalities might be crucial for further raising their efficiency as (1) at an intuitive level, entities are less complex objects than relations (which represent sets of pairs of entities) and therefore (2) entity embeddings might solely require a lower embedding dimensionality than relation embeddings. Since in real-world KGs, the number of entities is typically much higher than the number of relations, a lower entity dimensionality might further raise the model’s efficiency.

Since gKGEs naturally provide a geometric interpretation of their learned patterns, how to automatically and efficiently mine these learned patterns

from the embeddings — to make the implicitly learned knowledge explicit and further raise the model’s transparency — remains an open challenge and forms an exciting branch for future work. Finally, another interesting direction for future work points at how to integrate knowledge graph embeddings in novel practical applications, such as aligning their learned knowledge with the latent representations of large language models.

9 Ethical Impact

We designed SpeedE with the goal of finding a highly resource-efficient model for KGC that, at the same time, provides a geometric interpretation of its captured patterns. Therefore, our work aligns with two pressing challenges of the machine learning community in general and the KGC community in particular, namely, (1) raising the resource efficiency of KGC models while (2) offering some degree of explainability via the geometric interpretation of captured patterns. Specifically, SpeedE reduces the training time — and thus the total compute — of the SotA ExpressivE model on WN18RR to one-fourth while sustaining ExpressivE’s KGC performance and geometric interpretation. Therefore, we do not foresee any negative impact, but even expect a potential positive *environmental* (see 1) and *social impact* (see 2) of our work by introducing a highly resource-efficient model that allows for some degree of explainability.

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A Organization

This appendix includes complete proofs, experimental setup details, and additional results. In particular, Section B lists the complete low-dimensional benchmark results. Section C provides an overview of SpeedE’s modifications and their impact on SpeedE’s efficiency and prediction performance. Section D studies the relevance of the distance slope parameters by performing an ablation study. Section E reports the KGC performance of SpeedE and SotA gKGEs under high-dimensional conditions. Section F briefly summarizes the notation that is used throughout this paper. Section G formally defines vital concepts for SpeedE that we will use in our proofs. Based on the introduced concepts, Section H proves Theorem 5.1. Finally, Section I lists details on reproducing our results and on our implementation, training setup, evaluation protocol, and estimated CO2 emissions.

B Complete Low-Dimensional KGC Results

This section reports the complete KGC performance of SotA gKGEs under low-dimensional conditions (i.e., $d = 32$). Table 6 displays these results, where the results for SpeedE, Min_SpeedE, and ExpressivE were obtained by us; for ConE are from (Bai et al., 2021), for HAKE are from (Zheng et al., 2022), for TuckER are from (Wang et al., 2021), and for any other gKGE are from (Chami et al., 2020). Table 6 reveals that on YAGO3-10 — the largest benchmark, containing over a million triples (see Appendix I.2, Table 11) — SpeedE outperforms any considered gKGE by a relative difference of 7% on H@1, providing strong evidence for SpeedE’s scalability to large KGs. Furthermore, it shows that our enhanced SpeedE model is competitive with SotA gKGEs on FB15k-237 and even outperforms any competing gKGE on WN18RR by a large margin. Furthermore, SpeedE’s performance gain over Min_SpeedE on the highly hierarchical dataset WN18RR provides strong empirical evidence for the effectiveness of the distance slope parameters for representing hierarchical relations under low-dimensional conditions.

Table 6: KGC performance under low dimensionalities ($d = 32$) of SpeedE, Min_SpeedE, ExpressivE, and SotA gKGEs on WN18RR, FB15k-237, and YAGO3-10 split by embedding space.

| 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 | 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 |
| | 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 |
| | 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 | - | - | - | - | - | - | - | - |

C SpeedE’s Advancements

When we theoretically analyzed ExpressivE, we noticed that (1) its space and time efficiency and (2) its prediction performance could significantly be increased by (a) replacing its width vector with a scalar and (b) adding flexibility to its distance function by enhancing it with learnable parameters that (c) are constrained in such a way that the intuitive geometric interpretation of its embeddings is preserved. The advancements of Points (a), (b), and (c) (discussed in Section 5) are highly non-trivial and need significant theoretical and empirical effort to show that they do not have a negative impact but even a significant

positive impact on SpeedE’s prediction performance and resource efficiency. The following paragraphs briefly discuss each reported evidence for SpeedE’s advancements over SotA gKGEs.

Min_SpeedE’s Inference Capabilities. Surprisingly, there is no theoretical downside to replacing ExpressivE’s relation-wise width parameters w_j with a constant width w , as shown in Theorem 5.1 (proven in Appendix H). Specifically, it shows that Min_SpeedE, a model that replaces ExpressivE’s width vector with a scalar, still captures all core inference patterns and, thus, does not lose any of its inference capabilities.

Min_SpeedE’s Prediction Performance. Furthermore, Min_SpeedE has no empirical downside compared to ExpressivE, as verified in Table 3. Specifically, Table 3 shows that Min_SpeedE performs similarly or slightly better than ExpressivE on KGC under low embedding dimensionalities, although Min_SpeedE replaces ExpressivE’s width vector with a scalar.

SpeedE’s Performance Boost Analysis. Recall, as explained in Section 3, hyperbolic gKGEs were proposed to capture hierarchical relations more effectively with low embedding dimensionalities, which was the key reason for their strong KGC performance under low-dimensional conditions (Chami et al., 2020). To test how well SpeedE performs on hierarchical relations, we evaluated SpeedE’s KGC performance on hierarchical relations of the highly hierarchical benchmark WN18RR and compared them to the KGC performance of SotA gKGEs. Table 4 presents the results of this analysis, showing that our SpeedE model outperforms the best-performing gKGEs on most hierarchical relations. Thus, SpeedE’s performance boost under low-dimensional conditions is likely due to SpeedE’s strong performance on hierarchical relations (see Table 4). Furthermore, Table 3 shows that SpeedE even outperforms Min_SpeedE by a large margin on WN18RR, which gives strong empirical evidence for the hypothesis that the added learnable parameters in SpeedE’s distance function boost SpeedE’s KGC performance in low-dimensional conditions. Even more, Table 3 reveals that SpeedE outperformed any competing gKGE by a large margin on the highly hierarchical benchmark WN18RR.

SpeedE’s Scalability and Efficiency Results. To test whether SpeedE’s prediction performance scales to larger KGs, we benchmarked SpeedE on the YAGO3-10 benchmark (which contains over one million triples) and reported the results in Table 3. We found that SpeedE outperforms any of the considered gKGEs on YAGO3-10 by a large margin, even outperforming the best-performing hyperbolic gKGE, namely AttH, on most metrics. These results provide strong empirical evidence for SpeedE’s scalability to large KGs with millions of triples. Moreover, we did not solely show that SpeedE reaches SotA KGC performance but that it even dramatically boosts the resource efficiency of any considered gKGE. Specifically, Table 1 shows that SpeedE preserves ExpressivE’s KGC performance on WN18RR with fewer parameters and a much smaller training time. In particular, SpeedE requires solely a fourth of ExpressivE’s number of parameters and only a fifth of its training time to reach the same KGC performance. Table 5 further emphasizes SpeedE’s efficiency benefits over SotA gKGEs, revealing that under the same configurations, SpeedE requires half of ExpressivE’s and about a sixth of RotH’s and AttH’s time per epoch on all benchmarks.

