Thompson Sampling and Compositions in Knowledge Bases with Uncertainty

ABSTRACT

A knowledge base construction consists of a two-step approach; extracting information from external sources, known as knowledge extraction, and inferring missing information through a statistical analysis on the extracted information, known as knowledge completion. In many cases, however, it is implausible to extract a fair amount of information from the external sources. An active knowledge acquisition via labelling of human experts can help to reduce the gap between two processes. In this paper, we propose a new probabilistic knowledge base factorisation that benefits from a compositionality of existing knowledge (e.g. syllogism). This explicit probabilistic formulation enable us to develop an active acquisition model based on exploitation-exploration strategies. We demonstrate that the compositional knowledge factorisation results a better performance on the knowledge completion, whereas the model performs worse in the active knowledge acquisition. The result leads to a counter-intuitive conclusion; a better predictive model does not guarantee to have a better active acquisition model. An additional experiment explains the degeneracy in terms of the exploitation-exploration regime in the active knowledge acquisition.

1. INTRODUCTION

Relational knowledge bases structuralise our understanding about the world into the form of *(entity1, relation, entity2)* triples that help reasoning and inferring in a wide range of tasks such as information retrieval, question answering, and semantic parsing [5, 9, 12, 23]. A construction of a knowledge base is a very active research area with many important and challenging research questions. The early stage of knowledge base construction relies on **knowledge extraction** task in which structured information from external sources are extracted, or human experts encode a prior knowledge manually. Despite the endeavour toward to construct a complete knowledge base, even the commercialised knowledge bases are still far from complete [6]. **Knowledge completion** task has been emerged as an complement of the knowledge extraction to scale up the knowledge base construction. Unlike the knowledge extraction task where the goal is to maximise the number of triples, the goal of knowledge completion is to maximise the predictive performance on unseen triples.

One major obstacle of knowledge base construction is a gap between knowledge extraction and completion. For example, when there is no external source to extract knowledge, the construction relies solely on the contribution of human experts. Manual labelling is often painful and tedious, therefore triples that will be labelled should be selected in an active way so that we can maximise the performance of following knowledge completion. Active learning may provide a systematic way of selecting a data point to be labelled with one of knowledge completion models [22]. However, it is not clear that which model should be used for the active selection because of the discrepancy between two different goals of knowledge extraction and completion.

We first re-formulate a bilinear tensor factorisation [17] in a probabilistic way, where the model embeds entities and relations into latent feature space. And then we propose a novel tensor factorisation model that incorporates the graph structure of knowledge base into the factorisation model. These two probabilistic models provide a natural way of embracing uncertainty of triples that is crucial to develop an active triple selection for the active knowledge extraction. With Thompson sampling [21] – an approach for solving the multi-armed bandit problem, the model find an optimal trade-off between exploration and exploitation when identifying new triples.

Based on experiments with three real-world datasets, we find that the models outperformed in the knowledge completion may not perform well in the active knowledge extraction. Because, for the knowledge completion, it is important to find a better latent structure given current observation, for the active extraction, however, it is more important to measure the uncertainty of a current model in order to explore the latent space efficiently over time. As far as we know, this is the first study that explicitly reveals how the knowledge completion models result in different conclusions in the active knowledge extraction.

The contributions of this paper can be summarised as follows:

- We propose a probabilistic re-formulation of bilinear tensor factorisation that allows us to predict and measure the uncertainty of unobserved triples in Section 3.

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- We incorporate a compositional structure of knowledge graph into the proposed factorisation by modelling a composition of relations as an algebraic operation in the probabilistic embedding space in Section 4.

- We propose an active knowledge extraction method that efficiently explore the factorised space guided by a principled way of exploration-exploitation via Thompson sampling algorithm in Section 5.

- Experiments on the knowledge completion with three real-world dataset show that the compositional model uncovers a better factorisation in Section 6.

- Experiments show the importance of uncertainty in the active acquisition. Especially, the better predictive model does not guarantee to have a better performance due to an improper uncertainty measure in Section 7.

2. RELATED WORK

The literature on data factorisation and vector space models for relational data is vast. We give a brief overview of related work along three design choices: the method, the learning strategy, and the data representation. We then use these dimensions to help position our work.

Probabilistic/Non-Probabilistic This refers to two broad classes of model formulation, whether the obtained model has a probabilistic interpretation or not.

Passive/Active This refers to two different learning strategies, of passively learning a model given labeled data points, or actively requesting data points to be labeled.

Matrix/Tensor/Composition Relational learning problems for operate on different data representations. Matrix representation is common when a dataset can be represented as a bi-partite graph, such as (user, item) tuples in the recommender systems setting. Tensor representation is handy when edges in the graph have labels, i.e. (entity1, relation, entity2). We can think of compositions as paths in the graph, i.e. entity1 – relation1 – entity2 – relation2 – entity3.

In Table 1, we summarise a sample of related recent work along all combinations in each dimension. Note that N,A,C, or Non-Bayesian Active Composition model, can be done by simply using the query strategies from [10] on the compositional model by [8]. Our work address a critical gap in Bayesian Tensor factorisation capable of learning in the Active setting with relation Compositions.

Given this position, our work is inspired by, and most closely related to: active multi-relational data construction (AMDC) with tensor factorisation [10], Thomson sampling for matrix factorisation [11], and compositions objectives in vector space [8]. Note that we re-formulate the compositions objectives probabilistically such that it can be used in an active setting; our approach for active learning is a generalisation of Thomson sampling from matrixes to tensors; AMDC find that reconstruction accuracy and recall cannot be achieved at the same time with strategies geared towards either exploit or reducing uncertainty, we show that the two objectives can be achieved at the same time with a properly designed exploration and exploitation scheme.

Table 1: The categorisation of factorisation problems with respect to three design considerations. The column headings are Bayesian(B)/Non-Bayesian(N) method, Passive(P)/Active(A) learning, and Matrix(M)/Tensor(T)/Compositional(C) structure. In this work, we tackle the problems denoted by an asterisk.

B/N	P/A	M/T/C	References
N	P	M	[14]
N	A	M	[19]
N	P	T	[18] [13]
N	A	T	[10]
N	P	C	[16] [8]
N	A	C	–
B	P	M	[15]
B	A	M	[11] [24]
B	P	T	*, [26] [20]
B	A	T	*
B	P	C	*
B	A	C	*

3. PROBABILISTIC RESCAL

A relational knowledge base consists of a set triples in the form of (i, k, j) where i, j are entities, and k is a relation. A triple can be distinguished in a valid triple and invalid triple based on a semantic meaning of a triple. An example of valid triple in Freebase is (BarackObama, PresidentOf, U.S.), and an example of invalid triple is (BarackObama, PresidentOf, U.K.). A knowledge base can be represented in a three-way binary tensor $\mathcal{X} \in \{0,1\}^{N\times K\times N}$, where K is a number of relations, N is a number of entities, and $x_{ikj} \in \mathcal{X}$ indicates whether the triple is valid.

