# Binarized Knowledge Graph Embeddings

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**Abstract.** Tensor factorization has become an increasingly popular approach to knowledge graph completion (KGC), which is the task of automatically predicting missing facts in a knowledge graph. However, even with a simple model like CANDECOMP/PARAFAC (CP) tensor decomposition, KGC on existing knowledge graphs is impractical in resourcelimited environments, as a large amount of memory is required to store parameters represented as 32-bit or 64-bit floating point numbers. This limitation is expected to become more stringent as existing knowledge graphs, which are already huge, keep steadily growing in scale. To reduce the memory requirement, we present a method for binarizing the parameters of the CP tensor decomposition by introducing a quantization function to the optimization problem. This method replaces floating point-valued parameters with binary ones after training, which drastically reduces the model size at run time. We investigate the trade-off between the quality and size of tensor factorization models for several KGC benchmark datasets. In our experiments, the proposed method successfully reduced the model size by more than an order of magnitude while maintaining the task performance. Moreover, a fast score computation technique can be developed with bitwise operations.

**Keywords:** Knowledge graph completion  $\cdot$  Tensor factorization  $\cdot$  Model compression.

# 1 Introduction

Knowledge graphs, such as YAGO [25] and Freebase [2], have proven useful in many applications such as question answering [3], dialog [17] and recommender [22] systems. A knowledge graph consists of triples  $(e_i, e_j, r_k)$ , each of which represents a fact that relation  $r_k$  holds between subject entity  $e_i$  and object entity  $e_j$ . Although a typical knowledge graph may have billions of triples, it is still far from complete. Filling in the missing triples is of importance in carrying out various inference over knowledge graphs. Knowledge graph completion (KGC) aims to perform this task automatically.

In recent years, knowledge graph embedding (KGE) has been actively pursued as a promising approach to KGC. In KGE, entities and relations are embedded

in vector space, and operations in this space are used for defining a confidence score (or simply score) function  $\theta_{ijk}$  that approximates the truth value of a given triple  $(e_i, e_j, r_k)$ . Although a variety of KGE methods [4, 21, 24, 26, 6] have been proposed, Kazemi and Poole [11] and Lacroix et al. [14] found that a classical tensor factorization algorithm, known as the CANDECOMP/PARAFAC (CP) decomposition [10], achieves the state-of-art performances on several benchmark datasets for KGC.

In CP decomposition of a knowledge graph, the confidence score  $\theta_{ijk}$  for a triple  $(e_i, e_j, r_k)$  is calculated simply by  $\mathbf{a}_{i:}(\mathbf{b}_{j:} \circ \mathbf{c}_{k:})^{\mathrm{T}}$  where  $\mathbf{a}_{i:}, \mathbf{b}_{j:}$ , and  $\mathbf{c}_{k:}$  denote the D-dimensional row vectors representing  $e_i$ ,  $e_j$ , and  $r_k$ , respectively, and  $\circ$  is the Hadamard (element-wise) product. In spite of the model's simplicity, it needs to maintain  $(2N_e + N_r)$  D-dimensional 32-bit or 64-bit valued vectors, where  $N_e$ , and  $N_r$  denote the number of entities and relations, respectively. Because typical knowledge graphs contain enormous number of entities and relations, this leads to a significant memory requirement. As mentioned in [6], CP with D = 200 applied to Freebase will require about 66 GB of memory to store parameters. This large memory consumption poses issues especially when KGC is conducted on resource-limited devices. Moreover, the size of existing knowledge graphs is still growing rapidly, and a method for shrinking the embedding vectors is in strong demand.

To address the problem, this paper presents a new CP decomposition algorithm to learn compact knowledge graph embeddings. The basic idea is to introduce a quantization function built into the optimization problem. This function forces the embedding vectors to be binary, and optimization is done with respect to the binarized vectors. After training, the binarized embeddings can be used in place of the original vectors of floating-point numbers, which drastically reduces the memory footprint of the resulting model.

In addition, the binary vector representation contributes to efficiently computing the dot product by using bitwise operations. This fast computation allows the proposed model to substantially reduce the amount of time required to compute the confidence scores of triples.

Note that our method only improves the run-time (i.e., predicting missing triples) memory footprint and speed but not those for training a prediction model. However, the reduced memory footprint of the produced model enables KGC to be run on many affordable resource-limited devices (e.g., personal computers). Unlike research-level benchmarks in which one is required to compute the scores of a small set of test triples, completion of an entire knowledge graph requires computing the scores of all missing triples in a knowledge graph, whose number is enormous because knowledge graphs are sparse. Thus, improved memory footprints and reduced score computation time are of practical importance, and these are what our proposed model provides.