Conclusion. In this section, we have very comprehensively shown that SpeedE’s modifications did not solely lead to significant KGC performance boosts as verified in Theorem 5.1, Figure 2, and Tables 3 and 4, but also that SpeedE dramatically boosts the space and time efficiency of SotA gKGEs as shown in Tables 1 and 5.

D Ablation Study

To study the necessity of s_j^i and s_j^o in SpeedE, we introduce two versions of SpeedE: (1) Eq_SpeedE that forces $s_j^i = s_j^o$ and (2) Diff_SpeedE, where s_j^i and s_j^o can be different. We hypothesize that the flexibility of different s_j^i and s_j^o might be beneficial under lower dimensionalities, while under higher dimensionalities, reducing the number of parameters and thus setting $s_j^i = s_j^o$ might be beneficial. Figure 3 visualizes the result of this analysis, empirically supporting our hypothesis, as Diff_SpeedE outperforms Eq_SpeedE under low dimensionalities and vice-versa in high ones.

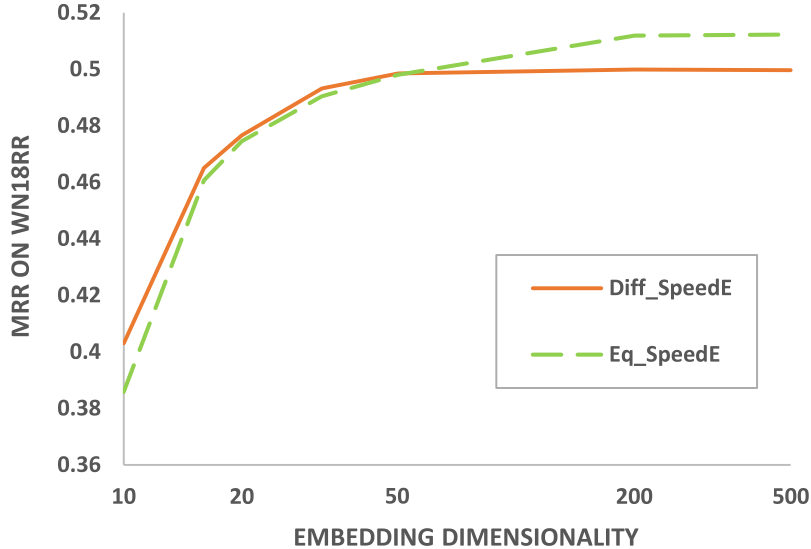


Figure 3: MRR of different ablations of SpeedE on WN18RR using $d \in \{10, 16, 20, 32, 50, 200, 500\}$

E High-Dimensional KGC Results

This section reports the KGC performance of SotA gKGEs under high-dimensional conditions (i.e., $d \geq 200$). Table 7 displays these results, where the results for SpeedE were obtained by us, for ExpressiveE are from (Pavlović and Sallinger, 2023b), for HAKE are from (Zhang et al., 2020), for ConE are from (Bai et al., 2021), for BoxE are from (Abboud et al., 2020), for MuRE and MuRP are from (Balazevic et al., 2019a; Chami et al., 2020), for DistMult are from (Dettmers et al., 2018), for RotatE are from (Sun et al., 2019), for TuckER are from (Balazevic et al., 2019b), and for any other gKGE are from (Chami et al., 2020). Table 7 reveals that on FB15k-237, SpeedE achieves highly competitive KGC performance compared to gKGEs of its own family while dramatically outperforming any competing gKGE on WN18RR.

Table 7: KGC performance under high dimensionalities of SpeedE and SotA gKGEs on WN18RR and FB15k-237 split by model family.

| Family | Model | WN18RR | | | | FB15k-237 | | | |
|----------------------|-------------|-------------|-------------|------|-------------|-------------|-------------|------|-------------|
| | | MRR | H@1 | H@3 | H@10 | MRR | H@1 | H@3 | H@10 |
| Functional / Spatial | SpeedE | .512 | <u>.460</u> | .531 | .615 | <u>.348</u> | <u>.253</u> | .386 | .536 |
| | ExpressiveE | .508 | .464 | .522 | .597 | .350 | .256 | .387 | .535 |
| | HAKE | .497 | .452 | .516 | .582 | .346 | .250 | .381 | .542 |
| | ConE | .496 | .453 | .515 | .579 | .345 | .247 | .381 | .540 |
| | BoxE | .451 | .400 | .472 | .541 | .337 | .238 | .374 | .538 |
| | MuRE | .475 | .436 | .487 | .554 | .336 | .245 | .370 | .521 |
| | RefE | .473 | .430 | .485 | .561 | .351 | .256 | .390 | <u>.541</u> |
| | RotE | .494 | .446 | .512 | .585 | .346 | .251 | .381 | .538 |
| | AttE | .490 | .443 | .508 | .581 | .351 | .255 | .386 | .543 |
| | MuRP | .481 | .440 | .495 | .566 | .335 | .243 | .367 | .518 |
| | RefH | .461 | .404 | .485 | .568 | .346 | .252 | .383 | .536 |
| | RotH | .496 | .449 | .514 | .586 | .344 | .246 | .380 | .535 |
| | AttH | .486 | .443 | .499 | .573 | <u>.348</u> | .252 | .384 | .540 |
| Bilinear | DistMult | .430 | .390 | .440 | .490 | .241 | .155 | .263 | .419 |
| | RotatE | .476 | .428 | .492 | .571 | .338 | .241 | .375 | .533 |
| | ComplEx-N3 | .480 | .435 | .495 | .572 | .357 | .264 | .392 | .547 |
| | QuatE | .488 | .438 | .508 | .582 | .348 | .248 | .382 | .550 |
| | TuckER | .470 | .443 | .482 | .526 | .358 | .266 | .394 | .544 |

F Notation

In this section, we give a brief overview of the most important notations we use. Note that, for ease of readability and comparability, we use exactly the same language as ExpressivE (Pavlović and Sallinger, 2023b).

- $v \dots$ non-bold symbols represent scalars
- $\mathbf{v} \dots$ bold symbols represent vectors, sets or tuples
- $\mathbf{0} \dots$ represents a vector of zeros (the same semantics apply to $\mathbf{0.5}$, $\mathbf{1}$, and $\mathbf{2}$)
- $\otimes \dots$ represents the element-wise division operator
- $\odot \dots$ represents the element-wise (Hadamard) product operator
- $\succeq \dots$ represents the element-wise greater or equal operator
- $\succ \dots$ represents the element-wise greater operator
- $\preceq \dots$ represents the element-wise less or equal operator
- $\prec \dots$ represents the element-wise less operator
- $\mathbf{x}^{|\cdot|} \dots$ represents the element-wise absolute value
- $\| \dots$ represents the concatenation operator

G Definition of Capturing

In this section, we introduce the formal semantics of SpeedE models. Note that, for ease of readability and comparability, we use exactly the same language as ExpressivE (Pavlović and Sallinger, 2023b). In places where SpeedE significantly differs from ExpressivE, we will explicitly note this and compare the two. Specifically, this section introduces the notions of capturing a pattern in a SpeedE model that we informally discussed in Section 2. Furthermore, it introduces some additional notations, which will help us simplify the upcoming proofs and present them intuitively.

Knowledge Graph. A tuple (G, E, R) is called a knowledge graph, where R is a finite set of relations, E is a finite set of entities, and $G \subseteq E \times R \times E$ is a finite set of triples. W.l.o.g., we assume that any relation is non-empty since removing any virtual entity pair embedding from a hyper-parallellogram would be trivial, just adding unnecessary complexity to the proofs.

SpeedE Model. We define a SpeedE model as a tuple $M^+ = (\epsilon, \sigma, w, \rho)$, where $\epsilon \subset 2^{\mathbb{R}^d}$ is the set of entity embeddings, $\sigma \subset 2^{\mathbb{R}^d}$ is the set of center embeddings, $w \in \mathbb{R}_{>0}$ represents the width constant, and $\rho \subset 2^{\mathbb{R}^d}$ is the set of slope vectors. Note that this definition is slightly different from an ExpressivE model $M = (\epsilon, \sigma, \delta, \rho)$, where instead of the width constant w , we have $\delta \subset 2^{\mathbb{R}^d}$ that represents the set of width embeddings.

Linking Embeddings to KGs. A SpeedE model $M^+ = (\epsilon, \sigma, w, \rho)$ and a KG (G, E, R) are linked via the following assignment functions: The entity assignment function $f_e : E \rightarrow \epsilon$ assigns to each entity $e_h \in E$ an entity embedding $e_h \in \epsilon$. Based on f_e , the virtual assignment function $f_v : E \times E \rightarrow \mathbb{R}^{2d}$ defines for any pair of entities $(e_h, e_t) \in E$ a virtual entity pair embedding $f_v(e_h, e_t) = (f_e(e_h) \| f_e(e_t))$, where $\|$ represents the concatenation operator. Furthermore, we define SpeedE’s relation assignment function $f_h^+(r_j) : R \rightarrow \mathbb{R}^{2d} \times \mathbb{R} \times \mathbb{R}^{2d}$ as $f_h^+(r_j) = (c_j^{ht}, w, s_j^{th})$, where $c_j^{ht} = (c_j^h \| c_j^t)$ with $c_j^h, c_j^t \in \sigma$ and where $s_j^{th} = (s_j^t \| s_j^h)$ with $s_j^t, s_j^h \in \rho$. Note that this is different from ExpressivE’s relation assignment function $f_h(r_j) : R \rightarrow \mathbb{R}^{2d} \times \mathbb{R}^{2d} \times \mathbb{R}^{2d}$, where $f_h(r_j) = (c_j^{ht}, w_j^{ht}, s_j^{th})$ with $w_j^{ht} = (w_j^h \| w_j^t)$ being two concatenated width embeddings.

Virtual Triple Space. To be able to assign a geometric interpretation to $f_h^+(r_j)$, we briefly recap the definition of the virtual triple space \mathbb{R}^{2d} introduced by Pavlović and Sallinger (2023b). Specifically, the virtual triple space is constructed by concatenating the head and tail entity embeddings. In detail, this means that any pair of entities $(e_h, e_t) \in E \times E$ defines a point in the virtual triple space by concatenating their entity embeddings $e_h, e_t \in \mathbb{R}^d$, i.e., $(e_h \| e_t) \in \mathbb{R}^{2d}$. We will henceforth call the first d dimensions of the virtual triple space the *head dimensions* and the second d dimensions the *tail dimensions*. A set of important sub-spaces of the virtual triple space are the 2-dimensional spaces created from the k -th

dimension of the head and tail dimensions — i.e., the k -th and $(d+k)$ -th virtual triple space dimensions. We call them *correlation subspaces* as they visualize the captured relation-specific dependencies of head and tail entity embeddings. Moreover, we call the correlation subspace spanned by the k -th and $(d+k)$ -th virtual triple space dimension the k -th correlation subspace. Now, the geometric interpretation of $\mathbf{f}_h^+(r_j)$ within the virtual triple space is a hyper-parallelgram whose edges are solely crooked in each correlation subspace, representing the relationship between head and tail entity embeddings.

Model Configuration. We call a SpeedE model M^+ together with a concrete relation assignment function \mathbf{f}_h^+ a relation configuration $\mathbf{m}_h^+ = (M^+, \mathbf{f}_h^+)$. If \mathbf{m}_h^+ additionally has a virtual assignment function \mathbf{f}_v , we call it a complete model configuration $\mathbf{m}^+ = (M^+, \mathbf{f}_h^+, \mathbf{f}_v)$. Note that an ExpressivE relation configuration $\mathbf{m}_h = (M, \mathbf{f}_h)$ and a complete ExpressivE model configuration $\mathbf{m} = (M, \mathbf{f}_h, \mathbf{f}_v)$ are defined differently by replacing M^+ and \mathbf{f}_h^+ with their ExpressivE equivalents, i.e., M and \mathbf{f}_h .

Definition of Truth. A triple $r_j(e_h, e_t)$ is captured to be true in some \mathbf{m}^+ , with $r_j \in \mathbf{R}$ and $e_h, e_t \in \mathbf{E}$ iff Inequality 5 holds for the assigned embeddings of h, t , and r . This means more precisely that Inequality 5 needs to hold for $\mathbf{f}_v(e_h, e_t) = (\mathbf{f}_e(e_h) \parallel \mathbf{f}_e(e_t)) = (e_h, e_t)$ and $\mathbf{f}_h^+(r_j) = (c_j^{ht}, w, s_j^{th})$. Note that, for ExpressivE, the definition of a triple's truth is slightly different, as w in Inequality 5 would be exchanged by the respective width embedding w_j^{ht} .

$$(e_{ht} - c_j^{ht} - s_j^{th} \odot e_{th})^{\cdot\cdot} \preceq w, \quad (5)$$

Intuition. At an intuitive level, a triple $r_j(e_h, e_t)$ is captured to be true by some complete SpeedE model configuration \mathbf{m}^+ iff the virtual pair embedding $\mathbf{f}_v(e_h, e_t)$ of entities e_h and e_t lies within the hyper-parallelgram of relation r_j defined by $\mathbf{f}_h^+(r_j)$.