We model the entities i as vectors e_i and the relations k as matrices R_k with an appropriately chosen latent dimension D. This follows a popular model for statistical relational learning, which is to factorise the tensor into a set of latent vector representations, such as the bilinear model RESCAL [18]. RESCAL aims to factorise each relational slice $X_{:k:}$ into a set of rank-D latent features as follows:

$$\mathcal{X}_{:k:} \approx E R_k E^\top, \qquad \text{for } k = 1, \ldots, K$$

Here, $E \in \mathbb{R}^{N\times D}$ contains the latent features of the entities $e_1, \ldots, e_N$ and $R_k \in \mathbb{R}^{D\times D}$ models the interaction of the latent features between entities in relation k.

We propose a probabilistic framework that directly generalises RESCAL by placing priors over the latent features. For each entity i, the latent feature of an entity $e_i \in \mathbb{R}^D$ is drawn from an isotropic multivariate-normal distribution.

$$e_i \sim N(\mathbf{0}, \sigma_e^2 I_D) \tag{1}$$

For each relation k, we draw matrix R_k from a zero-mean isotropic matrix normal distribution.

$$R_k \sim \mathcal{MN}_{D\times D}(\mathbf{0}, \sigma_r I_D, \sigma_r I_D) \tag{2}$$
$$\text{or equivalently } \; r_k = \text{vec}(R_k) \sim N(\mathbf{0}, \sigma_r^2 I_{D^2})$$

Table 2: Parameters for Gibbs updates. The conditional posterior of e_i and R_k follows the normal distribution with mean μ and precision matrix Λ. $\otimes$ is the Kronecker product.

var	μ	Λ	ξ
e_i	$\frac{1}{\sigma_x^2}\Lambda_i^{-1}\xi_i$	$\frac{1}{\sigma_x^2}\sum_{jk:x_{ikj}\in\mathcal{X}^t}(R_k e_j)(R_k e_j)^\top$	$\sum_{jk:x_{ikj}\in\mathcal{X}^t} x_{ikj}R_k e_j + \sum_{jk:x_{jki}\in\mathcal{X}^t} x_{jki}R_k^\top e_j.$
$vec(R_k)$	$\frac{1}{\sigma_x^2}\Lambda_k^{-1}\xi_k$	$\frac{1}{\sigma_x^2}\sum_{ij:x_{ikj}\in\mathcal{X}^t}(e_i\otimes e_j)(e_i\otimes e_j)^\top + \frac{1}{\sigma_r^2}I_{D^2}$	$\sum_{ij:x_{ikj}\in\mathcal{X}^t} x_{ikj}(e_i\otimes e_j).$

where vec(R_k) denotes the flattening of the matrix.

We consider two models for x_{ikj}: a real or random variable. By placing a normal distribution over x_{ikj},

$$x_{ikj}|e_i, e_j, R_k \sim \mathcal{N}(e_i^\top R_k e_j, \sigma_x^2) \tag{3}$$

we can control the confidence on different observations through the variance parameter σ_x^2. The role of this parameter will be further discussed in the compositional model section.

We develop an efficient Gibbs sampler to perform inference for the probabilistic RESCAL (PPRESCAL). The key for achieving efficiency are the two conditional posteriors for latent features. The Gibbs updates are given by:

$$p(e_i|E_{-i}, \mathcal{R}, \mathcal{X}^t, \sigma_e, \sigma_x) = \mathcal{N}(e_i|\mu_i, \Lambda_i^{-1}) \tag{4}$$

$$p(R_k|E, \mathcal{X}, \sigma_r, \sigma_x) = \mathcal{N}(\text{vec}(R_k)|\mu_k, \Lambda_k^{-1}) \tag{5}$$

where the negative subscript $-i$ indicates the every other entity variables except e_i. The means and precision matrices are listed in Table 2, where we have used the identity $e_i^\top R_k e_j = r_k^\top e_i \otimes e_j$.

Alternatively, we may want to more closely model the fact that the observations are binary. Therefore we model x_{ikj} as a binomial distributed random variable whose probability is determined by logistic regression.

$$p(x_{ikj} = 1) = \sigma(e_i^\top R_k e_j),$$

where σ is a sigmoid function. We approximate the conditional posterior of E and R by Laplace approximation [1]. The maximum a posterior estimate of e_i or R_k given the rest can be computed through the standard logistic regression solvers with regularisation parameters. Given the maximum a posteriori parameters e_i^*, the posterior covariance S_i of entity i takes the form

$$S_i^{-1} = \sum_{x_{ikj}} \sigma(e_i^{*\top} R_k e_j)(1 - \sigma(e_i^{*\top} R_k e_j)) R_k e_j (R_k e_j)^\top + \sum_{x_{jki}} \sigma(e_j^\top R_k e_i^*)(1 - \sigma(e_j^\top R_k e_i^*)) R_k^\top e_i^* (R_k^\top e_i^*)^\top + I\sigma_e^{-1}.$$

The posterior covariance of R_k can be computed in the same way, and is shown in the appendix.

There are many advantages to a Bayesian view of tensor factorisation, such as the quantification of uncertainty by the predictive distribution, the ability to utilise priors, and the availability of principled model selection. We show in the empirical experiments that PRESCAL outperforms standard RESCAL. In the following, we focus on the predictive distribution, which enables us to improve sequential knowledge acquisition.

4. COMPOSITIONAL RELATIONS

In this section, we propose a compositional relation model that exploit the compositional structure of knowledge graph to capture the latent semantic structure of the entities and relations. While previously suggested vector space models provide a statistical way to infer the latent semantic structure of entities and relations, but lack consideration of a graph structure of a knowledge base itself.

The compositionality represents a semantic meaning of a path over a knowledge graph that corresponds to a sequence of composable triples. For example, given two triples, "Barack Obama is a 44th president of U.S." (BarackObama, PresidentOf, U.S) and "Joe Biden was a running mate of Barack Obama" (JoeBiden, RunningMateOf, BarackObama), one can naturally deduce that the "Joe Biden is a vice president of U.S." (JoeBiden, VicePresidentOf, U.S.). Here the composition of two relations, president of, and running mate of, yield to a compositional relation, vice president of. More formally, if there is a sequence of triples where the target entity of a former triple is a source entity of a latter triple in a consecutive pair of triples in the sequence, then we can form a compositional triples as follows. Given the sequence of triples (i_1, k_1, j_1), (i_2, k_2, j_2), (i_2, k_2, j_2) ... (i_n, k_n, j_n), where $i_k = j_{k+1}$ for all k, we form a compositional triple $(i_1, c(k_1, k_2, \ldots, k_n), j_n)$, where c denotes the compositional relation of the sequence of relations.

Let $\mathcal{C}^L$ be a set of all possible compositions of which length is up to L, $c \in \mathcal{C}$ be a sequence of relations, $c(i)$ be ith index of a relation in sequence c and $|c|$ be the length of the sequence. With set of compositions $\mathcal{C}^L$, we can expand set of observed triples $\mathcal{X}^t$ to set of compositional triples $\mathcal{X}^{\mathcal{C}^L(t)}$ in which compositional triple x_{icj} is an indicator variable that show the existence of the path from entity i to entity j through sequence of relations c in $\mathcal{X}^t$. Note that the compositional relation c is an abstract relation, and there might be a multiple possible paths from i_1 to j_n.

