Scalable Probabilistic Matrix Factorization with Graph-Based Priors

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Abstract

In matrix factorization, available graph side-information may not be well suited for the matrix completion problem, having edges that disagree with the latent-feature relations learnt from the incomplete data matrix. We show that removing these contested edges improves prediction accuracy and scalability. We identify the contested edges through a highly-efficient graphical lasso approximation. The identification and removal of contested edges adds no computational complexity to state-of-the-art graph-regularized matrix factorization, remaining linear with respect to the number of non-zeros. Computational load even decreases proportional to the number of edges removed. Formulating a probabilistic generative model and using expectation maximization to extend graph-regularised alternating least squares (GRALS) guarantees convergence. Rich simulated experiments illustrate the desired properties of the resulting algorithm. On real data experiments we demonstrate improved prediction accuracy with fewer graph edges (empirical evidence that graph side-information is often inaccurate). A 300 thousand dimensional graph with three million edges (Yahoo music side-information) can be analyzed in under ten minutes on a standard laptop computer demonstrating the efficiency of our graph update.

1 Introduction

Matrix factorization (MF) is popular in a number of domains including recommender systems\cite{Koren2009, Mehta2017}, bioinformatics
Brunet et al. [2004], Jacoby and Brown [2018], Stein-O’Brien et al. [2018], Zakeri et al. [2018], Zheng et al. [2013], image restoration Xue et al. [2017] and many more Davenport and Romberg [2016]. Much of the data is of a very large scale and sparse, and additional (side-)information is usually available. Therefore, many methods focus on scalability Davenport and Romberg [2016], Mnih and Salakhutdinov [2008], Sardianos et al. [2019] and the addition of side information (SI) Chiang et al. [2015, 2018], Gönen et al. [2013], Ma et al. [2011], Zakeri et al. [2018], Zhou et al. [2012], Zhao et al. [2015], and more recently scalable methods with SI Monti et al. [2017], Rao et al. [2015], Yao and Li [2018].

Empirical evidence shows that prediction accuracy is significantly improved by graph SI, where edges in the graph represent similarity between connected nodes Cai et al. [2011], Ma et al. [2011], Monti et al. [2017], Rao et al. [2015], Yao and Li [2018], Zhou et al. [2012], Zhao et al. [2015]. MF (or low-rank matrix completion) has theoretical guarantees for exact completion without and with noise Candes and Plan [2010], Candès and Recht [2009]. Introducing noisy SI is shown to reduce sample-complexity, and is reduced even further handling the noise Chiang et al. [2015]. Reduction in sample complexity through the introduction of graph SI has also been shown Ahn et al. [2018], Rao et al. [2015], as a function of graph quality. However, to the best of our knowledge there is no work on scalable methods to handle the noise in the graph SI.

Mnih and Salakhutdinov [2008] introduced probabilistic matrix factorisation (PMF), which is equivalent to $\ell_2$-regularised (alternating least squares) MF. Probabilistic interpretations for MF with graph SI are kernelized PMF (KPMF Zhou et al. [2012]) and kernelized Bayesian MF (KBMF Gönen et al. [2013]): placing priors over the columns of the latent feature matrices. This type of prior models the pairwise relation between rows, where these rows correspond to rows or columns of the incomplete data matrix. KPMF and KBMF showed good results on moderate-sized data but failed to scale to large data.

To address scalability, graph-regularised least squares (GRALS Rao et al. [2015]) was proposed, with conjugate gradient descent exploiting the sparsity in the data matrix and the graphs, resulting in linear computational complexity and fast convergence. Recently there has been progress on applying deep learning to matrix completion, with and without side information, with good accuracy and showing potential for scalability Berg et al. [2017], Hartford et al. [2018], Monti et al. [2017], Yao and Li [2018].

All of the non-Bayesian or scalable methods incorporating graph SI Cai et al. [2011], Ma et al. [2011], Monti et al. [2017], Rao et al. [2015], Zhou et al. [2012] fix the edges in the graph, considering them as true. However, these graphs are known to be uncertain Adar and Re [2007], Asthana et al. [2004], and furthermore, the similarities they represent (e.g. homophily McPherson et al. [2001]) are rarely specific to the matrix factorization task leaving no guarantee that correlations correspond Ma et al. [2011], Singla and Richardson [2008]. