TuckER: Tensor Factorization for Knowledge Graph Completion

Ivana Balažević ¹ Carl Allen ¹ Timothy M. Hospedales ¹

Abstract

Knowledge graphs are structured representations of real world facts. However, they typically contain only a small subset of all possible facts. Link prediction is a task of inferring missing facts based on existing ones. We propose TuckER, a relatively simple but powerful linear model based on Tucker decomposition of the binary tensor representation of knowledge graph triples. TuckER outperforms all previous state-of-the-art models across standard link prediction datasets. We prove that TuckER is a fully expressive model, deriving the bound on its entity and relation embedding dimensionality for full expressiveness which is several orders of magnitude smaller than the bound of previous state-of-the-art models ComplEx and SimplE. We further show that several previously introduced linear models can be viewed as special cases of TuckER.

1. Introduction

Vast amounts of information available in the world can be represented succinctly as *entities* and *relations* between them. *Knowledge graphs* are large, graph-structured databases which store facts in triple form (e_s, r, e_o) , with e_s and e_o representing subject and object entities and r a relation between them. Knowledge graphs are used for a wide range of natural language processing and information extraction tasks. However, far from all available information is stored in existing knowledge graphs and manually adding new information is costly, which creates the need for algorithms that are able to automatically infer missing facts based on existing ones.

Knowledge graphs can be represented by a third-order binary tensor, where each element corresponds to a triple, 1 indicating a true fact and 0 indicating the unknown (either a false or a missing fact). One of the most important tasks in relational machine learning is *link prediction*: predicting

Preprint. Work in progress.

whether two entities are related, based on known relations already present in a knowledge graph. The task of link prediction is thus to infer which of the 0 entries in the tensor are indeed false, and which are missing but actually true.

A large number of approaches to link prediction so far have been linear, based on various methods of factorizing the third-order binary tensor (Nickel et al., 2011; Yang et al., 2015; Trouillon et al., 2016; Kazemi & Poole, 2018). Recently, state-of-the-art results have been achieved using non-linear convolutional models (Dettmers et al., 2018; Balažević et al., 2018). Despite achieving very good performance, the fundamental problem with deep, non-linear models is that they are non-transparent and poorly understood, as opposed to more mathematically principled and widely studied tensor decomposition models.

In this paper, we introduce TuckER (E stands for entities, R for relations), a simple linear model for link prediction in knowledge graphs, based on Tucker decomposition (Tucker, 1966) of the third-order binary tensor of triples. Tucker decomposition factorizes a tensor into a core tensor multiplied by a matrix along each mode. It can be thought of as a form of higher-order singular value decomposition (HOSVD) in the special case where matrices are orthogonal and the core tensor is "all-orthogonal" (Kapteyn et al., 1986; Kroonenberg & De Leeuw, 1980; Kolda & Bader, 2009). In our case, rows of the three matrices contain entity and relation embedding vectors, while entries of the core tensor determine the level of interaction between them. Further, subject and object entity embedding matrices are assumed equivalent, i.e. we make no distinction between the embeddings of an entity depending on whether it appears as a subject or as an object in a particular triple.

Given that knowledge graphs contain several relation types (symmetric, asymmetric, transitive, etc.), it is important for a link prediction model to have enough expressive power to accurately represent all of them. We thus show that TuckER is *fully expressive*, i.e. given any ground truth over the triples, there exists an assignment of values to the entity and relation embeddings that accurately separates the true triples from false ones. We also derive a bound on the entity and relation embedding dimensionality that guarantees full expressiveness, finding it to be several orders of magnitude lower than the bound of previous state-of-the-art models

¹School of Informatics, University of Edinburgh, United Kingdom. Correspondence to: Ivana Balažević <ivana.balazevic@ed.ac.uk>.

ComplEx (Trouillon et al., 2016) and SimplE (Kazemi & Poole, 2018). This enables TuckER to achieve better results with much smaller embedding sizes than needed by those models, important for efficiency in downstream tasks.

Finally, we show that several previous state-of-the-art linear models, RESCAL (Nickel et al., 2011), DistMult (Yang et al., 2015), ComplEx (Trouillon et al., 2016) and SimplE (Kazemi & Poole, 2018), are special cases of TuckER.

In summary, the main contributions of this paper are:

- proposing TuckER, a new *linear* model for link prediction in knowledge graphs, that is simple, expressive and achieves *state-of-the-art results* across all standard datasets;
- proving that TuckER is *fully expressive* and deriving a bound on the entity and relation embedding dimensionality for full expressiveness which is several orders of magnitude lower than the bound of previous state-ofthe-art models ComplEx and SimplE; and
- showing that TuckER subsumes several previously proposed tensor factorization approaches to link prediction, i.e. that RESCAL, DistMult, ComplEx and SimplE are all special cases of our model.

2. Related Work

Several *linear* models for link prediction have previously been proposed:

RESCAL An early linear model, RESCAL (Nickel et al., 2011), optimizes a scoring function containing a bilinear product between vector embeddings for each subject and object entity and a full rank matrix for each relation. Although a very expressive and powerful model, RESCAL is prone to overfitting due to its large number of parameters, which increases quadratically in the embedding dimension with the number of relations in a knowledge graph.

DistMult DistMult (Yang et al., 2015) is a special case of RESCAL with a diagonal matrix per relation, so the number of parameters of DistMult grows linearly with respect to the embedding dimension, reducing overfitting. However, the linear transformation performed on subject entity embedding vectors in DistMult is limited to a stretch. Given the equivalence of subject and object entity embeddings for the same entity, third-order binary tensor learned by DistMult is symmetric in the subject and object entity mode and thus DistMult cannot model asymmetric relations.

