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# Knowledge Graph Analysis

## Solutions to Exercise Sheet 4

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### 1 IN CLASS

#### 1. Tensors: notation and terminology

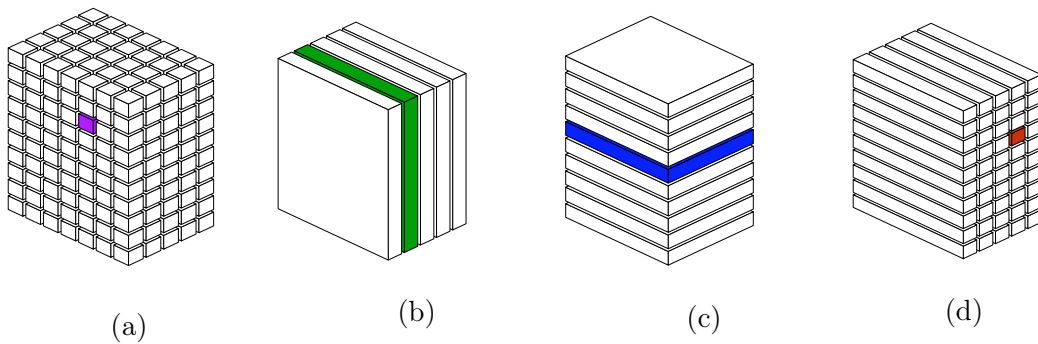


Figure 1.1: (a) - the tensor entry  $\mathcal{T}_{3,5,1}$ , (b) - 2nd frontal slice  $\mathcal{T}_{::,2}$ , (c) - the fifth horizontal slice  $\mathcal{T}_{5,::}$ , and (d) - the mode-2 fiber  $\mathcal{T}_{4,::4}$

## 2. Adjacency tensors

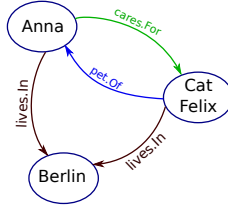


Figure 1.2: Knowledge graph described by the adjacency tensor.

## 3. Convert Tensor into Matrix

$$\mathbf{X}_{(1)} = \begin{bmatrix} 1 & 3 & 5 & 7 \\ 2 & 4 & 6 & 8 \end{bmatrix} \quad (1.1)$$

$$\mathbf{X}_{(2)} = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{bmatrix} \quad (1.2)$$

$$\mathbf{X}_{(3)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix} \quad (1.3)$$

## 4. Matrix factorization

For

$$\mathbf{X} = \begin{bmatrix} 5 & 3 & 0 & 1 \\ 4 & 0 & 0 & 1 \\ 1 & 1 & 0 & 5 \\ 1 & 0 & 0 & 4 \\ 0 & 1 & 5 & 4 \end{bmatrix}$$

the prediction based on the factorization into 2 latent dimensions is given by

$$\hat{\mathbf{X}} = \begin{bmatrix} 5.01 & 2.59 & 5.44 & 1.02 \\ 3.88 & 1.97 & 4.23 & 0.99 \\ 2.11 & 1.08 & 3.94 & 4.65 \\ 1.66 & 0.85 & 3.13 & 3.74 \\ 3.28 & 1.67 & 4.83 & 3.99 \end{bmatrix} = \begin{bmatrix} 2.25 & 0.97 \\ 1.68 & 0.82 \\ 0.26 & 1.97 \\ 0.19 & 1.58 \\ 0.92 & 1.86 \end{bmatrix} \begin{bmatrix} 1.91 & 0.97 & 1.65 & -0.6 \\ 0.82 & 0.42 & 1.78 & 2.44 \end{bmatrix}$$

## 5. Loss function for matrix factorization

The Mean Squared Error (MSE) is given by

$$\begin{aligned} \|\mathbf{X} - \hat{\mathbf{X}}\|^2 &= \sum_{ij} (X_{ij} - \hat{X}_{ij})^2 \\ &= 0.1^2 + 0.2^2 + 0.1^2 + 0.3^2 + 0.1^2 + 0.1^2 \\ &= 0.17 \end{aligned}$$

## 6. Outer product

Given are the following three vectors

$$\mathbf{a} = [1 \ 3 \ 2]$$

$$\mathbf{b} = [4 \ 2 \ 1]$$

$$\mathbf{c} = [1 \ 3 \ 4]$$

The  $\mathcal{T}_{:,1,1}$  fiber of the rank-3 tensor  $\mathcal{T}$  resulting from the outer product of the vectors

$$\mathcal{T} = \mathbf{a} \circ \mathbf{b} \circ \mathbf{c} .$$

is given by

$$[4 \ 12 \ 8]^T ,$$

since the  $ijk$ -th element of  $\mathcal{T}$  is given by  $\mathcal{T}_{ijk} = a_i * b_j * c_k$  and

$$\mathcal{T}_{:,1,1} = [a_1 * b_1 * c_1 \ a_2 * b_1 * c_1 \ a_3 * b_1 * c_1]^T = [a_1 * 4 \ a_2 * 4 \ a_3 * 4]^T .$$

## 7. Collective learning in bipartite model

In a bipartite model (like CP) for each entity two latent representations are learned, one describing its role as a subject the other its role as an object of relations. In a unipartite model (Like RESCAL) an unique latent representation is learned for each entity. This enables information flow and improves the ability for collective learning.