The quantization technique has been commonly used in the community of deep neural networks to shrink network components [5, 8]. To the best of our knowledge, this technique has not been studied in the field of tensor factorization. The main contribution of this paper is that we introduce the quantization

function to a tensor factorization model for the first time. This is also the first study to investigate the benefits of the quantization for KGC. Our experimental results on several KGC benchmark datasets showed that the proposed method reduced the model size nearly 10- to 20-fold compared to the standard CP decomposition without a decrease in the task performance. Besides, with bitwise operations, B-CP got a bonus of speed-up in score computation time.

# 2 Related Work

Approaches to knowledge graph embedding (KGE) can be classified into three types: models based on bilinear mapping, translation, and neural network-based transformation.

RESCAL [21] is a bilinear-based KGE method whose score function is formulated as  $\theta_{ijk} = \mathbf{a}_{e_i}^{\mathrm{T}} \mathbf{B}_{r_k} \mathbf{a}_{e_j}$ , where  $\mathbf{a}_{e_i}, \mathbf{a}_{e_j} \in \mathbb{R}^D$  are the vector representations of entities  $e_i$  and  $e_j$ , respectively, and matrix  $\mathbf{B}_{r_k} \in \mathbb{R}^{D \times D}$  represents a relation  $r_k$ . Although RESCAL is able to output non-symmetric score functions, each relation matrix  $B_{r_k}$  holds  $D^2$  parameters. This can be problematic both in terms of overfitting and computational cost. To avoid this problem, several methods have been proposed recently. DistMult [27] restricts the relation matrix to be diagonal,  $B_{r_k} = \text{diag}(b_{r_k})$ . However, this form of function is necessarily symmetric in i and j; i.e.,  $\theta_{ijk} = \theta_{jik}$ . To reconcile efficiency and expressiveness, Trouillon et al. (2016) [26] proposed ComplEx, using the complex-valued representations and Hermitian inner product to define the score function, which unlike DistMult, can be nonsymmetric in i and j. Hayashi and Shimbo (2017) [9] found that ComplEx is equivalent to another state-of-the-art KGE method, holographic embeddings (HolE) [19]. ANALOGY [16] is a model that can be view as a hybrid of ComplEx and DistMult. Manabe et al. (2018) [18] reduced redundant parameters of ComplEx with L1 regularizers. Lacroix et al. (2018) [14] and Kazemi and Pool (2018) [11] independently showed that CP decomposition (called SimplE in [11]) achieves a comparable KGC performance to other bilinear methods such as ComplEx and ANALOGY. To achieve this performance, they introduced an "inverse" triple  $(e_j, e_i, r_k^{-1})$  to the training data for each existing triple  $(e_i, e_j, r_k)$ , where  $r_k^{-1}$  denotes the inverse relation of  $r_k$ .

TransE [4] is the first KGE model based on vector translation. It employs the principle  $\mathbf{a}_{e_i} + \mathbf{b}_{r_k} \approx \mathbf{a}_{e_j}$  to define a distance-based score function  $\theta_{ijk} = -\|\mathbf{a}_{e_i} + \mathbf{b}_{r_k} - \mathbf{a}_{e_j}\|^2$ . Since TransE was recognized as too limited to model complex properties (e.g., symmetric/reflexive/one-to-many/many-to-one relations) in knowledge graphs, many extended versions of TransE have been proposed.

Neural-based models, such as NTN [24] and ConvE [6], employ non-linear functions to define score function, and thus they have a better expressiveness. Compared to bilinear and translation approaches, however, neural-based models require more complex operations to compute interactions between a relation and two entities in vector space.

It should be noted that the binarization technique proposed in this paper can be applied to other KGE models besides CP decomposition, such as those mentioned above. Our choice of CP as the implementation platform only reflects the fact that it is one of the strongest baseline KGE methods.

Numerous recent publications have studied methods for training quantized neural networks to compact the models without performance degradation. The Binary Connect algorithm [5] is the first study to show that binarized neural networks can achieve almost the state-of-the-art results on datasets such as MNIST and CIFAR-10 [8]. BinaryConnect uses the binarization function  $Q_1(x)$  to replace floating point weights of deep neural networks with binary weights during the forward and backward propagation. Lam (2018) [15] used the same quantization method as BinaryConnect to learn compact word embeddings. To binarize knowledge graph embeddings, this paper also applied the quantization method to the CP decomposition algorithm. To the best of our knowledge, this paper is the first study to examine the benefits of the quantization for KGC.

#### 3 Notation and Preliminaries

We follow the notation and terminology established in [12] for the most part. These are summarized below mainly for third-order tensors, by which a knowledge graph is represented (see Section 4.1).