Simplifying Notations. Therefore, to simplify the upcoming proofs, we denote with $\mathbf{f}_v(e_h, e_t) \in \mathbf{f}_h^+(r_j)$ that the virtual pair embedding $\mathbf{f}_v(e_h, e_t)$ of an entity pair $(e_h, e_t) \in \mathbf{E} \times \mathbf{E}$ lies within the hyper-parallelgram $\mathbf{f}_h^+(r_j)$ of some relation $r_j \in \mathbf{R}$ in the virtual triple space. Accordingly, for sets of virtual pair embeddings $\mathbf{P} := \{\mathbf{f}_v(e_{h_1}, e_{t_1}), \dots, \mathbf{f}_v(e_{h_n}, e_{t_n})\}$, we denote with $\mathbf{P} \subseteq \mathbf{f}_h^+(r_j)$ that all virtual pair embeddings of \mathbf{P} lie within the hyper-parallelgram of the relation r_j . Furthermore, we denote with $\mathbf{f}_v(e_h, e_t) \notin \mathbf{f}_h^+(r_j)$ that a virtual pair embedding $\mathbf{f}_v(e_h, e_t)$ does not lie within the hyper-parallelgram of a relation r_j and with $\mathbf{P} \not\subseteq \mathbf{f}_h^+(r_j)$ we denote that an entire set of virtual pair embeddings \mathbf{P} does not lie within the hyper-parallelgram of a relation r_j .

Capturing Inference Patterns. Based on the previous definitions, we define capturing patterns formally: A relation configuration \mathbf{m}_h^+ captures a pattern ψ *exactly* if for any ground pattern $\phi_{B_1} \wedge \dots \wedge \phi_{B_m} \Rightarrow \phi_H$ within the deductive closure of ψ and for any instantiation of \mathbf{f}_e and \mathbf{f}_v the following conditions hold:

- if ϕ_H is a triple and if \mathbf{m}_h^+ captures the body triples to be true — i.e., $\mathbf{f}_v(\text{args}(\phi_{B_1})) \in \mathbf{f}_h^+(\text{rel}(\phi_{B_1})), \dots, \mathbf{f}_v(\text{args}(\phi_{B_m})) \in \mathbf{f}_h^+(\text{rel}(\phi_{B_m}))$ — then \mathbf{m}_h^+ also captures the head triple to be true — i.e., $\mathbf{f}_v(\text{args}(\phi_H)) \in \mathbf{f}_h^+(\text{rel}(\phi_H))$.
- if $\phi_H = \perp$, then \mathbf{m}_h^+ captures at least one of the body triples to be false — i.e., there is some $j \in \{1, \dots, m\}$ such that $\mathbf{f}_v(\text{args}(\phi_{B_j})) \notin \mathbf{f}_h^+(\text{rel}(\phi_{B_j}))$.

where $\text{args}()$ is the function that returns the arguments of a triple, and $\text{rel}()$ is the function that returns the relation of the triple. Furthermore, a relation configuration \mathbf{m}_h^+ captures a pattern ψ *exactly* and *exclusively* if (1) \mathbf{m}_h^+ exactly captures ψ and (2) \mathbf{m}_h^+ does not capture any *positive* pattern ϕ (i.e., $\phi \in \{\text{symmetry}, \text{inversion}, \text{hierarchy}, \text{intersection}, \text{composition}\}$) such that $\psi \not\models \phi$ except where the body of ϕ is not satisfied over \mathbf{m}_h^+ .

Discussion. The next paragraphs provide some intuition of the above definition of capturing a pattern.

Capturing a pattern *exactly* is defined straightforwardly by adhering to the semantics of logical implication $\phi := \phi_B \Rightarrow \phi_H$, i.e., a relation configuration \mathbf{m}_h^+ needs to be found such that for any complete model configuration \mathbf{m}^+ over \mathbf{m}_h^+ if the body ϕ_B of the pattern is satisfied, then its head ϕ_H can be inferred.

Capturing a pattern *exactly* and *exclusively* imposes additional constraints. Here, the aim is not solely to capture a pattern but additionally to showcase that a pattern can be captured independently from any other pattern. Therefore, some notion of minimality/exclusiveness of a pattern is needed. As in [Abboud et al. \(2020\)](#); [Pavlović and Sallinger \(2023b\)](#), we define minimality by means of *solely* capturing those positive patterns ϕ that directly follow from the deductive closure of the pattern ψ , except for those ϕ that are captured trivially, i.e., except for those ϕ where their body is not satisfied over the constructed m_h^+ .

The authors of ([Pavlović and Sallinger, 2023b](#)) have shown that any core inference patterns (given in Section 2) can be expressed by means of spatial relations of the corresponding relation hyper-parallelgrams in the virtual triple space. Therefore, *exclusiveness* is formulated intuitively as the ability to limit the intersection of hyper-parallelgrams to only those intersections that directly follow from the captured pattern ψ for any known relation $r_j \in \mathbf{R}$, which is in accordance with the notion of exclusiveness of the literature ([Abboud et al., 2020](#); [Pavlović and Sallinger, 2023b](#)).

Note that the definition of capturing patterns solely depends on relation configurations. This is vital for SpeedE to capture patterns in a *lifted* manner, i.e., SpeedE shall be able to capture patterns without grounding them first. Furthermore, being able to capture patterns in a lifted way is not only efficient but also natural, as the aim is to capture patterns between relations. Thus, it would be unnatural if constraints on entity embeddings were necessary to capture such relation-specific patterns.

As outlined in the previous paragraphs, the definition of capturing patterns is in accordance with the literature ([Abboud et al., 2020](#); [Pavlović and Sallinger, 2023b](#)), focuses on efficiently capturing patterns, and gives us a formal foundation for the upcoming proofs, which will show that SpeedE can capture the core inference patterns.

H Proof of Theorem 5.1

In Section 2, we have already briefly introduced inference patterns. To prove that SpeedE captures the core inference patterns exactly and exclusively (Theorem 5.1), let us now first recall the full, formal definition of these patterns.

Definition H.1. ([Abboud et al., 2020](#); [Pavlović and Sallinger, 2023b](#)) *Let the inference patterns be defined as follows:*

- Patterns of the form $r_1(X, Y) \Rightarrow r_1(Y, X)$ with $r_1 \in \mathbf{R}$ are called symmetry patterns.
- Patterns of the form $r_1(X, Y) \wedge r_1(Y, X) \Rightarrow \perp$ with $r_1 \in \mathbf{R}$ are called anti-symmetry patterns.
- Patterns of the form $r_1(X, Y) \Leftrightarrow r_2(Y, X)$ with $r_1, r_2 \in \mathbf{R}$ and $r_1 \neq r_2$ are called inversion patterns.
- Patterns of the form $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$ with $r_1, r_2, r_3 \in \mathbf{R}$ and $r_1 \neq r_2 \neq r_3$ are called (general) composition patterns.
- Patterns of the form $r_1(X, Y) \Rightarrow r_2(X, Y)$ with $r_1, r_2 \in \mathbf{R}$ and $r_1 \neq r_2$ are called hierarchy patterns.
- Patterns of the form $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$ with $r_1, r_2, r_3 \in \mathbf{R}$ and $r_1 \neq r_2 \neq r_3$ are called intersection patterns.
- Patterns of the form $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$ with $r_1, r_2 \in \mathbf{R}$ and $r_1 \neq r_2$ are called mutual exclusion patterns.