## 8. RESCAL

A) Given the entity matrix

$$\mathbf{A} = \begin{bmatrix} 0.1 & 0.8 & 0.1 \\ 0.7 & 0.2 & 0.1 \end{bmatrix} \quad (1.4)$$

and the  $k$ -th frontal slice of the relation tensor

$$\mathbf{R}_{::,k} = \begin{bmatrix} 1 & 0 & 1.2 \\ 1 & 1.2 & 0 \\ 0.1 & 0 & 1 \end{bmatrix} \quad (1.5)$$

the  $k$ -th slice of approximated tensor is give by

$$\mathbf{A}\mathbf{R}_{::,k}\mathbf{A}^T = \begin{bmatrix} 0.881 & 0.851 \\ 0.377 & 0.779 \end{bmatrix} . \quad (1.6)$$

The result describes the confidence of the model that the two entities are connected via the  $k$ -th relation (entries close to 1/0 indicate that a relation exists/not exists).

B)

$$\mathbf{A} = \begin{bmatrix} \textit{latent - representations - of - CatFelix} \\ \textit{latent - representations - of - Anna} \\ \textit{latent - representations - of - Berlin} \end{bmatrix} . \quad (1.7)$$

$$\mathbf{R}_{caresFor} \quad (1.8)$$

$$\mathbf{R}_{petOf} \quad (1.9)$$

$$\mathbf{R}_{livesIn} \quad (1.10)$$

$$P(X|A, \mathbf{R}) = \prod_{i=1}^n \prod_{j=1}^n \prod_{k=1}^m P(x_{ijk} | \mathbf{a}_i^T \mathbf{R}_k \mathbf{a}_j).$$

## 9. Applications of RESCAL

a) **Link Prediction:** Let

$$\mathcal{T}_{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \quad (1.11)$$

be the 1-mode presentation of a tensor and

$$\hat{\mathcal{T}}_{(1)} = \begin{bmatrix} 1.2 & 0.02 & 0.03 & 0.89 & 0.9 & 0.01 & 0.1 & 1.04 & 0.03 \\ 0 & 0.95 & 0.04 & 0.07 & 0.11 & 1.1 & 0.07 & 1.05 & 0.0 \\ 1.1 & 1 & 0.01 & 0.2 & 1.2 & 1 & 0.1 & 0.08 & 0.09 \end{bmatrix} \quad (1.12)$$

its approximation gained by a tensor decomposition technique.

check here for details how to fold back the tensor and get the predicted links [https://sewiki.iai.uni-bonn.de/\\_media/teaching/lectures/kga/2017/tensor\\_ex\\_3-9.jpg](https://sewiki.iai.uni-bonn.de/_media/teaching/lectures/kga/2017/tensor_ex_3-9.jpg)

New links in the knowledge graph are  $(e_1, r_2, e_1)$  (corresponding to  $\hat{\mathcal{T}}_{112} = 0.89$ ),  $(e_2, r_1, e_2)$  (corresponding to  $\hat{\mathcal{T}}_{221} = 0.95$ ), and  $(e_2, r_2, e_2)$  (corresponding to  $\hat{\mathcal{T}}_{322} = 1.2$ ).

Links that got removed are  $(e_2, r_1, e_3)$  (corresponding to  $\hat{\mathcal{T}}_{231} = 0.04$ ) and  $(e_2, r_3, e_1)$  (corresponding to  $\hat{\mathcal{T}}_{213} = 0.07$ ).

b) **Entity Similarity:** Let

$$\mathbf{A} = \begin{bmatrix} 0.8 & 0.3 & 1.7 \\ 0.9 & 0.4 & 1.6 \\ 0.2 & 0.2 & 0.3 \\ 1.0 & 0.3 & 1.5 \end{bmatrix} \quad (1.13)$$

be the entity matrix gained by RESCAL. Entities 1,2 and 4 corresponding to the latent features  $\mathbf{a}_1 = (0.8, 0.3, 1.7)$ ,  $\mathbf{a}_2 = (0.9, 0.4, 1.6)$  and  $\mathbf{a}_3 = (1.0, 0.3, 1.5)$  respectively are similar to each other (since similarity of entities can be measured based on the similarity of their latent representations).