Vectors are represented by boldface lowercase letters, e.g., a. Matrices are represented by boldface capital letters, e.g., A. Third-order tensors are represented by boldface calligraphic letters, e.g.,  $\mathcal{X}$ .

The *i*th row of a matrix A is represented by  $a_{i:}$ , and the *j*th column of Ais represented by  $a_{ij}$ , or simply as  $a_j$ . The symbol  $\circ$  represents the Hadamard product for matrices and also for vectors, and  $\otimes$  represents the outer product.

A third-order tensor  $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times I_3}$  is rank one if it can be written as the outer product of three vectors, i.e.,  $\mathcal{X} = a \otimes b \otimes c$ . This means that each element  $x_{i_1i_2i_3}$  of  $\mathcal{X}$  is the product of the corresponding vector elements:

$$x_{i_1 i_2 i_3} = a_{i_1} b_{i_2} c_{i_3}$$
 for  $i_1 \in [I_1], i_2 \in [I_2], i_3 \in [I_3],$ 

where  $[I_n]$  denotes the set of natural numbers  $1, 2, \dots, I_n$ . The norm of a tensor  $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times \dots \times I_k}$  is the square root of the sum of the squares of all its elements, i.e.,

$$\|\mathcal{X}\| = \sqrt{\sum_{i_1 \in [I_1]} \sum_{i_2 \in [I_2]} \cdots \sum_{i_k \in [I_k]} x_{i_1 i_2 \cdots i_k}^2}.$$

For a matrix (or a second-order tensor), this norm is called the Frobenius norm and is represented by  $\|\cdot\|_F$ .

#### Tensor Factorization for Knowledge Graphs 4

# Knowledge Graph Representation

A knowledge graph  $\mathcal{G}$  is a labeled multigraph  $(\mathcal{E}, \mathcal{R}, \mathcal{F})$ , where  $\mathcal{E} = \{e_1, \dots, e_{N_e}\}$ is the set of entities (vertices),  $\mathcal{R} = \{r_1, \dots, r_{N_r}\}$  is the set of all relation types

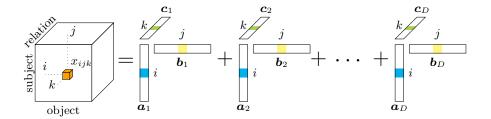


Fig. 1. Illustration of a D-component CP model for a third-order tensor  $\mathcal{X}$ .

(edge labels), and  $\mathcal{F} \subset \mathcal{E} \times \mathcal{E} \times \mathcal{R}$  denotes the observed instances of relations over entities (edges). The presence of an edge, or a triple,  $(e_i, e_j, r_k) \in \mathcal{F}$  represents the fact that relation  $r_k$  holds between subject entity  $e_i$  and object entity  $e_j$ .

A knowledge graph can be represented as a boolean third order tensor  $\mathcal{X} \in \{0,1\}^{N_e \times N_e \times N_r}$  whose elements are set such as

$$x_{ijk} = \begin{cases} 1 & \text{if } (e_i, e_j, r_k) \in \mathcal{F} \\ 0 & \text{otherwise} \end{cases}.$$

KGC is concerned with incomplete knowledge graphs, i.e.,  $\mathcal{F} \subsetneq \mathcal{F}^*$ , where  $\mathcal{F}^* \subset \mathcal{E} \times \mathcal{E} \times \mathcal{R}$  is the unobservable set of ground truth facts (and a superset of  $\mathcal{F}$ ). KGE has been recognized as a promising approach to predicting the truth value of unknown triples in  $\mathcal{F}^* \setminus \mathcal{F}$ . KGE can be generally formulated as the tensor factorization problem and defines a score function  $\theta_{ijk}$  using the latent vectors of entities and relations.

# 4.2 CP Decomposition

CP decomposition [10] factorizes a given tensor as a linear combination of D rankone tensors. For a third-order tensor  $\mathcal{X} \in \mathbb{R}^{N_e \times N_e \times N_r}$ , its CP decomposition is

$$m{\mathcal{X}}pprox \sum_{d\in [D]}m{a}_d\otimes m{b}_d\otimes m{c}_d\;,$$

where  $\boldsymbol{a}_d \in \mathbb{R}^{N_e}$ ,  $\boldsymbol{b}_d \in \mathbb{R}^{N_e}$  and  $\boldsymbol{c}_d \in \mathbb{R}^{N_r}$ . Figure 1 illustrates CP for third-order tensors, which demonstrates how we can formulate knowledge graphs. The elements  $x_{ijk}$  of  $\boldsymbol{\mathcal{X}}$  can be written as

$$x_{ijk} \approx \boldsymbol{a}_{i:}(\boldsymbol{b}_{j:} \circ \boldsymbol{c}_{k:})^{\mathrm{T}} = \sum_{d \in [D]} a_{id}b_{jd}c_{kd} \quad \text{for } i, j \in [N_e], \ k \in [N_r].$$