ComplEx ComplEx (Trouillon et al., 2016) extends Dist-Mult to the complex domain. Even though each relation matrix of ComplEx is still diagonal, subject and object entity embeddings for the same entity are no longer equivalent, but complex conjugates, which introduces asymmetry into the tensor decomposition and thus enables ComplEx to model asymmetric relations.

SimplE SimplE (Kazemi & Poole, 2018) is a linear model based on Canonical Polyadic (CP) decomposition (Hitchcock, 1927). In CP decomposition, subject and object entity embeddings for the same entity are independent (note that DistMult is a special case of CP, where subject and object entity embeddings are equivalent). SimplE's scoring function alters CP to make subject and object entity embedding vectors dependent on each other, i.e. it computes the average of two terms, first of which is a bilinear product of the head embedding of the subject entity, relation embedding and tail embedding of the head embedding of the object entity, inverse relation embedding and tail embedding of the subject entity.

Recently, state-of-the-art results have been achieved with *non-linear* models:

ConvE ConvE (Dettmers et al., 2018) is the first non-linear model that significantly outperformed the preceding linear models. In ConvE, a global 2D convolution operation is performed on the subject entity and relation embedding vectors, after they are reshaped to matrices and concatenated. The obtained feature maps are flattened, transformed through a fully connected layer, and the inner product is taken with all object entity vectors to generate a score for each triple. Whilst results achieved by ConvE are impressive, its reshaping and concatenating of vectors as well as using 2D convolution on word embeddings is unintuitive.

HypER HypER (Balažević et al., 2018) is a simplified convolutional model, that uses a hypernetwork to generate 1D convolutional filters for each relation, extracting relation-specific features from subject entity embeddings. The authors show that convolution is a way of introducing sparsity and parameter tying and that HypER can be understood in terms of tensor factorization up to a non-linearity, thus placing HypER closer to the well established family of factorization models. The drawback of HypER is that it sets most elements of the core weight tensor to 0, which amounts to hard regularization, rather than letting the model learn which parameters to use via a soft regularization approach.

Scoring functions of all models described above and TuckER are summarized in Table 1.

3. Background

Let $\mathcal E$ denote the set of all entities and $\mathcal R$ the set of all relations present in a knowledge graph. A triple is represented as (e_s, r, e_o) , with $e_s, e_o \in \mathcal E$ denoting subject and object entities respectively and $r \in \mathcal R$ the relation between them.

Table 1. Scoring functions of state-of-the-art link prediction models, the dimensionality of their relation parameters, and significant terms of their space complexity. d_e and d_r are the dimensionalities of entity and relation embeddings, while n_e and n_r denote the number of entities and relations respectively. $\mathbf{\bar{e}}_o \in \mathbb{C}^{d_e}$ is the complex conjugate of \mathbf{e}_o , $\mathbf{\underline{e}}_s$, $\mathbf{\underline{w}}_r \in \mathbb{R}^{d_w \times d_h}$ denote a 2D reshaping of \mathbf{e}_s and \mathbf{w}_r respectively, \mathbf{h}_{e_s} , $\mathbf{t}_{e_s} \in \mathbb{R}^{d_e}$ are the head and tail entity embedding of entity e_s , and $\mathbf{w}_{r-1} \in \mathbb{R}^{d_r}$ is the embedding of relation r^{-1} which is the inverse of relation r. * is the convolution operator, $\langle \cdot \rangle$ denotes the dot product and \times_n denotes the tensor product along the n-th mode, f is a non-linear function, and $\mathcal{W} \in \mathbb{R}^{d_e \times d_e \times d_r}$ is the core tensor of a Tucker decomposition.

Model	Scoring Function	Relation Parameters	Space Complexity		
RESCAL (Nickel et al., 2011)	$\mathbf{e}_s^\top \mathbf{W}_r \mathbf{e}_o$	$\mathbf{W}_r \in \mathbb{R}^{{d_e}^2}$	$\mathcal{O}(n_e d_e + n_r d_r^2)$		
DistMult (Yang et al., 2015)	$\langle \mathbf{e}_s, \mathbf{w}_r, \mathbf{e}_o angle$	$\mathbf{w}_r \in \mathbb{R}^{d_e}$	$\mathcal{O}(n_e d_e + n_r d_e)$		
ComplEx (Trouillon et al., 2016)	$\operatorname{Re}(\langle \mathbf{e}_s, \mathbf{w}_r, \overline{\mathbf{e}}_o angle)$	$\mathbf{w}_r \in \mathbb{C}^{d_e}$	$\mathcal{O}(n_e d_e + n_r d_e)$		
ConvE (Dettmers et al., 2018)	$f(\text{vec}(f([\underline{\mathbf{e}}_s;\underline{\mathbf{w}}_r]*w))\mathbf{W})\mathbf{e}_o$	$\mathbf{w}_r \in \mathbb{R}^{d_r}$	$\mathcal{O}(n_e d_e + n_r d_r)$		
HypER (Balažević et al., 2018)	$f(\text{vec}(\mathbf{e}_s*\text{vec}^{-1}(\mathbf{w}_r\mathbf{H}))\mathbf{W})\mathbf{e}_o$	$\mathbf{w}_r \in \mathbb{R}^{d_r}$	$\mathcal{O}(n_e d_e + n_r d_r)$		
SimplE (Kazemi & Poole, 2018)	$rac{1}{2}(\langle\mathbf{h}_{e_s},\mathbf{w}_r,\mathbf{t}_{e_o} angle+\langle\mathbf{h}_{e_o},\mathbf{w}_{r^{-1}},\mathbf{t}_{e_s} angle)$	$\mathbf{w}_r \in \mathbb{R}^{d_e}$	$\mathcal{O}(n_e d_e + n_r d_e)$		
TuckER (ours)	$\mathcal{W} \times_1 \mathbf{e}_s \times_2 \mathbf{w}_r \times_3 \mathbf{e}_o$	$\mathbf{w}_r \in \mathbb{R}^{d_r}$	$\mathcal{O}(n_e d_e + n_r d_r)$		

3.1. Link Prediction

In link prediction, we are given a subset of all true triples and the aim is to learn a $scoring\ function\ \phi$ that assigns a score $s=\phi(e_s,r,e_o)\in\mathbb{R}$ to each triple, indicating whether that triple is true or false, with the ultimate goal of being able to correctly score all missing triples. The scoring function is either a specific form of tensor factorization in the case of linear models or a more complex (deep) neural network architecture in the case of non-linear models. Typically, a positive score for a particular triple indicates a true fact predicted by the model, while a negative score indicates a false one. With most recent models, a non-linearity such as the logistic sigmoid function is typically applied to the score to give a corresponding probability prediction $p=\sigma(s)\in[0,1]$ as to whether a certain fact is true.

3.2. Tucker Decomposition

Tucker decomposition, named after Ledyard R. Tucker (Tucker, 1964) and refined in his subsequent work (Tucker, 1966), decomposes a tensor into a set of matrices and a smaller core tensor. In a three-mode case, given the original tensor $\mathcal{X} \in \mathbb{R}^{I \times J \times K}$, Tucker decomposition outputs a tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$ and three matrices $\mathbf{A} \in \mathbb{R}^{I \times P}$, $\mathbf{B} \in \mathbb{R}^{J \times Q}$, $\mathbf{C} \in \mathbb{R}^{K \times R}$ (Kolda & Bader, 2009):

$$\mathcal{X} \approx \mathcal{Z} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C} = \sum_{p=1}^P \sum_{q=1}^Q \sum_{r=1}^R z_{pqr} \mathbf{a}_p \otimes \mathbf{b}_q \otimes \mathbf{c}_r,$$
(1)

with \times_n indicating the tensor product along the n-th mode and \otimes the vector inner product. Factor matrices \mathbf{A} , \mathbf{B} and \mathbf{C} , when orthogonal, can be thought of as the principal components in each mode. Elements of the core tensor \mathcal{Z} show the level of interaction between the different components. Typically, P, Q, R are smaller than I, J, K respectively, so \mathcal{Z} can be thought of as a compressed version of \mathcal{X} . Tucker decomposition is not unique, i.e. we can transform \mathcal{Z} without affecting the fit if we apply the inverse of that

transformation to the factor matrices. Imposing additional constraints on the structure of \mathcal{Z} , such as sparsity, making its elements small or making the core "all-orthogonal", can lead to improved uniqueness (Kolda & Bader, 2009).

4. Tucker Decomposition for Link Prediction

We propose a model that uses Tucker decomposition for link prediction on the third-order binary tensor representation of a knowledge graph, with entity embedding matrix ${\bf E}$ that is equivalent for subject and object entities, i.e. ${\bf E}={\bf A}={\bf C}\in\mathbb{R}^{n_e\times d_e}$ and relation embedding matrix ${\bf R}={\bf B}\in\mathbb{R}^{n_r\times d_r}$, where n_e and n_r represent the number of entities and relations and d_e and d_r the dimensionality of entity and relation embedding vectors respectively.

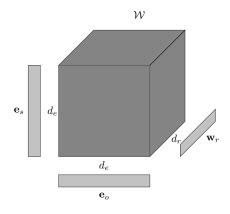


Figure 1. Visualization of the TuckER architecture.

We define the scoring function for TuckER as:

$$\phi(e_s, r, e_o) = \mathcal{W} \times_1 \mathbf{e}_s \times_2 \mathbf{w}_r \times_3 \mathbf{e}_o \tag{2}$$

where $\mathbf{e}_s, \mathbf{e}_o \in \mathbb{R}^{d_e}$ are the rows of \mathbf{E} representing the subject and object entity embedding vectors, $\mathbf{w}_r \in \mathbb{R}^{d_r}$ the rows of \mathbf{R} representing the relation embedding vector, $\mathcal{W} \in \mathbb{R}^{d_e \times d_r \times d_e}$ is the core tensor of Tucker decomposition

and \times_n is the tensor product along the n-th mode. We apply logistic sigmoid to each score $\phi(e_s,r,e_o)$ to obtain the predicted probability $p=\sigma(\phi(e_s,r,e_o))$ of a triple being true. Visualization of the TuckER model architecture can be seen in Figure 1.

As proven in Section 5.1, TuckER is *fully expressive*, i.e. given sufficient entity and relation embedding dimensionality, it is able to assign values to the embeddings that correctly separate any combination of ground truth true triples from the false ones. The number of parameters of TuckER increases *linearly* with respect to entity and relation embedding dimensionality d_e and d_r , as the number of entities and relations (n_e and n_r respectively) increases, since the number of parameters of core tensor \mathcal{W} depends only on the entity and relation embedding dimensionality and not on the number of entities or relations. By having the core tensor \mathcal{W} , unlike simpler models such as DistMult, ComplEx and SimplE, TuckER does not encode all the learned knowledge into the embeddings; some is stored in the core tensor and shared between all entities and relations.

4.1. Training

Given we cannot use analytical methods for computing the tensor factorization, since the tensor being factorized is comprised of ∞ and $-\infty$ (after applying the inverse of logistic sigmoid), we use numerical methods to train TuckER. Following the training procedure introduced by Dettmers et al. (2018) with the goal of speeding up training and increasing accuracy, we use 1-N scoring, i.e. we simultaneously score a pair e_s and r with all entities $e_o \in \mathcal{E}$, in contrast to 1-1 scoring, where individual triples (e_s, r, e_o) are trained one at a time. This way we make use of the local-closed world assumption (Nickel et al., 2016), where we assume that a knowledge graph is only locally complete, i.e. we include only the non-existing triples (e_s, r, \cdot) and (\cdot, r, e_o) of the observed pairs e_s , r and r, e_o respectively as negative samples and all observed triples as positive samples. We train our model to minimize the Bernoulli negative log-likelihood loss function:

$$L(\mathbf{p}, \mathbf{y}) = -\frac{1}{n_e} \sum_{i=1}^{n_e} (\mathbf{y}^{(i)} \log(\mathbf{p}^{(i)}) + (1 - \mathbf{y}^{(i)}) \log(1 - \mathbf{p}^{(i)})),$$
(3)

where $\mathbf{p} \in \mathbb{R}^{n_e}$ is the vector of probabilities predicted by the model and $\mathbf{y} \in \mathbb{R}^{n_e}$ is the label vector of ones for true and zeros for false triples.

5. Theoretical Analysis

5.1. Bound on Embedding Dimensionality for Full Expressiveness

As previously stated in Section 4, a tensor factorization model is said to be fully expressive if for any ground truth over all entities and relations, there exist entity and relation embeddings that accurately separate the true triples from the false ones.

As shown in (Trouillon et al., 2017), ComplEx is fully expressive with the bound on entity and relation embedding dimensionality of $d_e = d_r = n_e \cdot n_r$ for achieving full expressiveness. Similarly to ComplEx, Kazemi & Poole (2018) show that SimplE is fully expressive with entity and relation embeddings of size $d_e = d_r = \min(n_e \cdot n_r, \gamma + 1)$, with γ representing the number of true facts. The authors further prove other models are not fully expressive: DistMult, because it cannot model asymmetric relations; and transitive models such as TransE (Bordes et al., 2013) and its variants FTransE (Feng et al., 2016) and STransE (Nguyen et al., 2016), because of certain contradictions that they impose between different relation types.

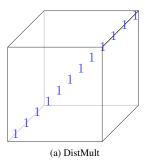
By Theorem 1, we establish the bound on entity and relation embedding dimensionality (i.e. rank of the decomposition) that guarantees full expressiveness of TuckER.

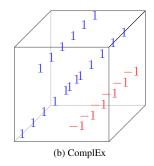
Theorem 1. Given any ground truth over a set of entities \mathcal{E} and relations \mathcal{R} , there exists a TuckER model with subject and object entity embeddings of dimensionality $d_e = n_e$ and relation embeddings of dimensionality $d_r = n_r$, where $n_e = |\mathcal{E}|$ is the number of entities and $n_r = |\mathcal{R}|$ the number of relations, that accurately represents that ground truth.

Proof. Let \mathbf{e}_s and \mathbf{e}_o be the n_e -dimensional one-hot binary vector representations of subject and object entities e_s and e_o respectively and \mathbf{w}_r the n_r -dimensional one-hot binary vector representation of a relation r. For each subject entity $e_s^{(i)}$, relation $r^{(j)}$ and object entity $e_o^{(k)}$, we let the i-th, j-th and k-th element respectively of the corresponding vectors \mathbf{e}_s , \mathbf{w}_r and \mathbf{e}_o be 1 and all other elements 0. Further, we set the ijk element of the tensor $\mathcal{W} \in \mathbb{R}^{n_e \times n_r \times n_e}$ to 1 if the fact (e_s, r, e_o) holds and -1 otherwise. Thus the tensor product of these entity embeddings and the relation embedding with the core tensor, after applying the logistic sigmoid, accurately represents the original tensor.

Theorem 1 shows that it is straightforward to prove that the required dimensionality of TuckER embeddings to ensure full expressiveness is lower than the required dimensionality for SimplE and ComplEx by a factor of n_r for entity embeddings and by a factor of n_e for relation embeddings. Existing knowledge graphs usually contain tens of thousands of entities and hundreds or even thousands of relations. This allows TuckER to be fully expressive with entity and relation embedding dimensionalities several orders of magnitude smaller than those of ComplEx and SimplE.

In practice, we expect the entity and relation embedding dimensionality needed for full reconstruction of the underlying binary tensor to be much smaller than the bound stated





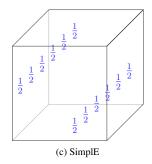


Figure 2. Constraints imposed on the values of core tensor $\mathcal{Z} \in \mathbb{R}^{d_e \times d_e \times d_e}$ for DistMult and $\mathcal{Z} \in \mathbb{R}^{2d_e \times 2d_e \times 2d_e}$ for ComplEx and SimplE. White represents elements that are set to 0.

above, since the assignment of values to the tensor is not random but follows a certain structure, otherwise nothing unknown could be predicted. Even more so, low decomposition rank is actually a desired property, forcing the model to learn that structure and generalize to new data, rather than simply memorizing the input. We expect TuckER to perform better than ComplEx and SimplE with embeddings of lower dimensionality due to parameter sharing in the core tensor (shown empirically in Section 6.4), which could be of importance for efficiency in downstream tasks.

5.2. Relation of TuckER to Previous Tensor Factorization Approaches

Several previous state-of-the-art models can be viewed as a special case of TuckER:

RESCAL (Nickel et al., 2011) Following the notation introduced in Section 3.2, the RESCAL scoring function has the form:

$$\mathcal{X} \approx \mathcal{Z} \times_1 \mathbf{A} \times_3 \mathbf{C}. \tag{4}$$

This corresponds to Equation 1 with $I=K=n_e, P=R=d_e, Q=J=n_r$ and $\mathbf{B}=\mathbf{I}_J$ the $J\times J$ identity matrix, i.e the second dimension of original tensor $\mathcal{X}\in\mathbb{R}^{n_e\times n_r\times n_e}$ is not reduced by $\mathcal{Z}\in\mathbb{R}^{d_e\times n_r\times d_e}$. This is also known as Tucker2 decomposition (Kolda & Bader, 2009). As is the case with TuckER, the entity embedding matrix of RESCAL is shared between subject and object entities, i.e. $\mathbf{E}=\mathbf{A}=\mathbf{C}\in\mathbb{R}^{n_e\times d_e}$ and the relation matrices $\mathbf{W}_r\in\mathbb{R}^{d_e\times d_e}$ are the $d_e\times d_e$ slices of the core tensor \mathcal{Z} .

