Non-Negative Tensor Factorization with RESCAL

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Abstract. Non-negative data is generated by a broad range of applications, e.g in gene expression analysis and in imaging. Many factorization techniques have been extended to account for this natural constraint and have become very popular, mainly due to the improved interpretability of the latent factors. Relational data, like data from protein interaction networks or social networks, can also be seen as being naturally non-negative. In this work, we extend the RESCAL tensor factorization, which has shown state-of-the-art results for multi-relational learning, to account for non-negativity by employing multiplicative update rules. We study the performance of non-negative RESCAL on various benchmark datasets and show that non-negativity constraints lead to very sparse factors at a slight loss in predictive performance, if compared to unconstraint RESCAL.

Keywords: RESCAL, non-negative matrix factorization, non-negative tensor factorization, Kullback-Leibler-Divergence, relational learning, multiplicative updates, sparsity

1 Introduction

When mining non-negative datasets like document collections, gene expression data or imaging data, matrix and tensor decompositions are often employed for low rank approximations of the original data matrix/tensor to perform tasks like clustering [1] or for predicting items that might be interesting for a user in a recommendation environment [2]. Other interesting applications arise in the field of image processing, e.g., compression. As the original data is non-negative, a non-negative constraint on the computed factors of the decomposition seems also very natural. In contrast to, e.g., SVD-based decompositions, a non-negative decomposition results in an additive representation that tends to be naturally sparse and memory efficient. Another important benefit of non-negative factors comes from their interpretability, which has been demonstrated in various applications like text-processing [3] or image processing [4], where the factors could be interpreted as latent topics in the former case or as image structures like eyes, ears or noses, in the latter case.

In contrast to an SVD, a non-negative decomposition is generally not unique and converges into local minima. As a consequence, the initialization of the factor matrices becomes critical. In the past, different methods have been proposed for initializing one or more of the factors matrices (see [3] for a summary and [5]). Out of a set of candidate solutions, some authors argue that one should prefer the sparsest solution.

In the past, non-negative matrix factorization (NMF) has been extended to tensor decompositions like PARAFAC/CP [6][7] and TUCKER[8] by employing multiplicative update rules as introduced by [9]. As relational datasets from protein interactions or social networks also impose a natural non-negativity constraint, we propose to extend NMF to the recently introduced RESCAL model [10]. RESCAL is a three-way-tensor factorization model that has been shown to lead to very good results in various canonical relational learning tasks like link prediction, entity resolution and collective classification [10]. One main feature of RESCAL is that it can exploit a collective learning effect when used on relational data.

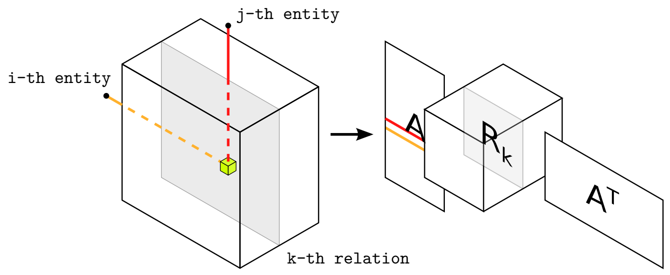


Fig. 1. Graphical illustration of the RESCAL tensor factorization into the factor matrix A and the core tensor $\mathcal{R}$ [11].

The RESCAL decomposition decomposes a tensor $\mathcal{X}$ of shape $n \times n \times m$, into a factor matrix A of shape $n \times r$ and a core tensor R of shape $r \times r \times m$, where each of the m frontal slices of $\mathcal{X}$ can be seen as a binary adjacency-matrix between n entities for each of the m relations or observed subject-predicate-object RDF triples for m predicates (Figure 1). Each of the k frontal slices of $\mathcal{X}$ is factorized into

$$X_k = AR_kA^T, \text{for } k = 1, ..., m$$

The decomposition is computed by minimizing the regularized least-squares cost function

$$C_{LS}(\mathcal{X}, A, \mathcal{R}) = f_{LS}(\mathcal{X}, A, \mathcal{R}) + f_{L2}(A, \mathcal{R}) \tag{1}$$

$$\text{with } f_{LS}(\mathcal{X}, A, \mathcal{R}) = \sum_k \|X_k - AR_kA^T\|_F^2$$
$$f_{L2}(A, \mathcal{R}) = \lambda_A \|A\|_F^2 + \lambda_R \sum_k \|R_k\|_F^2$$

using Alternating Least Squares (ALS) with update functions for A and R_k:

$$A \leftarrow \left[\sum_k X_k A R_k^T + X_k^T A R_k\right] \left[\sum_k R_k A^T A R_k^T + R_k^T A^T A R_k + \lambda_A \mathbf{I}\right]^{-1}$$
$$R \leftarrow (Z^T Z + \lambda_R \mathbf{I})^{-1} Z^T \mathbf{vec}(X_k)$$
$$\text{with } Z = (A \otimes A)$$

This updates do not enforce a non-negative constraint on the factors.