A factor matrix refers to a matrix composed of vectors from the rank one components. We use  $\mathbf{A} = [\mathbf{a}_1 \ \mathbf{a}_2 \cdots \mathbf{a}_D]$  to denote the factor matrix, and likewise  $\mathbf{B}$ ,  $\mathbf{C}$ . Note that  $\mathbf{a}_{i:}$ ,  $\mathbf{b}_{j:}$  and  $\mathbf{c}_{k:}$  represent the D-dimensional embedding vectors of subject  $e_i$ , object  $e_j$ , and relation  $r_k$ , respectively.

### 4.3 Logistic Regression

Following literature [20], we formulate a logistic regression model for solving the CP decomposition problem. This model considers CP decomposition from a probabilistic viewpoint. We regard  $x_{ijk}$  as a random variable and compute the maximum a posteriori (MAP) estimates of A, B, and C for the joint distribution

$$p(\mathcal{X}|A, B, C) = \prod_{i \in [N_e]} \prod_{j \in [N_e]} \prod_{k \in [N_r]} p(x_{ijk}|\theta_{ijk}).$$

We define the score function  $\theta_{ijk} = a_{i:}(b_{j:} \circ c_{k:})^{\mathrm{T}}$  that represents the CP decomposition model's confidence that a triple  $(e_i, e_j, r_k)$  is a fact; i.e., that it must be present in the knowledge graph. By assuming that  $x_{ijk}$  follows the Bernoulli distribution,  $x_{ijk} \sim \text{Bernoulli}(\sigma(\theta_{ijk}))$ , the posterior probability is defined as the following equation

$$p(x_{ijk}|\theta_{ijk}) = \begin{cases} \sigma(\theta_{ijk}) & \text{if } x_{ijk} = 1\\ 1 - \sigma(\theta_{ijk}) & \text{if } x_{ijk} = 0 \end{cases},$$

where  $\sigma(x) = 1/(1 + \exp(-x))$  is the sigmoid function.

Furthermore, we minimize the negative log-likelihood of the MAP estimates, such that the general form of the objective function to optimize is

$$E = \sum_{i \in [N_e]} \sum_{j \in [N_e]} \sum_{k \in [N_r]} E_{ijk},$$

where

$$E_{ijk} = \underbrace{-x_{ijk} \log \sigma(\theta_{ijk}) + (x_{ijk} - 1) \log(1 - \sigma(\theta_{ijk}))}_{\ell_{ijk}} + \underbrace{\lambda_A \|\boldsymbol{a}_{i:}\|^2 + \lambda_B \|\boldsymbol{b}_{j:}\|^2 + \lambda_C \|\boldsymbol{c}_{k:}\|^2}_{\text{L2 regularizer}}.$$

 $\ell_{ijk}$  represents the logistic loss function for a triple  $(e_i, e_j, r_k)$ . While most knowledge graphs contain only positive examples, negative examples (false facts) are needed to optimize the objective function. However, if all unknown triples are treated as negative samples, calculating the loss function requires a prohibitive amount of time. To approximately minimize the objective function, following previous studies, we used negative sampling in our experiments.

The objective function is minimized with an online learning method based on stochastic gradient descent (SGD). For each training example, SGD iteratively updates parameters by  $\mathbf{a}_{i:} \leftarrow \mathbf{a}_{i:} - \eta \frac{\partial E_{ijk}}{\partial \mathbf{a}_{i:}}$ ,  $\mathbf{b}_{j:} \leftarrow \mathbf{b}_{j:} - \eta \frac{\partial E_{ijk}}{\partial \mathbf{b}_{j:}}$ , and  $\mathbf{c}_{k:} \leftarrow \mathbf{c}_{k:} - \eta \frac{\partial E_{ijk}}{\partial \mathbf{c}_{k:}}$  with a learning rate  $\eta$ . The partial gradient of the objective function with respect to  $\mathbf{a}_{i:}$  is

$$\frac{\partial E_{ijk}}{\partial \boldsymbol{a}_{i:}} = -x_{ijk} \exp\left(-\theta_{ijk}\right) \sigma(\theta_{ijk}) \boldsymbol{b}_{j:} \circ \boldsymbol{c}_{k:} + (1 - x_{ijk}) \sigma(\theta_{ijk}) \boldsymbol{b}_{j:} \circ \boldsymbol{c}_{k:} + 2\lambda_A \boldsymbol{a}_{i:}.$$

Those with respect to  $b_{j}$ : and  $c_{k}$ : can be calculated in the same manner.