With these extended compositional triples, we again model x_{icj} with a bilinear Gaussian distribution,

$$x_{(i,c(k_1,k_2),l)} \sim \mathcal{N}(e_i^\top R_{c(k_1,k_2)} e_j, \sigma_c^2), \tag{6}$$

where $R_{c(k_1,k_2)} \in \mathbb{R}^{D\times D}$ is a latent matrix of compositional relation c, and σ_c^2 is a covariance of the compositional triples. We keep the same latent vector e for each entity to model both normal triples and compositional triples. In the subsequent sections, we provide two different ways of modelling the compositional relation R_c.

4.1 Additive Compositionality

First, we define an additive compositional relation R_c as a sequence of normalized summation over relation matrices in composition c, i.e., $R_c = \frac{1}{|c|}(R_{c(1)} + R_{c(2)} + \cdots + R_{c(|c|)})$, then compositional triple x_{icj} is modeled as

$$\begin{aligned} x_{(i,c,j)} &\sim \mathcal{N}(e_i^\top R_c e_j, \sigma_c^2) \\ &= \mathcal{N}(e_i^\top \frac{1}{|c|}(R_{c(1)} + R_{c(2)} + \cdots + R_{c(|c|)}) e_j, \sigma_c^2). \end{aligned} \tag{7}$$

The conditional distribution of e_i given $E_{-i}, \mathcal{R}, \mathcal{X}^t, \mathcal{X}^{L(t)}$ is

expanded from the posterior of PRESCAL by incorporating compositional triples.

$$p(e_i|E_{-i}, \mathcal{R}, \mathcal{X}^t, \mathcal{X}^{L(t)}) = \mathcal{N}(e_i|\mu_i, \Lambda_i^{-1}). \quad (8)$$

To compute the conditional distribution of R_k, we first decompose R_c into two part where $R_c = \frac{1}{|c|}R_k + \frac{|c|-1}{|c|}R_{c/k}$, where $R_{c/k} = \sum_{k' \in c/k} R_{k'}$. The distribution of compositional triple is decomposed as follows:

$$x_{(i,c,l)} \sim \mathcal{N}(e_i^\top(\frac{1}{|c|}R_k + \frac{|c|-1}{|c|}R_{c/k})e_j, \sigma_c^2). \quad (9)$$

Then, the conditional distribution R_k given $R_{-k}, E, \mathcal{X}^t, \mathcal{X}^{L(t)}$ is

$$p(R_k|E, \mathcal{X}^t, \mathcal{X}^{L(t)}, \sigma_r, \sigma_x) = \mathcal{N}(\text{vec}(R_k)|\mu_k, \Lambda_k^{-1}). \quad (10)$$

The mean and precision are obtained by expanding out the sum across $\mathcal{X}^t$ and $\mathcal{X}^{L(t)}$. The details of the parameters are shown in the appendix.

4.2 Multiplicative Compositionality

Second, we define an multiplicative compositional relation R_c as a sequence of multiplication over relations in composition c, i.e. $R_c = R_{c(1)}R_{c(2)}\dots R_{c(|c|)}$, and the compositional triple as a bilinear Gaussian distribution with the compositional relation R_c,

$$x_{(i,c,j)} \sim \mathcal{N}(e_i^\top R_{c(1)}R_{c(2)}\dots R_{c(|c|-1)}R_{c(|c|)}e_j, \sigma_c^2) \quad (11)$$

The multiplicative compositionality can be understood as a sequence of linear transformation from the original entity i with the compositional relations, and the inner product between the transformed entity and target entity will form a value of the compositional triple.

Given a sequence of relations including relation k, R_k is placed in the middle of the compositional sequence, i.e., $e_i^\top R_{c(1)}R_{c(2)}\dots R_{c(\delta_k)}\dots R_{c(|c|-1)}R_{c(|c|)}e_j$, where δ_k is the index of relation k. For notational simplicity, we will denote the left side $e_i^\top R_{c(1)}R_{c(2)}\dots R_{c(\delta_k-1)}$ as $\bar{e}_{ic(:\delta_k)}^\top$, and the right side $R_{c(\delta_k+1)}\dots R_{c(|c|-1)}R_{c(|c|)}e_j$ as $\bar{e}_{ic(\delta_k:)}$, therefore we can rewrite the mean parameter as $\bar{e}_{ic(:\delta_k)}^\top R_k \bar{e}_{ic(\delta_k:)}$. With the simplified notations, the conditional of R_k is

$$p(R_k|E, \mathcal{X}, \sigma_r, \sigma_x) = \mathcal{N}(\text{vec}(R_k)|\mu_k, \Lambda_k^{-1}), \quad (12)$$

where the mean and precision are obtained by expanding out the product across $\mathcal{X}^t$ and $\mathcal{X}^{L(t)}$. The details of the parameters are shown in the appendix. The conditional distribution of e_i given the rest is the same as Equation 15.

As the length of sequence c increases, a small error in the first few multiplication will result a large differences in the final compositional relation. One way to mitigate the cascading error is to increase variance of compositional triples σ_c as the length of the sequence increases.

With the conditional distributions, both compositional models can use the same particle Thompson sampling scheme described in Algorithm 1. However, the model can only query the triples in the original tensor and not in the expanded tensor because the triples are not observable.

5. PARTICLE THOMPSON SAMPLING

Thompson sampling has been gaining an increasing attention because of a competitive empirical performance as well as its conceptual simplicity [21, 2]. Let $y_{1:t}$ be a sequence of rewards up to time t, and θ is an underlying parameter governing the rewards. With Thompson sampling, an agent choose action a according to its probability of being optimal:

$$\arg\max_a \int \mathbb{I}\Big[\mathbb{E}(r|a,\theta) = \max_{a'} \mathbb{E}(r|a',\theta)\Big] p(\theta|y_{1:t-1}) d\theta,$$

where $\mathbb{I}$ is an indicator function. Note that it is sufficient to draw a random sample from the posterior instead computing the integral.