As mentioned in Section 2, the drawback of RESCAL compared to TuckER is that its number of parameters grows quadratically in the entity embedding dimension d_e as the number of relations increases. Therefore, RESCAL tends to overfit for those relations for which only a small number of training triples is available.

DistMult (Yang et al., 2015) The scoring function of DistMult (see Table 1) can be viewed in two ways:

- as equivalent to that of TuckER (see Equation 1) with a core tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$, $P = Q = R = d_e$, which is *superdiagonal* with 1s on that superdiagonal, i.e. all elements z_{pqr} with p = q = r are 1 and all the other elements are 0 (as shown in Figure 2a); and
- as equivalent to that of RESCAL (see Equation 4) with a core tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$, $P = R = d_e, Q = n_r$, which is *diagonal* for every $d_e \times d_e$ slice, i.e. all elements apart from z_{pqr} with p = r are 0.

If we adopt the TuckER view of the DistMult scoring function, rows of $\mathbf{E} = \mathbf{A} = \mathbf{C} \in \mathbb{R}^{n_e \times d_e}$ contain subject and object entity embedding vectors $\mathbf{e}_s, \mathbf{e}_o \in \mathbb{R}^{d_e}$ and rows of $\mathbf{R} = \mathbf{B} \in \mathbb{R}^{n_r \times d_e}$ contain relation embedding vectors $\mathbf{w}_r \in \mathbb{R}^{d_e}$. By adopting the RESCAL view, entity embedding embedding vectors remain the same, but relation embedding vectors \mathbf{w}_r are now the diagonals of $d_e \times d_e$ slices of \mathcal{Z} .

It is interesting to note that the TuckER interpretation of the DistMult scoring function, given that matrices A and C are identical, can alternatively be interpreted as a special case of CP decomposition (Hitchcock, 1927), since Tucker decomposition with a superdiagonal core tensor becomes equivalent to CP decomposition.

Because of its simplicity, DistMult learns a binary tensor that is symmetric in the subject and object entity mode, so it cannot learn to represent asymmetric relations.

ComplEx (Trouillon et al., 2016) Bilinear models are a family of models where subject and object entity embeddings are represented by vectors $\mathbf{e}_s, \mathbf{e}_o \in \mathbb{R}^{d_e}$, a relation is represented by a matrix $\mathbf{W}_r \in \mathbb{R}^{d_e \times d_e}$ and the scoring function takes the form of a bilinear product between the two embedding vectors and the relation matrix, i.e. $\phi(e_s, r, e_o) = \mathbf{e}_s \mathbf{W}_r \mathbf{e}_o$.

It is trivial to show that both RESCAL and DistMult belong to the family of bilinear models. As explained by Kazemi & Poole (2018), ComplEx can be considered a bilinear model

with the real and imaginary part of an embedding for each entity concatenated in a single vector, $[\operatorname{Re}(\mathbf{e}_s); \operatorname{Im}(\mathbf{e}_s)] \in \mathbb{R}^{2d_e}$ for subject, $[\operatorname{Re}(\mathbf{e}_o); \operatorname{Im}(\mathbf{e}_o)] \in \mathbb{R}^{2d_e}$ for object, and a relation matrix $\mathbf{W}_r \in \mathbb{R}^{2d_e \times 2d_e}$, constrained in a way that its leading diagonal contains duplicated elements of $\operatorname{Re}(\mathbf{w}_r)$, its d_e -diagonal contains elements of $\operatorname{Im}(\mathbf{w}_r)$ and its $-d_e$ -diagonal has elements of $-\operatorname{Im}(\mathbf{w}_r)$, with all other elements set to 0, where d_e and $-d_e$ represent offsets from the leading diagonal. This makes the scoring function of ComplEx (see Table 1) equivalent to that of RESCAL with relation matrix \mathbf{W}_r constrained as described.

Therefore, similarly to DistMult, we can regard the scoring function of ComplEx in two ways:

- as equivalent to the scoring function of TuckER (see Equation 1), with core tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$, $P = Q = R = 2d_e$, where $3d_e$ elements on different tensor diagonals are set to 1, d_e elements on one tensor diagonal are set to -1 and all other elements are set to 0 (see Figure 2b); and
- as equivalent to the scoring function of RESCAL (see Equation 4), with core tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$, $P = R = 2d_e, Q = n_r$ where for each $2d_e \times 2d_e$ slice of \mathcal{Z} , all elements on the leading diagonal are set to $[\operatorname{Re}(\mathbf{w}_r); \operatorname{Re}(\mathbf{w}_r)]$, the d_e -diagonal is set to $\operatorname{Im}(\mathbf{w}_r)$, the $-d_e$ -diagonal is set to $-\operatorname{Im}(\mathbf{w}_r)$ and all other elements are set to 0.

This shows that the scoring function of ComplEx, which computes a bilinear product with complex entity and relation embeddings and disregards the imaginary part of the obtained result, is equivalent to a hard regularization of the core tensor of TuckER in the real domain.

SimplE (Kazemi & Poole, 2018) The authors show that SimplE belongs to the family of bilinear models by concatenating embeddings for head and tail entities for both subject and object into vectors $[\mathbf{h}_{e_s}; \mathbf{t}_{e_s}] \in \mathbb{R}^{2d_e}$ and $[\mathbf{h}_{e_o}; \mathbf{t}_{e_o}] \in \mathbb{R}^{2d_e}$ and constraining the relation matrix $\mathbf{W}_r \in \mathbb{R}^{2d_e \times 2d_e}$ so that it contains the relation embedding vector $\frac{1}{2}\mathbf{w}_r$ on its d_e -diagonal and the inverse relation embedding vector $\frac{1}{2}\mathbf{w}_{r-1}$ on its d_e -diagonal and 0s elsewhere.