The contribution of this paper is as follows: We derived and implemented non-negative tensor decompositions for the RESCAL model using regularized least-squares and Kullback-Leibler (KL) cost functions, by employing multiplicative update rules for A and $\mathcal{R}$. We give updates that feature combinations of L_1 and L_2 regularization of A and $\mathcal{R}$, as well as normalization of the factor matrix A as introduced by [9], [12] and [13].

Additionally we derived update rules for including attribute information of entities as proposed by [11]. The derived models are compared against the original RESCAL model without non-negative constraint using the Kinship, Nations and UMLS multirelational datasets. We show that non-negativity constraints lead to very sparse factors at a slight loss in predictive performance, if compared to unconstraint RESCAL.

2 Methods

In the next sections, $X \bullet Y$ and $\frac{X}{Y}$ will denote elementwise matrix-multiplication and division. XY will represent the regular matrix multiplication. Furthermore $\mathcal{R}$ or $\mathcal{X}$ will represent tensors whereas R, X will represent matrices. The matrix $\mathbf{J}^{ij}$ is defined as a single entry matrix, where $\mathbf{J}_{ij} = 1$ and zero otherwise. The matrix $\mathbf{E}^{n \times m}$ represents an $n \times m$ matrix filled with ones and $\mathbf{1}$ is a row vector of ones.

For deriving non-negative updates for A and R_k, we use multiplicative update rules as proposed in [9], having the general form of

$$\theta_i = \theta_i \left(\frac{\frac{\partial C(\theta)^-}{\partial \theta_i}}{\frac{\partial C(\theta)^+}{\partial \theta_i}}\right)^\alpha \tag{2}$$

Where $C(\theta)$ represents a cost function of the non-negative variables θ and $\frac{\partial C(\theta)^-}{\partial \theta_i}$ and $\frac{\partial C(\theta)^+}{\partial \theta_i}$ are the negative and positive parts of the derivative of $C(\theta)$ [13].

When initializing the factor matrices with non-negative values, these update functions guarantee non-negativity through only performing division, multiplication and additions on non-negative values. For $\alpha = 1$, [9] proved the convergence of the updates into local minima for non-negative factor matrices.

2.1 Non-Negative Updates for RESCAL with Least-Squares Cost Function

The partial derivatives of (1) with respect to A and $\mathcal{R}$ respectively are

$$\begin{aligned}
\frac{\partial C_{LS}(\mathcal{X}, A, \mathcal{R})}{\partial A} =& -2\left(\sum_k X_k A R_k^T + X_k^T A R_k\right) \\
&+ 2\left(\sum_k A R_k A^T A R_k^T + A R_k^T A^T A R_k\right) + \lambda_A A \\
\frac{\partial C_{LS}(\mathcal{X}, A, \mathcal{R})}{\partial R_k} =& -2\left(A^T X_k A\right) + 2\left(A^T A R_k A^T A + \lambda_R R_k\right)
\end{aligned}$$

Inserting this into (2) we get the updates for A and R_k in matricized form

$$A \leftarrow A \bullet \frac{\sum_k X_k A R_k^T + X_k^T A R_k}{A\left(\left[\sum_k R_k A^T A R_k^T + R_k^T A^T A R_k\right] + \lambda_A \mathbf{I}\right)} \tag{3}$$

$$R_k \leftarrow R_k \bullet \frac{A^T X_k A}{A^T A R_k A^T A + \lambda_R R_k} \tag{4}$$

2.2 Kullback-Leibler-Divergence Cost Function

The generalized Kullback-Leibler-divergence cost function for RESCAL with L_1 regularization is given by

$$C_{KL}(\mathcal{X}, A, \mathcal{R}) = f_{KL}(\mathcal{X}, A, \mathcal{R}) + f_{L1}(A, \mathcal{R}) \tag{5}$$

$$\begin{aligned}
\text{with } f_{KL}(\mathcal{X}, A, \mathcal{R}) &= \sum_{ijk}\left(X_{ij} \log \frac{X_{ij}}{(A R_k A^T)_{ij}} - X_{ij} + (A R_k A^T)_{ij}\right) \\
f_{L1}(A, \mathcal{R}) &= \lambda_A \|A\|_1 + \lambda_R \sum_k \|R_k\|_1
\end{aligned}$$