Algorithm 1 Particle Thompson sampling for probabilistic RESCAL with Gaussian output variable

Input: $\mathcal{X}^0, \sigma_x, \sigma_e, \sigma_r$.
for $t = 1, 2, \dots$ **do**
  Thompson Sampling:
  $h_t \sim \text{Cat}(\mathbf{w}^{t-1})$
  $(i,k,j) \leftarrow \arg\max p(x_{ikj}|E^{h_{t-1}}, \mathcal{R}^{h_{t-1}})$
  Query (i,k,j) and observe x_{ikj}
  $\mathcal{X}^t \leftarrow \mathcal{X}^{t-1} \cup \{x_{ikj}\}$
  Particle Filtering:
  $\forall h, w_h^t \propto p(x_{ikj}|E^h, \mathcal{R}^h)$ ▷ Reweighting
  if ESS$(\mathbf{w}^t) \leq N$ **then**
    resample particles
    $w_h^t \leftarrow 1/H$
  end if
  for $h = 1$ **to** H **do**
    $\forall k, R_k^{h_t} \sim p(R_k|\mathcal{X}^t, E^{h_{t-1}}, \mathcal{R}_{-k})$ ▷ see Table (2)
    $\forall i, e_i^{h_t} \sim p(e_i|\mathcal{X}^t, E_{-i}, \mathcal{R}^{h_t})$ ▷ see Table (2)
  end for
end for

We formulate Thompson sampling for active knowledge extraction system as follows. First, we assume there are optimal latent features E^* and R^*, and the triples are generated through Equation 1– 3. At time t, the system draws samples E^t and R^t from the posterior distribution, and then chooses an optimal triple $(i,k,j)^* = \arg\max_{i,k,j} e_i^\top R_k e_j$ to be queried. Finally, with the newly observed triple $x_{(i,k,j)^*}$, the system updates the posterior of the latent features.

The main difficulty of applying Thompson sampling to this task is a sequential update of the posterior distribution of the latent features with new observations over time. Unlike the point estimation algorithms such as the maximum likelihood estimate, computing a full posterior with MCMC requires extensive computational cost. To make the algorithm feasible, we employ a sequential Monte-Carlo (SMC) method for online posterior inference, generalising an algorithm proposed in [11] to tensors.

The SMC starts with H number of particles, each of which starts with likelihood weight $w_h = 1/H$, and a set of randomly sampled latent features E^{h_0} and $\mathcal{R}^{h_0}$. With a slight abuse of notation, let $\mathcal{X}^t$ be a set of observed triples up to time t. At time t, the system chooses one particle according to the particle weights, and then generates a new query via Thompson sampling from the selected particle. After observing a new variable, the system updates the posterior samples of every particle through the MCMC kernels with the new observation. We first sample the relation matrices using Equation 5, and sample the entity vectors using Equation 4. Under the mild assumption where $p(\Theta|\mathcal{X}^{t-1}) \approx p(\Theta|\mathcal{X}^t)$, $\Theta = \{E, \mathcal{R}\}$, the weight of each par-

Table 3: Description of datasets. Sparsity denotes the ration of valid triples to invalid triples.

Dataset	# rel	# entities	# triples	sparsity
Kinship	26	104	10,790	0.038
UMLS	49	135	6,752	0.008
Nation	56	14	2,024	0.184

ticle at time t can be computed as follows [4, 3]:

$$w_h^t = \frac{p(\mathcal{X}^t|\Theta)}{p(\mathcal{X}^{t-1}|\Theta)} = p(x^t|\Theta, \mathcal{X}^{t-1}) \tag{13}$$

To keep the posterior samples on regions of high probability mass, we resample the particles whenever an effective sample size (ESS) is less than a predefined threshold. The ESS can be computed as $(\sum_h w_h^2)^{-1}$, and we set the threshold to $N/2$ [7]. Resampling removes low weight particles with high probability, while keeping samples from the posterior. We summarise the particle Thompson sampling for PRESCAL with the Gaussian output variable in Algorithm 1.

We show that the Thompson sampling approach improves over passive PRESCAL in experiments with real and synthetic data. We also investigated the extension of the Rao-Blackwellisation approach as proposed in [11], but we did not observe any significant performance improvements. We describe our extension in the appendix.

6. MISSING TRIPLE PREDICTION

We evaluate the compositional models on three benchmark datasets and compare the performance to various baseline algorithms. We use three relational datasets: KINSHIP, UMLS, and NATION. Detailed description of each dataset is shown in Table 3 [1].

We first evaluate our model in a non-active setting, to measure the performance of PRESCAL with all non compositional and compositional variants.

For all experiments, we set the compositional length L to 2, split the dataset into 20% for validation and 30% for testing. We vary the proportion of training triples from 1% to 13% of datasets. For RESCAL, we use the authors' implementation, and measure performance over 10 runs with random initialisations. For PRESCAL and all the variants, we sample triples x_{ikj} from its posterior, and measure performance over 10 different samples. Given the test set, the performances of models are measured by ROC-AUC score:

$$\frac{1}{|\mathcal{X}_p||\mathcal{X}_n|} \sum_{\{i,k,j\}\in\mathcal{X}_p, \{i',k',j'\}\in\mathcal{X}_n} \mathbb{I}[\bar{x}_{ikj} > \bar{x}_{ikj}], \tag{14}$$

where X_p and X_n are the set of positive and negative triples in the test set, respectively, and $\bar{x}$ is a reconstructed triple.

Figure 1 shows the ROC-AUC scores of the compositional models with the various baseline models. We can see that PNORMAL or PLOGIT generally outperform RESCAL. We compare the compositional model with original RESCAL, PNORMAL, and PLOGIT. In general, PCOMP-MUL outperforms PCOMP-ADD, and performs better the other baseline models when the proportion of training set is small. For UMLS and NATION, BCOMP-MUL outperforms across the all training proportions. For KINSHIP, however, the model performs better when the training proportion is less than 7%.

[1]https://alchemy.cs.washington.edu/papers/kok07/

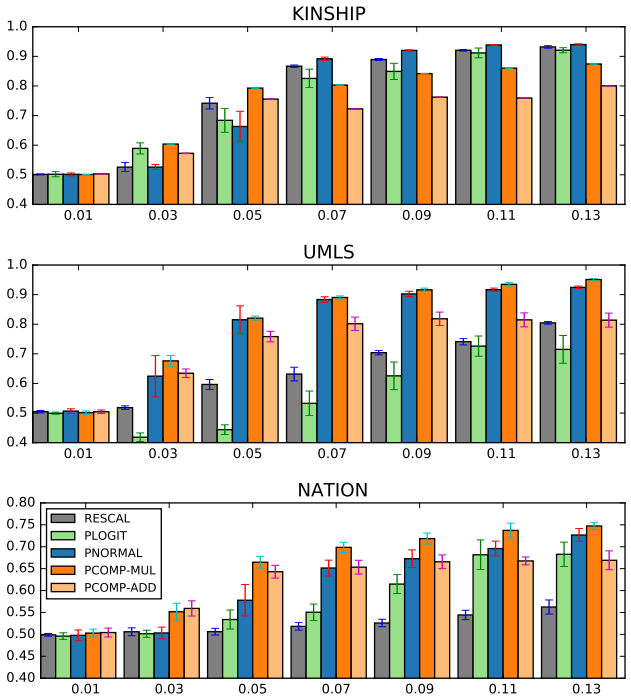


Figure 1: ROC-AUC scores of compositional models. The x-axis denotes the proportion of an observed triples including negative triples used for training models.

We visualise the multi-dimensional entities of the NATION dataset into the two-dimensional space through tSNE [25] in Figure 2.