Based on these definitions, we will prove that SpeedE captures the core inference patterns exactly and exclusively, thereby proving Theorem 5.1. To prove Theorem 5.1, we give the relevant propositions obtained from and proved by [Pavlović and Sallinger \(2023b\)](#) and adapt them to SpeedE. For each of them, we give proofs, which in some situations follow from the ones in [Pavlović and Sallinger \(2023b\)](#), and in other situations are entirely new constructions.

The key change of SpeedE that will be of our concern in the following proofs is fixing the width to a constant value, as this will require new proofs for some of the properties. Observe that SpeedE additionally changes the distance function of ExpressivE. However, this does not affect ExpressivE’s inference capabilities, i.e., which inference patterns can be captured. Careful inspection of the proofs of inference capabilities given in (Pavlović and Sallinger, 2023b) shows that the only property required of the distance function is that scores within the hyper-parallelgram are larger than those outside. As the newly defined distance function of SpeedE keeps this property, the change of distance function between the two models does not affect the proofs of the inference capabilities given in (Pavlović and Sallinger, 2023b). Hence, the same proof argument can be applied.

The other observation that we will make in general before giving the specific proofs is that the “exactly” part, proved in (Pavlović and Sallinger (2023b), Propositions F.1-F.7), of “exactly and exclusively” capturing patterns is not affected by the changes in the model. These proofs are all based on embedding pairs of entities as points in the virtual triple space and relations as hyper-parallelgrams, which is still the case in SpeedE. Thus, we now proceed to proving that SpeedE captures the core inference patterns exactly and exclusively.

Proposition H.2 (Inversion (Exactly and Exclusively)). *Let $m_h^+ = (M^+, f_h^+)$ be a relation configuration and $r_1, r_2 \in \mathbf{R}$ be relations where $r_1(X, Y) \Leftrightarrow r_2(Y, X)$ holds for any entities $X, Y \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \Leftrightarrow r_2(Y, X)$ exactly and exclusively.*

Proof. The proof of this property in Expressive (Pavlović and Sallinger (2023b), Proposition G.3) is based on a key assumption, namely that there is an m_h such that $f_h(r_1)$ is the mirror image of $f_h(r_2)$ with $f_h(r_1) \neq f_h(r_2)$. This is straightforward in ExpressivE but more complex in SpeedE. We will show this next.

Let us first observe that in SpeedE, it is not trivially given that there is an $m_h^+ = (M^+, f_h^+)$ such that $f_h^+(r_1)$ is the mirror image of $f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$, as $f_h(r_j)$ ’s width embedding w_j^{ht} has been replaced by a shared width constant w in $f_h^+(r_j)$ with $j \in \{1, 2\}$. Thus, what needs to be shown is that there is a relation configuration m_h^+ such that $f_h^+(r_1)$ is the mirror image of $f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$, as then the original proof of ExpressivE can be directly applied to prove Proposition H.2’s claim, i.e., that m_h^+ can capture $r_1(X, Y) \Leftrightarrow r_2(Y, X)$ exactly and exclusively. Now, it is interesting to see that fixing the width parameter in SpeedE as opposed to ExpressivE not only changes the model but actually allows a quite elegant construction witnessing this property.

Let us now give this construction, thereby showing the claim. Specifically, let $f_h^+(r_1) = (c_1^{ht}, w, s_1^{th})$ with $c_1^{ht} = (c_1^h || c_1^t) \in \mathbb{R}^{2d}$, $w \in \mathbb{R}_{>0}$, and $s_1^{th} = (s_1^t || s_1^h) \in \mathbb{R}^{2d}$. Furthermore, let $f_h^+(r_2) = (c_2^{ht}, w, s_2^{th})$ with $c_2^{ht} = (c_2^t || c_2^h) \in \mathbb{R}^{2d}$, $w \in \mathbb{R}_{>0}$, and $s_2^{th} = (s_2^h || s_2^t) \in \mathbb{R}^{2d}$. We will, in the following, show that the constructed $f_h(r_2)$ is the mirror image of $f_h(r_1)$ to prove our claim. Let $X, Y \in \mathbf{E}$ be arbitrary entities and let f_v be an arbitrary virtual assignment function defined over (X, Y) and (Y, X) with $f_v(X, Y) = e_{xy}$ and $f_v(Y, X) = e_{yx}$. Then by Inequality 5, a triple $r_1(X, Y)$ is captured to be true by $m^+ = (M^+, f_h^+, f_v)$ if Inequality 6 is satisfied.

$$(e_{xy} - c_1^{ht} - s_1^{th} \odot e_{yx})^{|\cdot|} \preceq w \quad (6)$$

$$(e_{yx} - c_1^{th} - s_1^{ht} \odot e_{xy})^{|\cdot|} \preceq w \quad (7)$$

$$(e_{yx} - c_2^{ht} - s_2^{th} \odot e_{xy})^{|\cdot|} \preceq w \quad (8)$$

Since Inequality 6 is element-wise, one can equivalently reformulate it by arbitrarily exchanging its dimensions. Using this insight, we can replace the head and tail dimensions for each embedding, thereby obtaining Inequality 7. Finally, by our construction of $f_h^+(r_2)$, we have that $c_2^{ht} = c_2^{th}$ and $s_2^{th} = s_2^{ht}$. We substitute these equations into Inequality 7, thereby obtaining Inequality 8. Now, Inequality 8 states by the definition of a triple’s truth (i.e., Inequality 5) that $r_2(Y, X)$ is captured by m_h^+ . Since Inequalities 6-8

are all equivalent, we have shown that $f_h^+(r_1)$ is the mirror image of $f_h^+(r_2)$. Since, it is now easy to see that an m_h^+ exists such that $f_h^+(r_1)$ is the mirror image of $f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$, the proof of (Pavlović and Sallinger (2023b), Proposition G.4) can be directly applied to SpeedE. Thus, we have proven Proposition H.2, i.e., that m_h^+ can capture $r_1(X, Y) \Leftrightarrow r_2(Y, X)$ exactly and exclusively. \square

Table 8: Relation embeddings of a relation configuration m_h^+ that captures hierarchy (i.e., $r_1(X, Y) \Rightarrow r_2(X, Y)$) exactly and exclusively using width $w = 1$.

| | c^h | s^t | c^t | s^h |
|-------|-------|-------|-------|-------|
| r_1 | -2.5 | 0.5 | 1.5 | 0 |
| r_2 | 1 | -2 | 4.5 | 2 |

Proposition H.3 (Hierarchy (Exactly and Exclusively)). *Let $m_h^+ = (M^+, f_h^+)$ be a relation configuration and $r_1, r_2 \in \mathbf{R}$ be relations where $r_1(X, Y) \Rightarrow r_2(X, Y)$ holds for any entities $X, Y \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \Rightarrow r_2(X, Y)$ exactly and exclusively.*

Proof. The proof of this property in Expressive (Pavlović and Sallinger (2023b), Proposition G.4) is based on a key assumption, namely that there is an m_h such that $f_h(r_1) \subset f_h(r_2)$ with $f_h(r_1) \neq f_h(r_2)$. This is straightforward in ExpressivE but much more complex in SpeedE. We will show this next.