The elementwise partial derivatives of (5) with respect to A and R_k respectively are

$$\frac{\partial C_{KL}(\mathcal{X},A,\mathcal{R})}{\partial A_{ia}} = -\left[\sum_{jk}\frac{X_{ijk}}{(AR_kA^T)_{ij}}(J^{ia}R_kA^T)_{ij} + \frac{X^T_{jik}}{(AR_k^TA^T)_{ji}}(AR_kJ^{ai})_{ji}\right] + \left[\sum_{jk}(J^{ia}R_kA^T)_{ij} + (AR_kJ^{ai})_{ji}\right] + \lambda_A$$

$$\frac{\partial C_{KL}(\mathcal{X},A,\mathcal{R})}{\partial R_{rtk}} = -\left[\sum_{ij}(AJ^{rtk}A^T)_{ij}\frac{X_{ijk}}{(AR_kA^T)_{ij}}\right] + \left[\sum_{ij}(AJ^{rtk}A^T)_{ij}\right] + \lambda_R$$

Inserting this into (2) we get the elementwise updates for A and R_k:

$$A_{ia} \leftarrow A_{ia}\frac{\sum_{jk}\frac{X_{ijk}}{(AR_kA^T)_{ij}}(J^{ia}R_kA^T)_{ij} + \frac{X^T_{jik}}{(AR_k^TA^T)_{ji}}(AR_kJ^{ai})_{ji}}{\left[\sum_{jk}(J^{ia}R_kA^T)_{ij} + (AR_kJ^{ai})_{ji}\right] + \lambda_A}$$

$$R_{rtk} \leftarrow R_{rtk}\frac{\sum_{ij}\frac{X_{ijk}}{(AR_kA^T)_{ij}}(AJ^{rtk}A^T)_{ij}}{\left[\sum_{ij}(AJ^{rtk}A^T)_{ij}\right] + \lambda_R}$$

In matricized form the updates are

$$A \leftarrow A \bullet \frac{\sum_k \frac{X_k}{AR_kA^T}AR_k^T + \frac{X_k^T}{AR_k^TA^T}AR_k}{\sum_k \mathbf{E}^{n\times n}(AR_k^T + AR_k) + \lambda_A\mathbf{E}^{n\times r}} \tag{6}$$

$$R_k \leftarrow R_k \bullet \frac{A^T\frac{X_k}{AR_kA^T}A}{A^T\mathbf{E}^{n\times n}A + \lambda_R\mathbf{E}^{n\times r}} \tag{7}$$

2.3 Integrating L1 Regularization with Normalization of A

[12] proposed an algorithm for sparse NMF by penalizing the right factor matrix of the decomposition by the L_1 norm while keeping the column vectors of the left factor matrix normalized to unit length ($\widetilde{W}_{ir} = \frac{W_{ir}}{\|W_r\|_F}$). Originally this algorithm was proposed for a least squares cost function but was also derived for a generalized Kullback-Leibler divergence cost function by [13]. Applying this idea to the RESCAL cost functions based on least squares and KL-divergence leads to the following updates for A and R_k, respectively:

For a least squares cost function with L_1 penalty on R:

$$C^*_{LS}(\mathcal{X},A,\mathcal{R}) = f_{LS}(\mathcal{X},\widetilde{A},\mathcal{R}) + f_{L1}(\mathcal{R}) \tag{8}$$

$$\text{with } f_{LS}(\mathcal{X},\widetilde{A},\mathcal{R}) = \sum_k \|X_k - \widetilde{A}R_k\widetilde{A}^T\|_F^2$$

$$f_{L1}(\mathcal{R}) = \lambda_R\sum_k\|R_k\|_1$$

The updates are

$$A \leftarrow \widetilde{A} \bullet \frac{\sum_k \widetilde{B}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{C}_k \bullet \widetilde{A}\right]\right)}{\sum_k \widetilde{C}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{B}_k \bullet \widetilde{A}\right]\right)} \tag{9}$$

$$R_k \leftarrow R_k \bullet \frac{\widetilde{A}^T X_k \widetilde{A}}{\widetilde{A}^T \widetilde{A} R_k \widetilde{A}^T \widetilde{A} + \lambda_R \mathbf{E}^{r\times r}} \tag{10}$$

where

$$\widetilde{B}_k = X_k \widetilde{A} R_k^T + X_k^T \widetilde{A} R_k, \qquad \widetilde{C}_k = \widetilde{A}\left(R_k \widetilde{A}^T \widetilde{A} R_k^T + R_k^T \widetilde{A}^T \widetilde{A} R_k\right)$$