7. ACTIVE KNOWLEDGE ACQUISITION

In this section, we show results for Thomson sampling of the PRESCAL and its compositional variants, first, on two synthetic datasets, and then on three common benchmarks used in the knowledge graph completion task.

7.1 Thompson Sampling on synthetic data

We first synthesise two datasets following the model assumptions in Eq. 1 to 3. First, entities and relations are generated from zero-mean isotropic multivariate normal distribution, with variance parameters $\sigma_e = 1$, $\sigma_r = 1$, respectively. We generate two sets of output triples, with the logistic output and the Gaussian with σ_x set to 0.1, respectively (Sec 3).

To measure performance, we compute cumulative regret at each time n as $R(n) = \sum_{t=1}^{n} x_t - x_t^*$, where x_t^* is the highest-valued triple among triples that have not been chosen up to time t. Unlike the general bandit setting where one can select a single item multiple times, in our formulation, we can select one triple only once. So after selecting a triple at time t, the selected triple will be removed from a set of candidate triples.

Figure 3 shows the cumulative regret of the algorithm on the synthetic data with varying size of entities and relations.

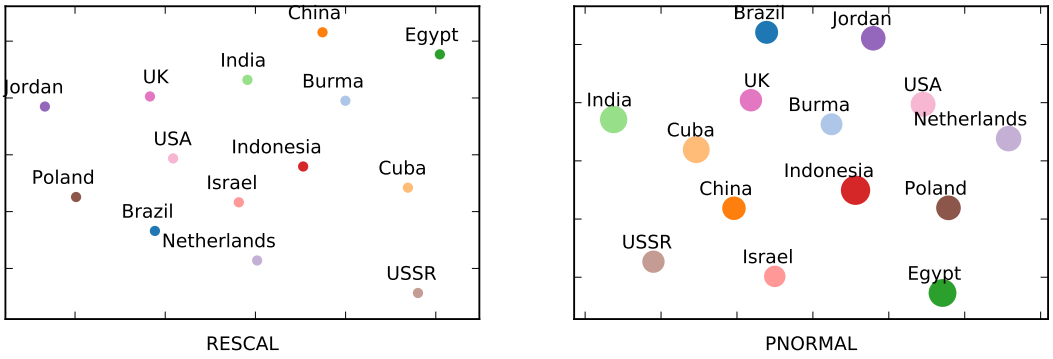
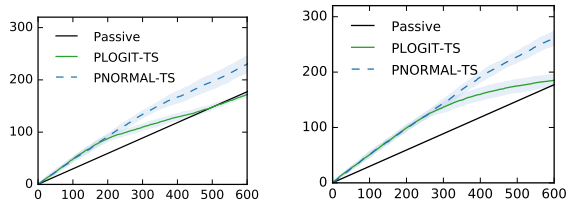
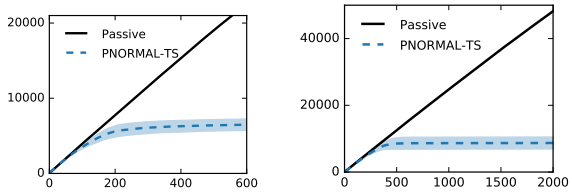


Figure 2: Embedding multi-dimensional entities of the NATION dataset into the two-dimensional space through tSNE [25]. The size of circle in PNORMAL is proportional to the uncertainty of entities in the embedded space.



(a) Logistic: N=10, K=10, D=5 (b) Logistic: N=20, K=10, D=5



(c) Gaussian: N=10, K=10, D=5 (d) Gaussian: N=20, K=10, D=5

Figure 3: Cumulative regret of particle Thompson sampling with Gaussian and logistic output (PNORMAL-TS, PLOGIT-TS) against Passive learning on synthetic datasets with logistic (top row, a, b) and Gaussian (bottom row, c, d) output variables. The averaged cumulative regrets over 10 runs are plotted with one standard error. As the model obtained more and more labeled samples from Thompson sampling, the cumulative regrets increase sublinearly.

We compare the cumulative regret of the particle Thompson sampling with the passive learning method where the model choose a random triple at each time. All results are averaged over 10 individual runs with different initialisations. Note that the dataset with binary logistic output variables can be used to train both logistic-output PRESCAL (PLOGIT) and Gaussian-output PRESCAL (PNORMAL) whereas the dataset with the Gaussian output can only be trained by PNORMAL. Figure 3(a) and 3(b) show that with the logistic synthetic dataset both models are capable to learn the latent features of the generated triples, with logistic outperforming

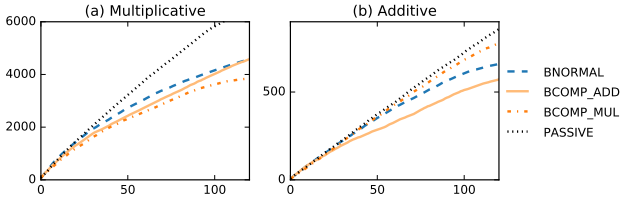


Figure 4: Cumulative regret of particle Thompson sampling of the compositional models on synthetic dataset with N=5, D=5. The synthetic dataset has three relations (K=3); the first two are independently generated, and the third relation is composed by the first two relations. The dataset used in (a) is generated by the multiplicative assumption, and the dataset used in (b) is generated by the additive assumption.

the Gaussian; Figure 3(c) and 3(d) show that PNORMAL outperform passive learning in the real valued dataset.

7.2 Thompson sampling for compositional models on synthetic data

We conduct a second experiment on synthetic dataset to understand how the Thompson sampling works for the compositional data. As in the first experiment, we first generate entities and relations from zero-mean multivariate normal with variance parameter $\sigma_e = 1$ and $\sigma_r = 1$. We generate a set of triples with Gaussian output as in Eq. 3. We then synthesise two sets of expanded tensors using the previously used entities and relations based on the multiplicative and additive compositional assumptions, defined in Sec 4, respectively. So we synthesise fully observable expanded tensor $\mathcal{X}^L$ where $L = 2$. We set both variance parameter σ_x and σ_c to 0.1. Note that in real world situation, the expanded tensor can be only constructed through the observed triples, and the triples in the expanded tensor cannot be queried.

To run the particle Thompson sampling on the synthetic dataset, we let the compositional models know which relation is composed by other relations. The non-compositional PNORMAL model assumes each relation is independent to one another. Therefore, the compositional model uses much

less number of parameters to model the same size of tensor to compare with the non-compositional model. With this fully observable expanded tensors, we run the Thompson sampling of the compositional models. Figure 4 shows the cumulative regrets on synthetic datasets. The multiplicative and additive compositionality are used to generate the dataset for Figure 4(a) and 4(b), respectively. The results correspond to our assumption: the multiplicative compositional model (BCOMP-MUL) shows lower regrets on the multiplicative data in Figure 4(a), and the additive compositional model (BCOMP-ADD) shows lower regrets on the additive compositional data in Figure 4(b), and both have lower regrets than passive learning or PNORMAL with no composition.

7.3 Thompson sampling on real datasets

Next, we evaluate particle Thompson sampling for both compositional and non-compositional models on real datasets.