#### 5 Binarized CP Decomposition

We propose a binarized CP decomposition algorithm to make CP factor matrices A, B and C binary, i.e., the elements of these matrices are constrained to only two possible values.

In this algorithm, we formulate the score function  $\theta_{ijk}^{(b)} = \sum_{d \in [D]} a_{id}^{(b)} b_{jd}^{(b)} c_{kd}^{(b)}$ , where  $a_{id}^{(b)}=Q_{\Delta}(a_{id}),\ b_{jd}^{(b)}=Q_{\Delta}(b_{jd}),\ c_{kd}^{(b)}=Q_{\Delta}(c_{kd})$  are obtained by binarizing  $a_{id},\ b_{jd},\ c_{kd}$  through the following quantization function

$$x^{(b)} = Q_{\Delta}(x) = \begin{cases} \Delta & \text{if } x \ge 0 \\ -\Delta & \text{if } x < 0 \end{cases}$$

where  $\Delta$  is a positive constant value. We extend the binarization function to vectors in a natural way:  $\mathbf{x}^{(b)} = Q_{\Delta}(\mathbf{x})$  whose ith element  $x_i^{(b)}$  is  $Q_{\Delta}(x_i)$ .

Using the new score function, we reformulate the loss function defined in Section 4.3 as follows

$$\ell_{ijk}^{(b)} = -x_{ijk} \log \sigma(\theta_{ijk}^{(b)}) + (x_{ijk} - 1) \log(1 - \sigma(\theta_{ijk}^{(b)})).$$

To train the binarized CP decomposition model, we optimize the same objective function E as in Section 4.3 except using the binarized loss function given above. We also employ the SGD algorithm to minimize the objective function. One issue here is that the parameters cannot be updated properly since the gradients of  $Q_{\Delta}$  are zero almost everywhere. To solve the issue, we simply use an identity matrix as the surrogate for the derivative of  $Q_{\Delta}$ :

$$\frac{\partial Q_{\Delta}(\boldsymbol{x})}{\partial \boldsymbol{x}} pprox \boldsymbol{I}.$$

The simple trick enables us to calculate the partial gradient of the objective function with respect to  $a_i$ ; through the chain rule:

$$\frac{\partial \ell_{ijk}^{(b)}}{\partial \boldsymbol{a}_{i:}} = \frac{\partial Q_{\Delta}(\boldsymbol{a}_{i:})}{\partial \boldsymbol{a}_{i:}} \frac{\partial \ell_{ijk}^{(b)}}{\partial Q_{\Delta}(\boldsymbol{a}_{i:})} \approx \boldsymbol{I} \frac{\partial \ell_{ijk}^{(b)}}{\partial Q_{\Delta}(\boldsymbol{a}_{i:})} = \frac{\partial \ell_{ijk}^{(b)}}{\partial \boldsymbol{a}_{i:}^{(b)}}$$

This strategy is known as Hinton's straight-through estimator [1] and has been developed in the community of deep neural networks to quantize network components [5,8]. Using this trick, we finally obtain the partial gradient as follows:

$$\frac{\partial E_{ijk}}{\partial \boldsymbol{a}_{i:}} = -x_{ijk} \exp\left(-\theta_{ijk}^{(b)}\right) \sigma(\theta_{ijk}^{(b)}) \boldsymbol{b}_{j:}^{(b)} \circ \boldsymbol{c}_{k:}^{(b)} + (1 - x_{ijk}) \, \sigma(\theta_{ijk}^{(b)}) \boldsymbol{b}_{j:}^{(b)} \circ \boldsymbol{c}_{k:}^{(b)} + 2\lambda_A \boldsymbol{a}_{i:}.$$

The partial gradients with respect to  $b_{j:}$  and  $c_{k:}$  can be computed similarly.

Binary vector representations bring benefits in faster computation of scores  $\theta_{ijk}^{(b)}$ , because the inner product between binary vectors can be implemented by bitwise operations: To compute  $\theta_{ijk}^{(b)}$ , we can use XNOR and Bitcount operations:

$$\theta_{ijk}^{(b)} = \boldsymbol{a}_{i:}^{(b)} (\boldsymbol{b}_{i:}^{(b)} \circ \boldsymbol{c}_{k:}^{(b)})^{\mathrm{T}} = \Delta^{3} \{2BitC - D\}$$

Table 1. Benchmark datasets for KGC.

	WN18	${ m FB15k}$	WN18RR	FB15k-237
$N_e$	40,943	14,951	40,559	14,505
$N_r$	18	1,345	11	237
# training triples	141,442	483,142	86,835	272,115
# validation triples	5,000	50,000	3,034	17,535
# test triples	5,000	59,071	3,134	20,466

**Table 2.** KGC results on WN18 and FB15k: Filtered MRR and Hits@ $\{1,3,10\}$  (%). Letters in boldface signify the best performers in individual evaluation metrics. \*, \*\* and \*\*\* indicate the results transcribed from [26], [6] and [11], respectively.