For a generalized KL-divergence based cost function we get

$$C^*_{KL}(\mathcal{X}, A, \mathcal{R}) = f_{KL}(\mathcal{X}, \widetilde{A}, \mathcal{R}) + f_{L1}(\mathcal{R}) \tag{11}$$

The updates are

$$A \leftarrow \widetilde{A} \bullet \frac{\sum_k \widetilde{E}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{F}_k \bullet \widetilde{A}\right]\right)}{\sum_k \widetilde{F}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{E}_k \bullet \widetilde{A}\right]\right)} \tag{12}$$

$$R_k \leftarrow R_k \bullet \frac{\widetilde{A}^T \frac{X_k}{\widetilde{A} R_k \widetilde{A}^T} \widetilde{A}}{\widetilde{A}^T \mathbf{E}^{n\times n} \widetilde{A} + \lambda_R \mathbf{E}^{n\times r}} \tag{13}$$

where

$$\widetilde{E}_k = \frac{X_k}{\widetilde{A} R_k \widetilde{A}^T} \widetilde{A} R_k^T + \frac{X_k^T}{\widetilde{A} R_k^T \widetilde{A}^T} \widetilde{A} R_k, \qquad \widetilde{F}_k = \mathbf{E}^{n\times n} \widetilde{A}(R_k^T + R_k)$$

2.4 Integrating Entity Attributes

In [11] an algorithm for efficiently including attributes of entities was proposed. For this reason, the original cost function was extended by a decomposition of the attributes matrix D into A and V ($D \approx AV$). Additionally a regularization penalty on V was added:

$$C_{LS_{attr}} = f_{LS_{attr}}(D, A, V) + f_{L2}(V) \tag{14}$$

$$\text{with } f_{LS_{attr}}(D, A, V) = \|D - AV\|_F^2$$
$$f_{L2}(V) = \|V\|_F^2$$

The idea can be used to extend the previous update rules such that they also include the information of entity attributes. The updates for R are unchanged but the updates of A have to be modified. Update rules for V can be easily derived from [9].

Updates for LS Cost Function with L_2-Regularization

$$A \leftarrow A \bullet \frac{\left[\sum_k X_k A R_k^T + X_k^T A R_k\right] + D V^T}{A(\left[\sum_k R_k A^T A R_k^T + R_k^T A^T A R_k\right] + \lambda_A \mathbf{I} + V V^T)} \tag{15}$$

$$V \leftarrow V \bullet \frac{A^T D}{(A^T A + \lambda_V \mathbf{I}) V} \tag{16}$$

Updates for LS Cost Function with Normalization of A and L_1-Regularization on $\mathcal{R}$ and V

$$A \leftarrow \widetilde{A} \bullet \frac{\widetilde{T_1} + D V^T + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{A} V V^T \bullet \widetilde{A}\right]\right)}{\widetilde{T_2} + \widetilde{A} V V^T + \widetilde{A}\ diag\left(\mathbf{1}\left[D V^T \bullet \widetilde{A}\right]\right)} \tag{17}$$

$$V \leftarrow V \bullet \frac{A^T D}{A^T A V + \lambda_V \mathbf{E}^{r \times m}} \tag{18}$$

where

$$\widetilde{T_1} = \sum_k \widetilde{B}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{C}_k \bullet \widetilde{A}\right]\right), \quad \widetilde{T_2} = \sum_k \widetilde{C}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{B}_k \bullet \widetilde{A}\right]\right)$$

Updates for KL-divergence with L_1-Regularization

$$A \leftarrow A \bullet \frac{\left[\sum_k \frac{X_k}{A R_k A^T} A R_k^T + \frac{X_k^T}{A R_k^T A^T} A R_k\right] + \frac{D}{AV} V^T}{\left[\sum_k \mathbf{E}^{n \times n}(A R_k^T + A R_k)\right] + \lambda_A \mathbf{E}^{n \times r} + \mathbf{E}^{n \times m} V^T} \tag{19}$$

$$V \leftarrow V \bullet \frac{A^T \frac{D}{AV}}{A^T \mathbf{E}^{n \times m} + \lambda_V \mathbf{E}^{r \times m}} \tag{20}$$