Experimental settings: We compare our model with AMDC, and passive learning with PRESCAL. AMDC model has been proposed to achieve two different active learning goals, constructing a predictive model and maximising the valid triples in a knowledge base, with two different querying strategies [10]. AMDC-PRED is a predictive model construction strategy and chooses a triple which is the most ambiguous (close to the decision boundary) at each time t. AMDC-POP is a population strategy which aims to maximise the number of valid triples in a knowledge base, choosing a triple with the highest expected value at each time. To train all models we only use the observed triples up to the current time. For the passive learning with PRESCAL, we generate a random sample at each time period. For the particle Thompson sampling models, we set variance parameter σ_e and σ_r to 1, σ_x to 0.1, and vary σ_c from 1 to 100.

We leave 30 % of triples as a test set to measure test error. At each time period, each model choose one triples to query, if the selected triple is in the test set then we choose the next highest expected triple which is not in the test set. All models start from zero observation. After every querying, the model obtains a label of the queried triples from an oracle, then the model updates the parameters.

Evaluation metric: We use two different evaluation metrics, ROC-AUC score, and cumulative gain, for the performance comparison. One goal of the Thompson sampling is to maximise the knowledge acquisition through the balanced querying strategy between exploration and exploitation. To measure how many triples are obtained through the querying stage, we fist compute the cumulative gain which is the number of valid triple obtained up to time t, and then compute the ROC-AUC score on test set to understand how this balanced querying strategy results in making a predictive model.

Exploitation and exploration: Figure 5 and 6 show the cumulative gains and ROC-AUC scores of the Thompson sampling on three real datasets. PNORMAL performs better than other baseline models for the cumulative gain, and shows comparable result for the ROC-AUC scores. Both compositional models perform worse than PNORMAL across all datasets.

In the original AMDC work [10], AMDC-POP model obtains more valid triples than AMDC-PRED, and AMDC-PRED shows high ROC-AUC scores than AMDC-POP. In our experiment, however, AMDC-POP shows comparable cumulative gain to AMDC-PRED and even worse than AMDC-PRED for the UMLS. We conjecture the initial observation results in the different performances: in the original experiment, the model starts from a small set of training data so this gives the model focusing on exploit and advantage, whereas in our experiment, we start from zero observation which makes the model hard to exploit the structure. This result shows the importance of balancing between exploitation and exploration.

We note that the compositional model performs worse than the model without composition in this active setting.

8. DISCUSSION

We have proposed a novel compositional relational model with uncertainty and presented the Thompson sampling for both compositional and non-compositional models to solve the active knowledge acquisition problem. The compositional model aims to infer the latent features of knowledge bases by incorporating an additional graph structure. In the passive learning scenario, the compositional model outperforms the other models, especially, when training size is relatively small. In the active learning scenario, probabilistic RESCAL achieves the highest cumulative gain across all datasets. Again, this result emphasise the importance of being balanced between exploration and exploitation.

Previous work such as the one by [10] views knowledge population and predictive model construction are separate problems. We find this observation true when the algorithm has a warm-start, i.e. already having a fair amount of data before active learning starts; when the information is sparse, the same strategy works for both maximizing recall and reducing uncertainty. Thompson sampling has been studied in the context of multi-armed bandit problems where the goal is to maximise cumulative gains or minimise cumulative regrets over time, whereas its performance on making a predictive model has not been widely discussed so far. Its performance on building a generalisable model was unclear. Throughout this work, we have empirically shown that maximising cumulative gain entails the predictive models as well. In the long run, we see this work as a promising step towards using a composition-aware knowledge completion system to connect with the knowledge extraction problem [6].

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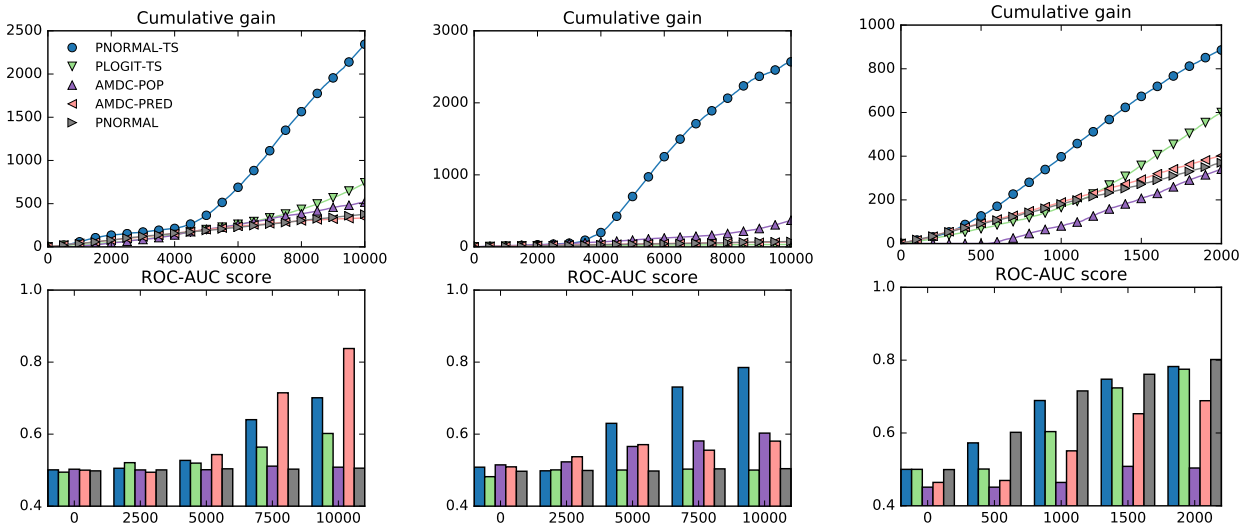

(a) KINSHIP (b) UMLS (c) NATION

Figure 5: Comparison between probabilistic RESCAL and greedy models.

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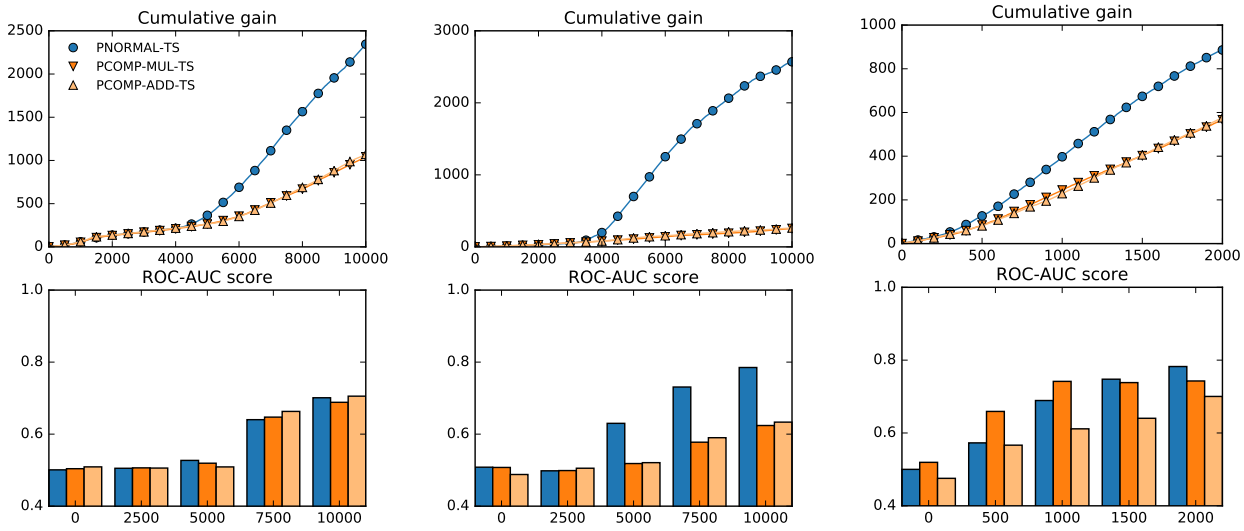