The SimplE scoring function is therefore equivalent to:

- that of TuckER (see Equation 1), with core tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$, $P = Q = R = 2d_e$, where $2d_e$ elements on two tensor diagonals are set to $\frac{1}{2}$ and all other elements are set to 0 (see Figure 2c); and
- that of RESCAL (see Equation 4), with core tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$, $P = R = 2d_e, Q = n_r$ where for each $2d_e \times 2d_e$ slice, elements on the d_e -diagonal are set to $\frac{1}{2}\mathbf{w}_r$, elements on the $-d_e$ -diagonal are set to $\frac{1}{2}\mathbf{w}_{r-1}$ and all other elements are 0.

5.3. Representing Asymmetric Relations

Each relation in a knowledge graph can be characterized by a certain set of properties, such as symmetry, reflexivity, transitivity, etc. A relation r is asymmetric if, for all subject entities that are related to their corresponding object entities through r, the reciprocal necessarily does not hold, i.e. none of the object entities are related to the subject entities through r.

So far, there have been two possible ways in which linear link prediction models introduce asymmetry into factorization of the binary tensor of triples. One is to have distinct (although possibly related) embeddings for subject and object entities and a diagonal matrix (or equivalently a vector) for each relation, as is the case with models such as ComplEx and SimplE. This puts a strict constraint on the relation matrix and imposes a hard limit on the type of transformation applied on entity embeddings. The other way of modeling asymmetry is for subject and object entity embeddings to be equivalent, but representing a relation as a full rank matrix, which is the case with RESCAL. The drawback of the latter approach is quadratic growth of parameter number with the number of relations, which often leads to overfitting, especially for relations with a small number of training triples.

TuckER introduces a novel approach to dealing with asymmetry: by representing relations as vectors \mathbf{w}_r , which makes the parameter number grow linearly with the number of relations n_r ; and by having an asymmetric relation-agnostic core tensor \mathcal{W} , which enables knowledge sharing between relations. Multiplying $\mathcal{W} \in \mathbb{R}^{d_e \times d_r \times d_e}$ with $\mathbf{w}_r \in \mathbb{R}^{d_r}$ along the second mode, we obtain a full rank relation-specific matrix $\mathbf{W}_r \in \mathbb{R}^{d_e \times d_e}$, which is capable of performing all possible linear transformations on the entity embeddings, i.e. rotation, reflection or stretch, and thus capable of modeling asymmetry. Regardless of what kind of transformation is needed for modeling a particular relation, TuckER is capable of learning it from the data, rather than through explicitly limiting the relation matrix.

6. Experiments and Results

6.1. Datasets

We evaluate TuckER using four standard link prediction datasets:

FB15k (Bordes et al., 2013) is a subset of Freebase, a large database of real world facts containing information about films, actors, sports, etc.

FB15k-237 (Toutanova et al., 2015) was created from FB15k by removing the inverse of many relations that are present in the training set from validation and test sets, mak-

Table 2. Link prediction results on WN18RR and FB15k-237.

		WN18RR				FB15k-237			
	Linear	MRR	Hits@10	Hits@3	Hits@1	MRR	Hits@10	Hits@3	Hits@1
DistMult (Yang et al., 2015)	yes	.430	.490	.440	.390	.241	.419	.263	.155
ComplEx (Trouillon et al., 2016)	yes	.440	.510	.460	.410	.247	.428	.275	.158
Neural LP (Yang et al., 2017)	no	_	_	_	_	.250	.408	_	_
R-GCN (Schlichtkrull et al., 2018)	no	_	_	_	_	.248	.417	.264	.151
MINERVA (Das et al., 2018)	no	_	_	_	_	_	.456	_	_
ConvE (Dettmers et al., 2018)	no	.430	.520	.440	.400	.325	.501	.356	.237
HypER (Balažević et al., 2018)	no	.465	.522	.477	.436	.341	.520	.376	.252
M-Walk (Shen et al., 2018)	no	.437	_	.445	.414	_	_	_	_
TuckER (ours)	yes	.470	.526	.482	.443	.358	.544	.394	.266

Table 3. Link prediction results on WN18 and FB15k.

		WN18				FB15k			
	Linear	MRR	Hits@10	Hits@3	Hits@1	MRR	Hits@10	Hits@3	Hits@1
TransE (Bordes et al., 2013)	no	_	.892	_	_	_	.471	_	_
DistMult (Yang et al., 2015)	yes	.822	.936	.914	.728	.654	.824	.733	.546
ComplEx (Trouillon et al., 2016)	yes	.941	.947	.936	.936	.692	.840	.759	.599
ANALOGY (Liu et al., 2017)	yes	.942	.947	.944	.939	.725	.854	.785	.646
Neural LP (Yang et al., 2017)	no	.940	.945	_	_	.760	.837	_	_
R-GCN (Schlichtkrull et al., 2018)	no	.819	.964	.929	.697	.696	.842	.760	.601
TorusE (Ebisu & Ichise, 2018)	no	.947	.954	.950	.943	.733	.832	.771	.674
ConvE (Dettmers et al., 2018)	no	.943	.956	.946	.935	.657	.831	.723	.558
HypER (Balažević et al., 2018)	no	.951	958	.955	.947	.790	.885	.829	.734
SimplE (Kazemi & Poole, 2018)	yes	.942	.947	.944	.939	.727	.838	.773	.660
TuckER (ours)	yes	.953	.958	.955	.949	.795	.892	.833	.741

ing it more difficult for simple models to do well.

WN18 (Bordes et al., 2013) is a subset of WordNet, a database containing lexical relations between words. WN18 follows a hierarchical structure.