Updates for KL-divergence with Normalization of A and L_1-Regularization on $\mathcal{R}$ and V

$$A \leftarrow \widetilde{A} \bullet \frac{\widetilde{T_3} + \frac{D}{\widetilde{A} V} V^T + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{A}^T \mathbf{E}^{n \times m} \bullet \widetilde{A}\right]\right)}{\widetilde{T_4} + \widetilde{A}^T \mathbf{E}^{n \times m} + \widetilde{A}\ diag\left(\mathbf{1}\left[\frac{D}{\widetilde{A} V} V^T \bullet \widetilde{A}\right]\right)} \tag{21}$$

$$V \leftarrow V \bullet \frac{\widetilde{A}^T \frac{D}{\widetilde{A} V}}{\widetilde{A}^T \mathbf{E}^{n \times m} + \lambda_V \mathbf{E}^{r \times m}} \tag{22}$$

where

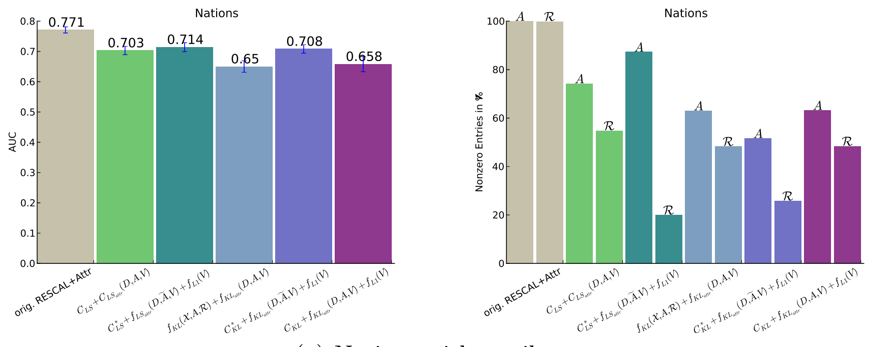
$$\widetilde{T_3} = \sum_k \widetilde{E}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{F}_k \bullet \widetilde{A}\right]\right), \quad \widetilde{T_4} = \sum_k \widetilde{F}_k + \widetilde{A}\ diag\left(\mathbf{1}\left[\widetilde{E}_k \bullet \widetilde{A}\right]\right)$$

3 Experiments

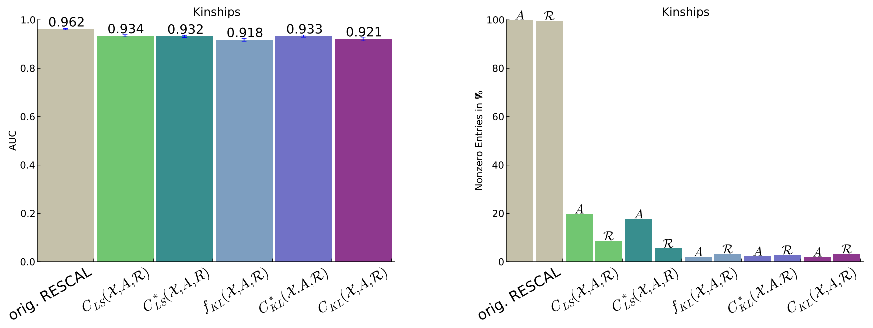
We conducted experiments on three different multi-relational datasets to evaluate the performance of the different non-negative extension of RESCAL:
Kinship $104 \times 104 \times 26$ multi-relational data that consist of several kinship relations within the Alwayarra tribe.
Nations $14 \times 14 \times 56$ multi-relational data that consist of relations between nations (treaties, immigration, etc). Additionally the dataset contains attribute information for each entity.
UMLS $135 \times 135 \times 49$ Multi-relational data that consist of biomedical relationships between categorized concepts of the Unified Medical Language System (UMLS).

To evaluate the different methods, we performed a 10-fold cross-validation and initialized the factor matrix A by using the initial factors calculated by the Non-negative Double Singular Value Decomposition method (NNDSVD) [5] for all datasets. The sets for the cross-validation were chosen by randomly selecting entries of the tensor. The results were evaluated by using the area under the precision-recall curve (AUC). To calculate the sparsity, nonzero entries were defined as entries smaller than -1.0e-9 or greater than 1.0e-9. The sparsity for each model was determined by taking the mean sparsity for A and $\mathcal{R}$ over all ten cross-validation iterations.