(a) KINSHIP (b) UMLS (c) NATION

Figure 6: Comparison between active PRESCAL, passive PRESCAL, and AMDC models.

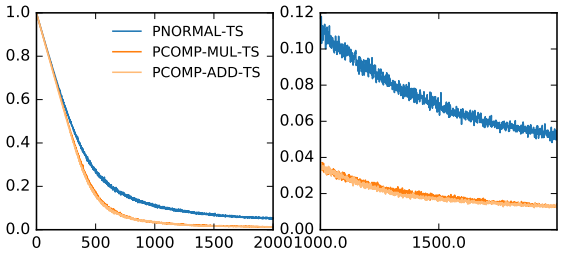

Figure 7: Trace plot of mean posterior variance of the non-compositional model and compositional models.

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APPENDIX

A. POSTERIOR COVARIANCE OF LOGISTIC OUTPUT

Let R_k^* is a maximum a posterior solution of R_k given E. Then, the conditional posterior covariance of relation matrix R_k has the form of:

$$S_i^{-1} = \sum_{x_{ikj}} \sigma(e_i^\top R_k^* e_j)(1 - \sigma(e_i^{*\top} R_k^* e_j))\bar{e}_{ij}\bar{e}_{ij}^\top + I\sigma_r^{-1},$$

where $\bar{e}_{ij} = e_i \otimes e_j$.

B. RAO-BLACKWELLISATION PARTICLE THOMPSON SAMPLING

We also develop Rao-Blackwellisation particle Thompson sampling algorithm for the RESCAL with the Gaussian output model. The outline of the algorithm is described in Algorithm 2. With the Rao-Blackwellisation, we marginalise out the relation matrix R_k while computing the weight of each particle, but we still keep the same MCMC kernel to generate the samples. In theory, this will reduce the degeneracy problems for long running particles, but in our experiment, the difference between two models is not significant.

C. POSTERIOR DISTRIBUTION OF COMPOSITIONAL RELATIONS

We provide the conditional posterior distributions of the compositional models.

C.1 Additive Compositionality

The conditional distribution of e_i given $E_{-i}, \mathcal{R}, \mathcal{X}^t, \mathcal{X}^{L(t)}$ is expanded from the posterior of BRESCAL by incorporating compositional triples.

$$p(e_i|E_{-i}, \mathcal{R}, \mathcal{X}^t, \mathcal{X}^{L(t)}) = \mathcal{N}(e_i|\mu_i, \Lambda_i^{-1}), \qquad (15)$$

Algorithm 2 Rao-Blackwellised Particle Thompson Sampling for Gaussian output

Input: $\sigma_x, \sigma_e, \sigma_r$.
for $t = 1, 2, \dots$ **do**
  Thompson Sampling:
  $h_t \sim \text{Cat}(\mathbf{w}^{t-1})$
  $(i, k, j) \leftarrow \arg\max p(x_{ikj}|E^{h_t})$
  Query (i, k, j) and observe x_{ikj}
  $\mathcal{X}^t \leftarrow \mathcal{X}^{t-1} \cup x_{ikj}$
  Particle Filtering:
  $\forall h, w_h^t \propto p(x_{ikj}|E^{h_t})$ ▷ Reweighting
  if $\text{ESS}(\mathbf{w}^t) \leq N$ **then**
    resample particles
    $w_h^t \leftarrow 1/H$
  end if
  for $h = 1$ **to** H **do**
    $\forall k, R_k^h \sim p(R_k|\mathcal{X}^t, E^{h_{t-1}})$ ▷ Auxiliary sampling
    $\forall i, e_i^h \sim p(e_i|\mathcal{X}^t, E_{-i}^h, \mathcal{R}^{h_t})$
  end for
end for

where

$$
\begin{aligned}
\mu_i &= \Lambda_i^{-1}\xi_i \\
\Lambda_i &= \frac{1}{\sigma_x^2}\sum_{jk:x_{ikj}\in\mathcal{X}^t}(R_k e_j)(R_k e_j)^\top \\
&\quad + \frac{1}{\sigma_x^2}\sum_{jk:x_{jki}\in\mathcal{X}^t}(R_k^\top e_j)(R_k^\top e_j)^\top \\
&\quad + \frac{1}{\sigma_c^2}\sum_{jc:x_{icj}\in\mathcal{X}^{L(t)}}(R_c e_j)(R_c e_j)^\top \\
&\quad + \frac{1}{\sigma_c^2}\sum_{jc:x_{jci}\in\mathcal{X}^{L(t)}}(R_c^\top e_j)(R_c^\top e_j)^\top + \frac{1}{\sigma_e^2}I_D \\
\xi_i &= \frac{1}{\sigma_x^2}\sum_{jk:x_{ikj}\in\mathcal{X}^t} x_{ikj}R_k e_j + \frac{1}{\sigma_x^2}\sum_{jk:x_{jki}\in\mathcal{X}^t} x_{jki}R_k^\top e_j \\
&\quad + \frac{1}{\sigma_c^2}\sum_{jc:x_{icj}\in\mathcal{X}^{L(t)}} x_{icj}R_c e_j + \frac{1}{\sigma_c^2}\sum_{jc:x_{jci}\in\mathcal{X}^{L(t)}} x_{jci}R_c^\top e_j
\end{aligned}
$$