WN18RR (Dettmers et al., 2018) is a subset of WN18, created by removing the inverse relations from validation and test sets.

Number of entities and relations for each dataset are summarized in Table 4.

Table 4. Dataset statistics.

Dataset	# Entities (n_e)	# Relations (n_r)
FB15k	14,951	1,345
FB15k-237	14,541	237
WN18	40,943	18
WN18RR	40,943	11

6.2. Implementation and Experiments

We implement TuckER in PyTorch (Paszke et al., 2017) and make our code available on Github ¹.

We choose all hyper-parameters by random search based on the validation set performance. For FB15k and FB15k-237, we set both entity and relation embedding dimensions to $d_e = d_r = 200$. For WN18 and WN18RR, which both contain a significantly smaller number of relations relative to the number of entities as well as a small number of relations compared to FB15k and FB15k-237, we set $d_e=200$ and $d_r = 30$. We use both batch normalization (Ioffe & Szegedy, 2015) and dropout (Srivastava et al., 2014) to control overfitting and improve predictions. We choose the learning rate from $\{0.01, 0.005, 0.003, 0.001, 0.0005\}$ and learning rate decay from $\{1, 0.995, 0.99\}$. We find the following combinations of learning rate and learning rate decay to give the best results: (0.003, 0.99) for FB15k, (0.0005, 1.0) for FB15k-237, (0.005, 0.995) for WN18 and (0.01, 1.0) for WN18RR. We train the model using Adam (Kingma & Ba, 2015) and set the batch size to 128.

We evaluate each triple from the test set as in (Bordes et al., 2013): for a given triple, we generate $2n_e$ test triples by keeping the subject entity e_s and relation r fixed and replacing the object entity e_o with all possible entities $\mathcal E$ and by keeping the object entity e_o and relation r fixed and replacing the subject entity e_s with all entities $\mathcal E$. We then rank the scores obtained. We use the filtered setting only, i.e. we remove all other true triples apart from the currently observed

https://github.com/ibalazevic/TuckER

test triple. For evaluation, we use two evaluation metrics used across the link prediction literature: mean reciprocal rank (MRR) and hits @k, $k \in \{1,3,10\}$. Mean reciprocal rank is the average of the inverse of a mean rank assigned to the true triple over all n_e generated triples. Hits @k measures the percentage of times the true triple is ranked in the top k of the n_e generated triples. The aim is for a model to achieve high MRR and hits @k.

6.3. Link Prediction Results

Link prediction results on all four datasets are shown in Tables 2 and 3. Overall, TuckER outperforms previous state-of-the-art models on all metrics across all datasets (apart from hits@10 on WN18 where a non-linear model, R-GCN, does better), which shows that this relatively simple yet fully flexible linear model leads to very good performance. Results achieved by TuckER are not only better than those of other linear models, such as DistMult, ComplEx and SimplE, but also better than the results of many more complex deep neural network and reinforcement learning architectures, e.g. R-GCN, MINERVA, ConvE and HypER, demonstrating the expressive power of linear models.

Even though TuckER has more parameters than some more simpler linear models (DistMult, ComplEx and SimplE) due to the presence of core tensor \mathcal{W} (containing $200 \times 200 \times 200 = 8$ million parameters for FB15k and FB15k-237 and $200 \times 30 \times 200 = 1.2$ million parameters for WN18 and WN18RR), it consistently obtains better results than any of those models. We believe this is achieved by exploiting knowledge sharing between relations through the core tensor and implicit regularization from dropout, which allows the model to learn which parameters to ignore rather than explicitly setting them to 0.

We find the value of the dropout parameter to have a significant influence on results, with lower dropout values (0.1,0.2) required for datasets with a higher number of training triples per relation and thus less risk of overfitting (WN18 and WN18RR) and higher dropout values (0.3,0.4,0.5) required for datasets with a large number of relations (FB15k and FB15k-237). We further note that TuckER improves the results of all previous linear models by a larger margin on datasets with a large number of relations (e.g. +14% improvement on FB15k results over ComplEx, +8% improvement over SimplE on the toughest hits@1 metric), which supports our belief that TuckER makes use of the parameters shared between similar relations to improve predictions by *multi-task learning*.

6.4. Influence of Embedding Dimensionality

In Section 5.1, we derive the bound on entity and relation embedding dimensionality for full expressiveness that is much lower for TuckER than for simpler linear models ComplEx and SimplE. This suggests TuckER should need a lower embedding dimensionality (i.e. lower rank of the decomposition) for obtaining good results than ComplEx or SimplE. To test this, we train ComplEx, SimplE and TuckER on FB15k-237 with embedding sizes $d_e = d_r \in \{20, 50, 100, 200\}$. Figure 3 shows the obtained MRR on the test set for each of the models.

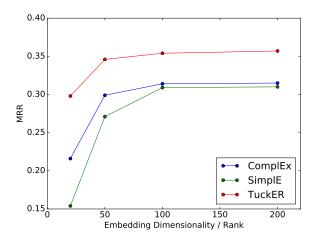


Figure 3. MRR for ComplEx, SimplE and TuckER for different embeddings sizes $d_e = d_r \in \{20, 50, 100, 200\}$ on FB15k-237.

We can see from Figure 3 that the difference between the MRRs of ComplEx, SimplE and TuckER is approximately constant for embedding sizes 100 and 200. However, for lower embedding sizes, the difference between MRRs increases by 0.7% for embedding size 50 and by 4.2% for embedding size 20 for ComplEx and by 3% for embedding size 50 and by 9.9% for embedding size 20 for SimplE. At embedding size 20, the performance of TuckER is almost as good as the performance of ComplEx and SimplE at embedding size 200, which supports our initial assumption.