	WN18			FB15k				
	MRR	Hits@		MRR	MRR. Hits@			
Models		1	3	10		1	3	10
TransE* DistMult* HolE* ComplEx* ANALOGY** CP*** ConvE**	45.4 82.2 93.8 94.1 94.2 94.2 94.3	8.9 72.8 93.0 93.6 93.9 93.9 93.5	82.3 91.4 94.5 94.5 94.4 94.4	93.4 93.6 94.9 94.7 94.7 94.7 <b>95.6</b>	38.0 65.4 52.4 69.2 72.5 72.7 65.7	23.1 54.6 40.2 59.9 64.6 66.0 55.8	47.2 73.3 61.3 75.9 <b>78.5</b> 77.3 72.3	64.1 82.4 73.9 84.0 <b>85.4</b> 83.9 83.1
$\begin{array}{c} {\rm CP} \ (D=200) \\ {\bf B\text{-}CP} \ (D=200) \\ {\bf B\text{-}CP} \ (D=400) \\ {\bf B\text{-}CP} \ (D=300\times3) \end{array}$	94.2 90.1 94.5 <b>94.6</b>	93.9 88.1 94.1 <b>94.2</b>	94.5 91.8 94.8 <b>95.0</b>	94.7 93.3 95.0 95.3	71.9 69.5 72.2 <b>72.9</b>	66.2 61.1 66.3 <b>66.5</b>	75.2 76.0 77.5 77.7	82.0 83.5 84.2 84.9

where  $BitC = \text{Bitcount}(\text{XNOR}(\overline{\mathbf{X}}\text{NOR}(\overline{\boldsymbol{a}}_{i:}^{(b)}, \overline{\boldsymbol{b}}_{j:}^{(b)}), \overline{\boldsymbol{c}}_{k:}^{(b)}))$ .  $\overline{\boldsymbol{x}}^{(b)}$  denotes the boolean vector whose ith element  $\overline{\boldsymbol{x}}_{i}^{(b)}$  is set to 1 if  $\boldsymbol{x}_{i}^{(b)} = \Delta$ , otherwise to 0. Bitcount returns the number of one-bits in a binary vector and XNOR represents the logical complement of the exclusive OR operation.

# 6 Experiments

### 6.1 Datasets and Evaluation Protocol

We evaluated the performance of our proposal in the standard knowledge graph completion (KGC) task. We used four standard datasets, WN18, FB15k [4], WN18RR, and FB15k-237 [6]. Table 1 shows the data statistics<sup>4</sup>.

We followed the standard evaluation procedure to evaluate the KGC performance: Given a test triple  $(e_i, e_j, r_k)$ , we corrupted it by replacing  $e_i$  or  $e_j$  with every entity  $e_\ell$  in  $\mathcal{E}$  and calculated  $\theta_{i,\ell,k}$  or  $\theta_{\ell,j,k}$ . We then ranked all these triples by their scores in decreasing order. To measure the quality of the ranking, we used the mean reciprocal rank (MRR) and Hits at N (Hits@N). We here report only results in the filtered setting [4], which provides a more reliable performance metric in the presence of multiple correct triples.

Following [11, 14], for each triple  $(e_i, e_j, r_k)$  observed in the training set, we added its inverse triple  $(e_j, e_i, r_k^{-1})$  also in the training set.

**Table 3.** KGC results on WN18RR and FB15k-237: Filtered MRR and Hits@ $\{1, 3, 10\}$  (%). \* indicates the results transcribed from [6].

	WN18RR			FB15k-237				
	MRR	Hits@		MRR	Hits@			
Models		1	3	10		1	3	10
DistMult* ComplEx* R-GCN* ConvE*	43.0 44.0 - 43.0	39.0 41.0 - 40.0	44.0 46.0 - 44.0	49.0 51.0 - 52.0	24.1 24.7 24.8 <b>32.5</b>	15.5 15.8 15.3 <b>23.7</b>	26.3 27.5 25.8 <b>35.6</b>	41.9 42.8 41.7 <b>50.1</b>
$\begin{array}{l} {\rm CP}\;(D=200)\\ {\bf B\text{-}CP}\;(D=200)\\ {\bf B\text{-}CP}\;(D=400)\\ {\bf B\text{-}CP}\;(D=300\times3) \end{array}$	44.0 45.0 45.0 <b>48.0</b>	42.0 43.0 43.0 <b>45.0</b>	46.0 46.0 46.0 <b>49.0</b>	51.0 50.0 52.0 <b>53.0</b>	29.0 27.8 29.2 30.3	19.8 19.4 20.8 21.4	32.2 30.4 31.8 33.3	47.9 44.6 46.1 48.2

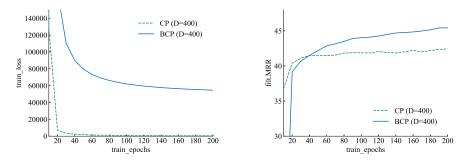


Fig. 2. Training loss and filtered MRR vs. epochs trained on WN18RR.