The detail derivation of the posterior distribution is as follows:

$$
\begin{aligned}
&p(R_k|E, R_{-k}, \mathcal{X}) \propto p(\mathcal{X}|R, E)p(R_k) \\
&\propto \prod_{x_{ikj}}\exp\Big\{-\frac{(x_{ikj}-e_i^\top R_k e_j)^2}{2\sigma_x^2}\Big\} \\
&\quad \prod_{x_{icj}}\exp\Big\{-\frac{(x_{icj}-e_i^\top R_c e_j)^2}{2\sigma_c^2}\Big\}\exp\Big\{-\frac{r_k^\top r_k}{2\sigma_r^2}\Big\} \\
&= \exp\Big\{-\frac{\sum_{x_{ikj}}(x_{ikj}-\bar{e}_{ij}^\top r_k)^2}{2\sigma_x^2} \\
&\quad -\frac{\sum_{x_{icj}}(x_{icj}-\bar{e}_{ij}^\top r_c)^2}{2\sigma_c^2} - \frac{r_k^\top r_k}{2\sigma_r^2}\Big\} \\
&= \exp\Big\{-\frac{\sum_{x_{ikj}}(x_{ikj}-\bar{e}_{ij}^\top r_k)^2}{2\sigma_x^2} \\
&\quad -\frac{\sum_{x_{icj}}(x_{icj}-\bar{e}_{ij}^\top(\frac{1}{|c|}r_k+\frac{|c|-1}{|c|})r_{c/k})^2}{2\sigma_c^2} - \frac{r_k^\top r_k}{2\sigma_r^2}\Big\} \\
&= \exp\Big\{-\frac{\sum_{x_{ikj}}-2x_{ikj}\bar{e}_{ij}^\top r_k + r_k^\top\bar{e}_{ij}\bar{e}_{ij}^\top r_k}{2\sigma_x^2} \\
&\quad -\frac{\sum_{x_{icj}}\frac{2}{|c|}r_k^\top(x_{icj}-\frac{(|c|-1)}{|c|}\bar{e}_{ij}^\top r_{c/k})+(\frac{1}{|c|^2}r_k^\top\bar{e}_{ij}\bar{e}_{ij}^\top r_k)}{2\sigma_c^2} \\
&\quad -\frac{r_k^\top r_k}{2\sigma_r^2} + const\Big\} \\
&\propto \exp\Big\{-\frac{1}{2}r_k^\top\big(\frac{1}{\sigma_x^2}\sum_{x_{ikj}}\bar{e}_{ij}\bar{e}_{ij}^\top + \frac{1}{|c|^2\sigma_c^2}\sum_{x_{icj}}\bar{e}_{ij}\bar{e}_{ij}^\top + \frac{1}{\sigma_r^2}I\big)r_k \\
&\quad - r_k^\top\Big(\frac{\sum_{x_{ikj}}-x_{ikj}\bar{e}_{ij}}{\sigma_x^2} + \frac{\sum_{x_{icj}}|c|^{-1}(x_{icj}-\frac{(|c|-1)}{|c|}\bar{e}_{ij}^\top r_{c/k})}{\sigma_c^2}\Big)
\end{aligned}
$$

Completing the square results Equation 17.

To compute the conditional distribution of R_k, we first decompose R_c into two part where $R_c = \frac{1}{|c|}R_k + \frac{|c|-1}{|c|}R_{c/k}$, where $R_{c/k} = \sum_{k'\in c/k} R_{k'}$. The distribution of compositional triple is decomposed as follows:

$$
x_{(i,c,l)} \sim \mathcal{N}(e_i^\top(\frac{1}{|c|}R_k + \frac{|c|-1}{|c|}R_{c/k})e_j, \sigma_c^2). \tag{16}
$$

Then, the conditional distribution R_k given $R_{-k}, E, \mathcal{X}^t, \mathcal{X}^{L(t)}$ is

$$
p(R_k|E, \mathcal{X}^t, \mathcal{X}^{L(t)}, \sigma_r, \sigma_x) = \mathcal{N}(\text{vec}(R_k)|\mu_k, \Lambda_k^{-1}), \tag{17}
$$

where

$$
\begin{aligned}
\mu_k &= \Lambda_k^{-1}\xi_k \\
\Lambda_k &= \frac{1}{\sigma_x^2}\sum_{ij:x_{ikj}\in\mathcal{X}^t}\bar{e}_{ij}\bar{e}_{ij}^\top + \frac{1}{\sigma_r^2}I_{D^2} \\
&\quad + \frac{1}{|c|^2\sigma_c^2}\sum_{ij:x_{icj}\in\mathcal{X}^{L(t)},\ k\in c}\bar{e}_{ij}\bar{e}_{ij}^\top \\
\xi_k &= \frac{1}{\sigma_x^2}\sum_{ij:x_{ikj}\in\mathcal{X}^t} x_{ikj}\bar{e}_{ij} \\
&\quad + \frac{1}{|c|\sigma_c^2}\sum_{ij:x_{icj}\in\mathcal{X}^{L(t)},\ k\in c} x_{icj}\bar{e}_{ij} - \frac{|c|-1}{|c|}\bar{e}_{ij}r_{c/k}^\top\bar{e}_{ij}
\end{aligned}
$$

$\bar{e}_{ij} = e_i \otimes e_j$.

Vectorisation of R_c and $R_{c/k}$ are represented as r_c and $r_{c/k}$, respectively.

C.2 Multiplicative Compositionality

Given a sequence of relations including relation k, R_k is placed in the middle of the compositional sequence, i.e., $e_i^\top R_{c(1)} R_{c(2)} \dots R_{c(\delta_k)} \dots R_{c(|c|-1)} R_{c(|c|)} e_j$, where δ_k is the index of relation k. For notational simplicity, we will denote the left side $e_i^\top R_{c(1)} R_{c(2)} \dots R_{c(\delta_k - 1)}$ as $\bar{e}_{ic(:\delta_k)}^\top$, and the right side $R_{c(\delta_k+1)} \dots R_{c(|c|-1)} R_{c(|c|)} e_j$ as $\bar{e}_{ic(\delta_k:)}$, therefore we can rewrite the mean parameter as $\bar{e}_{ic(:\delta_k)}^\top R_k \bar{e}_{ic(\delta_k:)}$. With the simplified notations, the conditional of R_k is

$$p(R_k|E, \mathcal{X}, \sigma_r, \sigma_x) = \mathcal{N}(\text{vec}(R_k)|\mu_k, \Lambda_k^{-1}), \tag{18}$$

where

$$\mu_k = \Lambda_k^{-1} \xi_k$$

$$\Lambda_k = \frac{1}{\sigma_x^2} \sum_{ij: x_{ikj} \in \mathcal{X}^t} (e_i \otimes e_j)(e_i \otimes e_j)^\top + \frac{1}{\sigma_r^2} I_{D^2}$$

$$+ \frac{1}{\sigma_c^2} \sum_{ij: x_{icj} \in \mathcal{X}^{L(t)},\ k \in c} (\bar{e}_{ic(:\delta_k)} \otimes \bar{e}_{jc(\delta_k:)})(\bar{e}_{ic(:\delta_k)} \otimes \bar{e}_{jc(\delta_k:)})^\top$$

$$\xi_k = \frac{1}{\sigma_x^2} \sum_{ij: x_{ikj} \in \mathcal{X}^t} x_{ikj} (e_j \otimes e_i)$$

$$+ \frac{1}{\sigma_c^2} \sum_{ij: x_{icj} \in \mathcal{X}^{L(t)},\ k \in c} x_{icj} (\bar{e}_{ic(:\delta_k)} \otimes \bar{e}_{jc(\delta_k:)}).$$

The conditional distribution of e_i given the rest is the same as the additive compositional case.