Let us first observe that in SpeedE, it is not trivially given that there is an $m_h^+ = (M^+, f_h^+)$ such that $f_h^+(r_1) \subset f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$, as $f_h(r_j)$'s width embedding w_j^{ht} has been replaced by a shared width constant w in $f_h^+(r_j)$ with $j \in \{1, 2\}$. Thus, what needs to be shown is that there is a relation configuration m_h^+ such that $f_h^+(r_1) \subset f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$, as then the original proof of ExpressivE can be directly applied to prove Proposition H.3's claim, i.e., that m_h^+ can capture $r_1(X, Y) \Rightarrow r_2(X, Y)$ exactly and exclusively. In the following, we construct such a relation configuration $m_h^+ = (M^+, f_h^+)$, where $f_h^+(r_1) \subset f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$ to prove the claim of Proposition H.3:

Figure 1 (given on Page 5 of the main body) visualizes the relation configuration $m_h^+ = (M^+, f_h^+)$ provided in Table 8. As can be easily seen in Figure 1, m_h^+ captures $f_h^+(r_1) \subset f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$. Thus, we have proven Proposition H.3, as (1) we have shown the existence of an m_h^+ that captures $f_h^+(r_1) \subset f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$ and (2) the proof of (Pavlović and Sallinger (2023b), Proposition G.4) can be directly applied to SpeedE since an m_h^+ exists such that $f_h^+(r_1) \subset f_h^+(r_2)$ with $f_h^+(r_1) \neq f_h^+(r_2)$. \square

Table 9: Relation embeddings of a relation configuration m_h^+ that captures intersection (i.e., $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$) exactly and exclusively using width $w = 1$.

| | c^h | s^t | c^t | s^h |
|-------|-------|-------|-------|-------|
| r_1 | -3.75 | 0.5 | 1 | 0 |
| r_2 | 1 | -2 | 5 | 2 |
| r_3 | -3.5 | 0.5 | 0.5 | -1 |

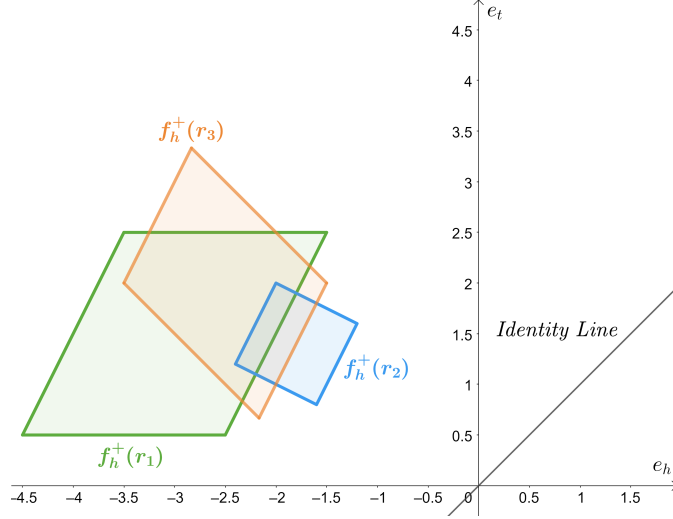


Figure 4: Relation embeddings of a relation configuration m_h that captures intersection (i.e., $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$) exactly and exclusively using width $w = 1$.

Proposition H.4 (Intersection (Exactly and Exclusively)). Let $m_h^+ = (M^+, f_h^+)$ be a relation configuration and $r_1, r_2, r_3 \in \mathbf{R}$ be relations where $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$ holds for any entities $X, Y \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$ exactly and exclusively.

Proof Sketch. This is similar in construction to the previous proof. Hence, we only give a proof sketch for ease of readability. To prove Proposition H.4, observe that in (Pavlović and Sallinger (2023b), Proposition G.5) an ExpressivE relation configuration m_h with several different width embeddings is constructed. However, the key observation we will make is that choosing the width embeddings differently is not necessary. In fact, an interested reader inspecting the original proof can obtain a proof applicable to SpeedE by following the proof of (Pavlović and Sallinger (2023b), Proposition G.5) analogously for the SpeedE relation configuration m_h^+ described in Table 9 and visualized by Figure 4. Thus, the proof for Proposition H.4 is straightforward given m_h^+ defined in Table 9 and (Pavlović and Sallinger (2023b), Proposition G.5). \square

Table 10: Relation embeddings of a relation configuration m_h^+ that captures composition (i.e., $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$) exactly and exclusively using width $w = 1$.

| | c^h | s^t | c^t | s^h |
|-------|-------|-------|-------|-------|
| r_1 | -7 | 3 | 5 | 1 |
| r_2 | -7.5 | 1 | 2 | 3 |
| r_3 | -19.5 | 2 | 13 | 2 |

Proposition H.5 (Composition (Exactly and Exclusively)). Let $r_1, r_2, r_3 \in \mathbf{R}$ be relations and let $m_h^+ = (M^+, f_h^+)$ be a relation configuration, where f_h^+ is defined over r_1, r_2 , and r_3 . Furthermore let r_3 be the composite relation of r_1 and r_2 , i.e., $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$ holds for all entities $X, Y, Z \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$ exactly and exclusively.

Proof Sketch. This is similar in construction to the proof of Proposition H.3. Hence, we only give a proof sketch for ease of readability. To prove Proposition H.5, observe that in (Pavlović and Sallinger (2023b), Proposition G.6), an ExpressivE relation configuration m_h with several different width embeddings is constructed. However, choosing the width embeddings differently is not necessary. In fact, an interested reader inspecting the original proof can obtain a proof applicable to SpeedE by following the proof of (Pavlović and Sallinger (2023b), Proposition G.6) analogously for the SpeedE relation configuration m_h^+