### 6.2 Experiment Setup

To train CP models, we selected the hyperparameters via grid search such that the filtered MRR is maximized on the validation set. For standard CP model, we tried all combinations of  $\lambda_A, \lambda_B, \lambda_C \in \{0.0001, 0\}$ , learning rate  $\eta \in \{0.025, 0.05\}$ , and the embedding dimension  $D \in \{15, 25, 50, 100, 150, 200, 300, 400, 500\}$  during grid search. For our binarized CP (B-CP) model, all combinations of  $\lambda_A, \lambda_B, \lambda_C \in \{0.0001, 0\}, \eta \in \{0.025, 0.05\}, \Delta \in \{0.3, 0.5\}$  and  $D \in \{100, 200, 300, 400, 500\}$  were tried. We randomly generated the initial values of the representation vectors from the uniform distribution  $U[-\frac{\sqrt{6}}{\sqrt{2D}}, \frac{\sqrt{6}}{\sqrt{2D}}]$  [7]. The maximum number of training epochs was set to 1000. For SGD training, negative samples were generated using the local closed-world assumption [4]. The number of negative samples generated per positive sample was 5 for WN18/WN18RR and 10 for FB15k/FB15k-237. In addition, to further take advantage of the benign run-time memory footprint of B-CP, we also tested the model ensemble of three independently trained B-CP models<sup>5</sup>, in which the final ranking is

<sup>&</sup>lt;sup>5</sup> As the original CP model has much larger memory consumption than B-CP, we did not test model ensemble with the CP model in our experiments.

Model	Div	Dir. 1.11	MRR		
	Bits per entity	Bits per relation	WN18RR	FB15k-237	
$DistMult^* (D = 200)$	6,400	6,400	43.0	24.1	
ComplEx* $(D = 200)$	12,800	12,800	44.0	24.7	
$ConvE^* (D = 200)$	6,400	6,400	43.0	32.5	
CP (D = 15)	960	480	40.0	22.0	
CP(D = 50)	3,200	1,600	43.0	24.8	
CP (D = 200)	12,800	6,400	44.0	29.0	
CP (D = 500)	32,000	16,000	43.0	29.2	
$VQ-CP \ (D=200)$	400	200	36.0	8.7	
VQ-CP (D = 500)	1,000	500	36.0	8.3	
<b>B-CP</b> $(D = 100)$	200	100	38.0	23.2	
<b>B-CP</b> $(D = 200)$	400	200	45.0	27.8	
<b>B-CP</b> $(D = 300)$	600	300	46.0	29.0	
<b>B-CP</b> $(D = 400)$	800	400	45.0	29.2	
<b>B-CP</b> $(D = 500)$	1,000	500	45.0	29.1	
<b>B-CP</b> $(D = 300 \times 3)$	1,800	900	48.0	30.3	

Table 4. Results on WN18RR and FB15k-237 with varying embedding dimensions.

computed by the sum of the scores of the three models. For this ensemble, the embedding dimension of each model was set to D=300, yet the total required run-time memory is still smaller than CP with D=200.

We implemented our CP decomposition systems in C++ and conducted all experiments on a 64-bit 16-Core AMD Ryzen Threadripper 1950x with 3.4GHz CPUs. The program codes were compiled using GCC 7.3 with -O3 option.

### 6.3 Results

Main Results We compared standard CP and B-CP models with other state-of-the-art KGE models. Table 2 shows the results on WN18 and FB15k, and Table 3 displays the results on WN18RR and FB15k-237. For most of the evaluation metrics, our B-CP model (D=400) outperformed or was competitive to the best baseline, although with a small vector dimension (D=200), B-CP showed tendency to degrade in its performance. In the table, B-CP ( $D=300\times3$ ) indicates an ensemble of three different B-CP models (each with D=300). This ensemble approach outperformed the baseline B-CP constantly on all datasets. Figure 2 shows training loss and accuracy versus epochs of training for CP (D=400) and B-CP (D=400) on WN18RR. The results indicate that CP is prone to overfitting with increased epochs of training. By contrast, B-CP appears less susceptible to overfitting than CP.