- c) **Relation Similarity:** Given are the  $k$ -th, the  $l$ -th, and the  $m$ -th frontal slice of the relation tensor of RESCAL

$$\mathbf{R}_{:,:,k} = \begin{bmatrix} 1.1 & 0.9 & 0.9 \\ 1.3 & 1.2 & 0.8 \\ 0.9 & 1.1 & 1.1 \end{bmatrix} \quad (1.14)$$

$$\mathbf{R}_{:,:,l} = \begin{bmatrix} 2 & 5 & 9 \\ 3 & 0.5 & 1 \\ 0.3 & 4 & 7 \end{bmatrix} \quad (1.15)$$

$$\mathbf{R}_{:,:,m} = \begin{bmatrix} 1.2 & 1.1 & 0.8 \\ 1.0 & 0.8 & 0.8 \\ 0.8 & 0.9 & 0.9 \end{bmatrix} \quad (1.16)$$

The  $m$ -th and the  $k$ -th relation are similar (since similarity of relations can be measured based on the similarity of their latent representations).

## 2 AT HOME

### 1. Singular value decomposition (SVD)

$$\lambda_1 u_1 \circ v_1 = 9.03 \times \begin{bmatrix} -0.44 \\ -0.3 \\ -0.52 \\ -0.4 \\ -0.52 \end{bmatrix} \times \begin{bmatrix} -0.47 & -0.78 & 0.17 & 0.37 \end{bmatrix} =$$

$$\begin{bmatrix} 1.867404 & 3.099096 & -0.675444 & -1.470084 \\ 1.27323 & 2.11302 & -0.46053 & -1.00233 \\ 2.206932 & 3.662568 & -0.798252 & -1.737372 \\ 1.69764 & 2.81736 & -0.61404 & -1.33644 \\ 2.291814 & 3.803436 & -0.828954 & -1.804194 \end{bmatrix}$$

$$\lambda_2 u_2 \circ v_2 = 6.23 \times \begin{bmatrix} -0.67 \\ -0.44 \\ 0.14 \\ 0.11 \\ 0.57 \end{bmatrix} \times \begin{bmatrix} -0.26 & -0.21 & 0.25 & -0.91 \end{bmatrix} =$$

$$\begin{bmatrix} 1.085266 & 0.876561 & -1.043525 & 3.798431 \\ 0.712712 & 0.575652 & -0.6853 & 2.494492 \\ -0.226772 & -0.183162 & 0.21805 & -0.793702 \\ -0.178178 & -0.143913 & 0.171325 & -0.623623 \\ -0.923286 & -0.745731 & 0.887775 & -3.231501 \end{bmatrix}$$

$$\lambda_3 u_3 \circ v_3 = 3.77 \times \begin{bmatrix} -0.3 \\ -0.05 \\ -0.05 \\ -0.48 \\ 0.61 \end{bmatrix} \times [-0.3 \quad 0.46 \quad 0.81 \quad 0.21] =$$

$$\begin{bmatrix} 0.3393 & -0.52026 & -0.91611 & -0.23751 \\ 0.05655 & -0.08671 & -0.152685 & -0.039585 \\ 0.05655 & -0.08671 & -0.152685 & -0.039585 \\ 0.54288 & -0.832416 & -1.465776 & -0.380016 \\ -0.68991 & 1.057862 & 1.862757 & 0.482937 \end{bmatrix}$$

$$\lambda_4 u_4 \circ v_4 = 1.84 \times \begin{bmatrix} -0.49 \\ 0.8 \\ -0.29 \\ 0.21 \\ 0.08 \end{bmatrix} \times [-0.78 \quad 0.37 \quad -0.5 \quad 0] =$$

$$\begin{bmatrix} 0.703248 & -0.333592 & 0.4508 & 0 \\ -1.14816 & 0.54464 & -0.736 & 0 \\ 0.416208 & -0.197432 & 0.2668 & 0 \\ -0.301392 & 0.142968 & -0.1932 & 0 \\ -0.114816 & 0.054464 & -0.0736 & 0 \end{bmatrix}$$

$$X = \sum_{i=1}^4 \lambda_i u_i \circ v_i = \begin{bmatrix} 3.995218 & 3.121805 & -2.184279 & 2.090837 \\ 0.894332 & 3.146602 & -2.034515 & 1.452577 \\ 2.452918 & 3.195264 & -0.466087 & -2.570659 \\ 1.76095 & 1.983999 & -2.101691 & -2.340079 \\ 0.563802 & 4.170031 & 1.847978 & -4.552758 \end{bmatrix}$$