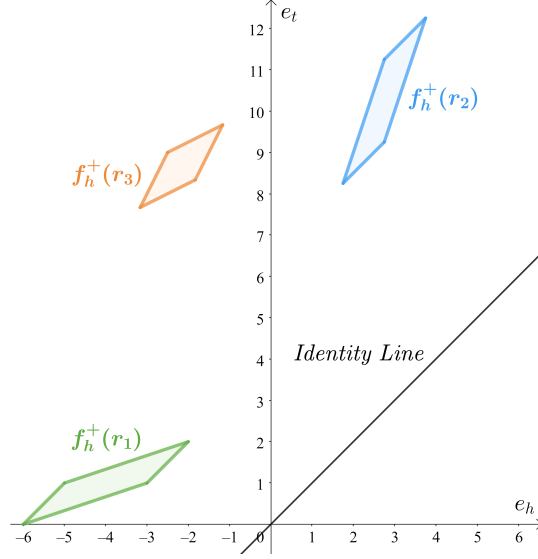


Figure 5: Relation embeddings of a relation configuration m_h that captures composition (i.e., $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$) exactly and exclusively using width $w = 1$.

described in Table 10 and visualized by Figure 5. Thus, the proof for Proposition H.5 is straightforward given m_h^+ defined in Table 10 and (Pavlović and Sallinger (2023b), Proposition G.6). \square

Proposition H.6 (Symmetry (Exactly and Exclusively)). *Let $m_h^+ = (M^+, f_h^+)$ be a relation configuration and $r_1 \in \mathbf{R}$ be a symmetric relation, i.e., $r_1(X, Y) \Rightarrow r_1(Y, X)$ holds for any entities $X, Y \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \Rightarrow r_1(Y, X)$ exactly and exclusively.*

Proposition H.7 (Anti-Symmetry (Exactly and Exclusively)). *Let $m_h^+ = (M^+, f_h^+)$ be a relation configuration and $r_1 \in \mathbf{R}$ be an anti-symmetric relation, i.e., $r_1(X, Y) \wedge r_1(Y, X) \Rightarrow \perp$ holds for any entities $X, Y \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \wedge r_1(Y, X) \Rightarrow \perp$ exactly and exclusively.*

The proofs for Proposition H.6-H.7 are straightforward and work analogously to the proofs of (Pavlović and Sallinger (2023b), Proposition G.1-G.2). This is the case, as (1) any of these patterns contain at most one relation, (2) thus we solely need to show that no unwanted patterns over at most one relation are captured, as any considered pattern over more than one relation (precisely inversion, hierarchy, intersection, and composition) requires by Definition H.1 at least two or three *distinct* relations and thus is not applicable, and (3) it is easy to see that, for instance, a relation hyper-parallelogram can be symmetric without being anti-symmetric, or vice versa (i.e., without capturing any unwanted pattern).

Proposition H.8 (Mutual Exclusion (Exactly and Exclusively)). *Let $m_h^+ = (M^+, f_h^+)$ be a relation configuration and $r_1, r_2 \in \mathbf{R}$ be mutually exclusive relations, i.e., $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$ holds for any entities $X, Y \in \mathbf{E}$. Then m_h^+ can capture $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$ exactly and exclusively.*

The proof for Proposition H.8 is trivial, as it is straight-forward to see that (1) there is an $m_h^+ = (M^+, f_h^+)$ such that $f_h^+(r_1) \cap f_h^+(r_2) = \emptyset$, thereby m_h^+ captures $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$ exactly, (2) neither $f_h^+(r_1)$ nor $f_h^+(r_2)$ need to be symmetric, thereby no unwanted symmetry pattern is captured, (3) $f_h^+(r_1)$ does not need to be the mirror image of $f_h^+(r_2)$, thus no unwanted inversion pattern is captured, and finally (4) since $f_h^+(r_1)$ and $f_h^+(r_2)$ are disjoint, neither $f_h^+(r_1)$ can subsume $f_h^+(r_2)$ nor vice versa, thus no unwanted hierarchy pattern is captured. Thus by Points 1-4, we have shown that m_h^+ captures $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$ exactly and that it does not capture any unwanted positive pattern that is applicable, i.e., requires at most two different relations (symmetry, inversion, and hierarchy). Thus, we have shown Proposition H.8, i.e., that m_h^+ can capture $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$ exactly and exclusively.

Finally, by Propositions H.2-H.8, we have shown Theorem 5.1, i.e., that SpeedE captures the core inference patterns exactly and exclusively.

I Experimental Details

The details of our experiment’s setup, benchmarks, and evaluation protocol are covered in this section. Specifically, details on SpeedE’s implementation and about reproducing our results are covered in Section I.1. Each benchmark’s properties are discussed in Section I.2. Our experimental setup is described in Section I.3, including details about the chosen learning setup, hardware, and hyperparameters. The evaluation protocol and the used metrics are discussed in Section I.4. Finally, the size of CO2 emissions resulting from our experiments is estimated in Section I.5.

I.1 Implementation Details & Reproducibility

Following Pavlović and Sallinger (2023b), we have implemented our gKGE using PyKEEN 1.7 (Ali et al., 2021), a Python library that runs under the MIT license and offers support for numerous benchmarks and gKGEs. In doing so, we facilitate the comfortable reuse of SpeedE for upcoming benchmarks and applications. To ease reproducing our findings, we provide SpeedE’s source code in a public GitHub repository². Additionally, the repository contains a ReadMe.md file stating library dependencies and running instructions.

I.2 Benchmarks and Licenses

The details of the three standard KGC benchmarks, WN18RR (Dettmers et al., 2018), FB15k-237 (Toutanova and Chen, 2015), and YAGO3-10 (Mahdisoltani et al., 2015) used in our experiments are discussed in this section. WN18RR is extracted from the WordNet database (Miller, 1995), representing lexical relations between English words, thus naturally containing many hierarchical relations (e.g., hypernym-of) (Chami et al., 2020). FB15k-237 is a subset of a collaborative database consisting of general knowledge (in English) called Freebase (Bollacker et al., 2007), which contains both hierarchical relations (e.g., part-of) and non-hierarchical ones (e.g., nationality) (Chami et al., 2020). YAGO3-10 is a subset of YAGO3, which is a KG describing people that, similarly to FB15k-237, contains both hierarchical relations (e.g., actedIn) and non-hierarchical relations (e.g., isMarriedTo). Table 2 (given on Page 6 of the main body) has already stated important characteristics of the benchmarks, including their number of entities, relations, and metrics describing how hierarchical the relations within the benchmark are. WN18RR, FB15k-237, and YAGO3-10 (Mahdisoltani et al., 2015) already provide a split into a training, validation, and testing set, which we directly adopted in any reported experiments. Table 11 lists characteristics of these splits, specifically the number of training, validation, and testing triples. Furthermore, the table lists the number of entities and relations of each benchmark. Finally, concerning licensing, we did not find a license for WN18RR nor its superset WN18 (Bordes et al., 2013). Also, we did not find a license for FB15k-237, but we found that its superset FB15k (Bordes et al., 2013) uses the CC BY 2.5 license. For YAGO3-10, we also did not find a license, but we found that its superset YAGO3 (Mahdisoltani et al., 2015) uses the CC BY 3.0 license.