KGC Performance vs. Model Size We also investigated how our B-CP method can maintain the KGC performance while reducing the model size. For a fair evaluation, we also examined a naive vector quantization method (VQ) [23] that can reduce the model size. Given a real valued matrix  $\mathbf{X} \in \mathbb{R}^{D_1 \times D_2}$ , the VQ method solves the following optimization problem:

$$\hat{\boldsymbol{X}}^{(b)}, \hat{\alpha} = \operatorname*{argmin}_{\boldsymbol{X}^{(b)}, \alpha} \|\boldsymbol{X} - \alpha \boldsymbol{X}^{(b)}\|_F^2$$

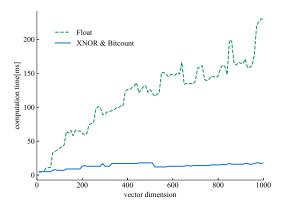


Fig. 3. CPU run time per 100,000-times score computations with single CPU thread.

where  $\boldsymbol{X}^{(b)} \in \{+1,-1\}^{D_1 \times D_2}$  is a binary matrix and  $\alpha$  is a positive real value. The optimal solutions  $\hat{\boldsymbol{X}}^{(b)}$  and  $\hat{\alpha}$  are given by  $Q_1(\boldsymbol{X})$  and  $\frac{1}{D_1 \times D_2} \|\boldsymbol{X}\|_1$ , respectively, where  $\|\cdot\|_1$  denotes  $l_1$ -norm, and  $Q_1(\boldsymbol{X})$  is a sign function whose behavior in each element x of  $\boldsymbol{X}$  is as per the sign function  $Q_1(x)$ . After obtaining factor matrices  $\boldsymbol{A}$ ,  $\boldsymbol{B}$  and  $\boldsymbol{C}$  via CP decomposition, we solved the above optimization problem independently for each matrix. We call this method VQ-CP.

Table 4 shows the results when the dimension size of the embeddings was varied. While CP requires  $64 \times D$  and  $32 \times D$  bits per entity and relation, respectively, both B-CP and VQ-CP have only to take one thirty-second of them. Obviously, the task performance dropped significantly after vector quantization (VQ-CP). The performance of CP also degraded when reducing the vector dimension from 200 to 15 or 50. While simply reducing the number of dimensions degraded the accuracy, B-CP successfully reduced the model size nearly 10- to 20-fold compared to CP and other KGE models without performance degradation. Even in the case of B-CP ( $D=300 \times 3$ ), the model size was 6 times smaller than that of CP (D=200).

Computation Time As described in Section 5, the B-CP model can accelerate the computation of confidence scores by using the bitwise operations (XNOR and Bitcount). To compare the score computation speed between CP (Float) and B-CP (XNOR and Bitcount), we calculated the confidence scores 100,000 times for both CP and B-CP, varying the vector size D from 10 to 1000 at 10 increments. Figure 3 clearly shows that bitwise operations provide significant speed-up compared to standard multiply-accumulate operations.

Table 5. Results on the Freebase-music dataset.

	Accuracy	Model size
CP (D = 15)	50.3	0.4GB
CP (D = 200)	89.2	4.8GB
<b>B-CP</b> $(D = 400)$	<b>92.8</b>	<b>0.3GB</b>

### 6.4 Evaluation on Large-scale Freebase

To verify the effectiveness of B-CP over larger datasets, we also conducted experiments on the Freebase-music data<sup>6</sup>. To reduce noises, we removed triples from the data whose relation and entities occur less than 10 times. The number of the remaining triples were 18,482,832 which consist of 138 relations and 3,025,684 entities. We split them randomly into three subsets: 18,462,832 training, 10,000 validation, and 10,000 test triples. We randomly generated 20,000 triples that are not in the knowledge graph, and used them as negative samples; half of them were placed in the validation set, and the other half in the test set. Experiments were conducted under the same hyperparameters and negative samples setting we achieved the best results on the FB15k dataset. We here report the triple classification accuracy. Table 5 gives the results. As it was with the small datasets, the performance of CP (D=15) was again poor. Meanwhile, B-CP successfully reduced the model size while achieving better performance than CP (D=200). These results show that B-CP is robust to the data size.

### 7 Conclusion

In this paper, we showed that it is possible to obtain binary vectors of relations and entities in knowledge graphs that take 10–20 times less storage/memory than the original representations with floating point numbers. Additionally, with the help of bitwise operations, the time required for score computation was considerably reduced. Tensor factorization arises in many machine learning applications such as item recommendation [22] and web link analysis [13]. Applying our B-CP algorithm to the analysis of other relational datasets is an interesting avenue for future work.

The program codes for the binarized CP decomposition algorithm proposed here will be provided on the first author's GitHub page <sup>7</sup>.

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