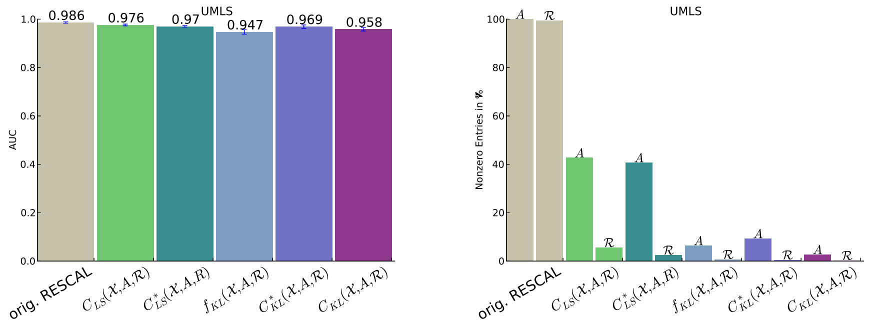
In Figure 2 the results on the three datasets, Kinships, Nations and UMLS are shown. In case of the Kinships and UMLS dataset, the non-negative realizations of RESCAL are quite close to the AUC results of the original RESCAL model (left plots). RESCAL achieves 0.962 in Kinships and 0.986 in the UMLS dataset, where the non-negative least-squares approach with L_2 regularization has an AUC of 0.934 and 0.976, respectively, closely followed by the two normalized (A) variations. In case of the Nations dataset, the difference is more severe. RESCAL achieves an AUC of 0.771, where the best non-negative model achieves only 0.714. Between the different non-negative approaches, there is not much difference in AUC. Only the update functions for the KL-divergence without regularization seem to perform a little bit worse than the other non-negative approaches. Regarding the sparsity of the factor matrix A and the core tensor $\mathcal{R}$ the difference between the non-negative decompositions and RESCAL are more significant. As expected, the decomposition of the original RESCAL algorithm is almost completely dense (density: 99.9% for A and 99.8% for $\mathcal{R}$ in all datasets). It can be seen that in the case of the non-negative decompositions, the sparsity of the factor matrix A and the core tensor $\mathcal{R}$ increases dramatically with the size of the original matrix (and the factor matrices respectively). Taking the regularized KL-divergence-based results for instance (rightmost), the density between the Nations and the UMLS dataset drops for A from 62% to 2.7% and for $\mathcal{R}$ from 48% to 0.2%. By comparing the results of the least-squares and KL-divergence based factorizations where A is kept normalized during minimization, it also seems that in the KL-divergence based cost functions, sparsity of the factors is more enforced during minimization, especially for A. When factorizing the UMLS dataset, A has a density of about 40% (about 20% in Kinships) in the



(a) Nations with attributes



(b) Kinships



(c) UMLS

Fig. 2. The plots on the left show the area under the precision-recall curve results of the different non-negative models and the original version of RESCAL on the Nations (a), Kinships (b) and UMLS (c) datasets. The plots on the rights show the amount of nonzero entries in the factor matrix A and the core tensor $\mathcal{R}$, respectively. The labels of the methods are explained in Section 2. From left to right: 1) Original version of RESCAL. 2) LS cost function with L_2-regularization on A and $\mathcal{R}$. 3) LS cost function with normalized A and L_1-regularization on $\mathcal{R}$. 4) KL-divergence cost function without regularization. 5) KL-divergence cost function with normalized A and L_1-regularization on $\mathcal{R}$. 6) KL-divergence cost function with L_1-regularization on A and $\mathcal{R}$. In case of the Nations dataset the attributes of the entities were included.

least-squares case, but at most 9% (2.5% in the Kinships) in the KL-divergence case.

4 Conclusion

We extended non-negative matrix factorization to relational learning tasks using the RESCAL model, by employing multiplicative update rules. We showed that the non-negative constraint can be introduced into the model with little loss in terms of predictive performance but with a significant gain in sparsity of the latent factor representations. Additionally we presented different update rules for the factor matrices based on least-squares or the Kullback-Leibler cost functions.

A great advantage of the multiplicative update rules is that they can exploit data sparsity in the same way as the original RESCAL updates. In practice, although, the multiplicative update rules enforcing non-negativity converge much slower than the original RESCAL updates. A more accurate analysis of this issue is planned for the near future.

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