Table 11: Benchmark split characteristics: Number of entities, relations, and training, validation, and testing triples.

| Dataset | $ E $ | $ R $ | #training triples | #validation triples | #testing triples |
|-----------|---------|-------|-------------------|---------------------|------------------|
| FB15k-237 | 14,541 | 237 | 272,115 | 17,535 | 20,466 |
| WN18RR | 40,943 | 11 | 86,835 | 3,034 | 3,134 |
| YAGO3-10 | 123,143 | 37 | 1,079,040 | 4,978 | 4,982 |

I.3 Training Setup

Training Details. We have trained each model on one of four GeForce RTX 2080 Ti GPUs of our internal cluster. In particular, during the training phase, we optimize the self-adversarial negative sampling loss (Sun et al., 2019) using the Adam optimizer (Kingma and Ba, 2015). We use gradient descent to optimize SpeedE’s parameters, stopping the training after 1000 epochs early if the H@10 score did not rise by at

²<https://github.com/AleksVap/SpeedE>

least 0.5% for WN18RR and YAGO3-10 and 1% for FB15k-237. Any experiment was run three times to average over light performance variations. We will discuss the optimization of hyperparameters in the following paragraph.

Hyperparameter Optimization. Following similar optimization principles as Balazevic et al. (2019a); Chami et al. (2020); Pavlović and Sallinger (2023b), we manually tuned the following hyperparameters within the listed ranges: (1) the learning rate $\lambda \in \{b * 10^{-c} \mid b \in \{1, 2, 5\} \wedge c \in \{2, 3, 4, 5, 6\}\}$, (2) the negative sample size $n \in \{100, 150, 200, 250\}$, (3) the loss margin $\gamma \in \{2, 3, 4, 5, 6\}$, (4) the adversarial temperature $\alpha \in \{1, 2, 3, 4\}$, (5) the batch size $b \in \{100, 250, 500, 1000, 2000\}$, and (6) constraining the distance slope parameters to be equal — i.e., $s_j^i = s_j^o$ for each relation $r_j \in \mathbf{R}$ — or not $EqDS \in \{true, false\}$. Following the literature (Chami et al., 2020; Lu and Hu, 2020), we used for the large YAGO3-10 benchmark a wider range for the negative sampling size n , in particular $n \in \{100, 200, 500, 1000, 2000\}$. Similar to Lu and Hu (2020), we also increased the range for margins γ to include 50 and 100 for YAGO3-10. In accordance with Pavlović and Sallinger (2023b), we chose self-adversarial negative sampling (Sun et al., 2019) for generating negative triples. We list the best hyperparameters for SpeedE split by benchmark and embedding dimensionality in Table 12. Following Chami et al. (2020), we used one parameter set for any low-dimensional experiment (i.e., $d \leq 50$) and one parameter set for any high-dimensional experiment (i.e., $d > 50$). Furthermore, for ExpressivE, we used the hyperparameters of Pavlović and Sallinger (2023b) under high-dimensional conditions, as they report the best-published results for ExpressivE. For low-dimensional conditions, ExpressivE’s best hyperparameter setting was unknown. Thus, we optimized ExpressivE’s hyperparameters manually, finding the hyperparameters of Table 13 to produce the best KGC results for ExpressivE under low dimensionalities. For RotH, we used the hyperparameters of Chami et al. (2020), as they report the best-published results for RotH. Finally, we used the same hyperparameters for each of SpeedE’s model variants to directly compare SpeedE to them, i.e., Min_SpeedE, Diff_SpeedE, and Eq_SpeedE.

Table 12: Hyperparameters of SpeedE models that achieve the best performance on WN18RR, FB15k-237, and YAGO3-10 split by low-dimensional (i.e., $d \leq 50$) and high-dimensional setting (i.e., $d > 50$).

| Dataset | Embedding Dimensionality | Margin | Learning Rate | Adversarial Temperature | Negative Sample Size | Batch Size | EqDS |
|-----------|--------------------------|--------|---------------|-------------------------|----------------------|------------|-------|
| WN18RR | $d \leq 50$ | 3 | $5 * 10^{-3}$ | 2 | 200 | 250 | false |
| WN18RR | $d > 50$ | 3 | $1 * 10^{-3}$ | 2 | 200 | 250 | true |
| FB15k-237 | $d \leq 50$ | 2 | $5 * 10^{-4}$ | 4 | 250 | 100 | false |
| FB15k-237 | $d > 50$ | 4 | $1 * 10^{-4}$ | 4 | 150 | 1000 | false |
| YAGO3-10 | $d \leq 50$ | 100 | $1 * 10^{-2}$ | 2 | 2000 | 2000 | false |

Table 13: Hyperparameters of ExpressivE that achieve the best performance on WN18RR, FB15k-237, and YAGO3-10 under low-dimensional conditions (i.e., $d \leq 50$).

| Dataset | Embedding Dimensionality | Margin | Learning Rate | Adversarial Temperature | Negative Sample Size | Batch Size |
|-----------|--------------------------|--------|---------------|-------------------------|----------------------|------------|
| WN18RR | $d \leq 50$ | 2 | $5 * 10^{-3}$ | 3 | 200 | 250 |
| FB15k-237 | $d \leq 50$ | 2 | $5 * 10^{-4}$ | 4 | 250 | 100 |
| YAGO3-10 | $d \leq 50$ | 100 | $1 * 10^{-2}$ | 2 | 2000 | 2000 |

I.4 Evaluation Protocol

Following the standard KGC evaluation protocol as described by Sun et al. (2019); Balazevic et al. (2019b); Chami et al. (2020); Pavlović and Sallinger (2023b), we have evaluated ExpressivE by measuring

the ranking quality of each test set triple $r_i(e_h, e_t)$ over all possible heads e'_h and tails e'_t : $r_i(e'_h, e_t)$ for all $e'_h \in \mathbf{E}$ and $r_i(e_h, e'_t)$ for all $e'_t \in \mathbf{E}$. The typical metrics for evaluating the KGC performance are the mean reciprocal rank (MRR) and H@k (Bordes et al., 2013). In particular, we have presented the filtered metrics (Bordes et al., 2013), i.e., all triples occurring in the training, validation, and testing set are deleted from the ranking (apart from the test triple that must be ranked), as scoring these triples highly does not indicate a wrong inference. The most used metrics for assessing gKGEs are the filtered MRR, H@1, and H@10 (Sun et al., 2019; Trouillon et al., 2016; Balazevic et al., 2019b; Abboud et al., 2020). Finally, we will briefly review how these metrics are defined: The proportion of true triples among the predicted triples whose rank is at maximum k is represented by H@k, whereas the MRR reflects the average of inverse ranks ($1/\text{rank}$).

I.5 CO2 Emissions

The sum of all reported experiments took less than 150 GPU hours. This corresponds to an estimate of approximately $16.20\text{kg } CO_2\text{-eq}$, based on the OECD’s 2014 carbon efficiency average of $0.432\text{kg}/\text{kWh}$ and the usage of an RTX 2080 Ti on private infrastructure. We computed these estimates using the MachineLearning Impact calculator (Lacoste et al., 2019).