7. Conclusion

In this work, we introduce TuckER, a relatively simple yet highly flexible linear model for link prediction in knowledge graphs based on the Tucker decomposition of a third-order binary tensor of training set triples, which achieves state-of-the-art results on standard link prediction datasets. As well as being fully expressive, TuckER's number of parameters grows linearly with respect to embedding dimension as the number of entities or relations in a knowledge graph increases. We further show that previous linear state-of-the-art models, RESCAL, DistMult, ComplEx and SimplE, are all special cases of our model.

Future work might include exploring various means of softly regularizing the model other than dropout and finding a way to incorporate background knowledge on individual relation properties into the existing model.

References

- Balažević, I., Allen, C., and Hospedales, T. M. Hypernetwork Knowledge Graph Embeddings. *arXiv* preprint *arXiv*:1808.07018, 2018.
- Bordes, A., Usunier, N., Garcia-Duran, A., Weston, J., and Yakhnenko, O. Translating Embeddings for Modeling Multi-relational Data. In Advances in Neural Information Processing Systems, 2013.
- Das, R., Dhuliawala, S., Zaheer, M., Vilnis, L., Durugkar, I., Krishnamurthy, A., Smola, A., and McCallum, A. Go for a Walk and Arrive at the Answer: Reasoning over Paths in Knowledge Bases Using Reinforcement Learning. In *International Conference on Learning Representations*, 2018.
- Dettmers, T., Minervini, P., Stenetorp, P., and Riedel, S. Convolutional 2D Knowledge Graph Embeddings. In *Association for the Advancement of Artificial Intelligence*, 2018.
- Ebisu, T. and Ichise, R. TorusE: Knowledge Graph Embedding on a Lie Group. In *Association for the Advancement of Artificial Intelligence*, 2018.
- Feng, J., Huang, M., Wang, M., Zhou, M., Hao, Y., and Zhu, X. Knowledge Graph Embedding by Flexible Translation. In *KR*, pp. 557–560, 2016.
- Hitchcock, F. L. The Expression of a Tensor or a Polyadic as a Sum of Products. *Journal of Mathematics and Physics*, 6(1-4):164–189, 1927.
- Ioffe, S. and Szegedy, C. Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. In *International Conference on Machine Learning*, 2015.
- Kapteyn, A., Neudecker, H., and Wansbeek, T. An Approach To n-Mode Components Analysis. *Psychometrika*, 51(2):269–275, 1986.
- Kazemi, S. M. and Poole, D. SimplE Embedding for Link Prediction in Knowledge Graphs. In Advances in Neural Information Processing Systems, 2018.
- Kingma, D. P. and Ba, J. Adam: A Method for Stochastic Optimization. In *International Conference on Learning Representations*, 2015.
- Kolda, T. G. and Bader, B. W. Tensor Decompositions and Applications. *SIAM review*, 51(3):455–500, 2009.
- Kroonenberg, P. M. and De Leeuw, J. Principal Component Analysis of Three-Mode Data by Means of Alternating Least Squares Algorithms. *Psychometrika*, 45(1):69–97, 1980.

- Liu, H., Wu, Y., and Yang, Y. Analogical Inference for Multirelational Embeddings. In *International Conference on Machine Learning*, 2017.
- Nguyen, D. Q., Sirts, K., Qu, L., and Johnson, M. STransE: a Novel Embedding Model of Entities and Relationships in Knowledge Bases. In *Proceedings of NAACL-HLT*, 2016.
- Nickel, M., Tresp, V., and Kriegel, H.-P. A Three-Way Model for Collective Learning on Multi-Relational Data. In *International Conference on Machine Learning*, 2011.
- Nickel, M., Murphy, K., Tresp, V., and Gabrilovich, E. A Review of Relational Machine Learning for Knowledge Graphs. *Proceedings of the IEEE*, 104(1):11–33, 2016.
- Paszke, A., Gross, S., Chintala, S., Chanan, G., Yang, E., DeVito, Z., Lin, Z., Desmaison, A., Antiga, L., and Lerer, A. Automatic Differentiation in PyTorch. In NIPS-W, 2017.
- Schlichtkrull, M., Kipf, T. N., Bloem, P., van den Berg, R., Titov, I., and Welling, M. Modeling Relational Data with Graph Convolutional Networks. In *European Semantic Web Conference*, 2018.
- Shen, Y., Chen, J., Huang, P.-S., Guo, Y., and Gao, J. M-Walk: Learning to Walk over Graphs using Monte Carlo Tree Search. In Advances in Neural Information Processing Systems, 2018.
- Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. *Journal of Machine Learning Research*, 15(1):1929–1958, 2014.
- Toutanova, K., Chen, D., Pantel, P., Poon, H., Choudhury, P., and Gamon, M. Representing Text for Joint Embedding of Text and Knowledge Bases. In *Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing*, 2015.
- Trouillon, T., Welbl, J., Riedel, S., Gaussier, É., and Bouchard, G. Complex Embeddings for Simple Link Prediction. In *International Conference on Machine Learning*, 2016.
- Trouillon, T., Dance, C. R., Gaussier, É., Welbl, J., Riedel, S., and Bouchard, G. Knowledge Graph Completion via Complex Tensor Factorization. *The Journal of Machine Learning Research*, 18(1):4735–4772, 2017.
- Tucker, L. R. The Extension of Factor Analysis to Three-Dimensional Matrices. *Contributions to Mathematical Psychology*, 110119, 1964.
- Tucker, L. R. Some Mathematical Notes on Three-Mode Factor Analysis. *Psychometrika*, 31(3):279–311, 1966.

- Yang, B., Yih, W.-t., He, X., Gao, J., and Deng, L. Embedding Entities and Relations for Learning and Inference in Knowledge Bases. In *International Conference on Learning Representations*, 2015.
- Yang, F., Yang, Z., and Cohen, W. W. Differentiable Learning of Logical Rules for Knowledge Base Reasoning. In *Advances in Neural Information Processing Systems*, 2017.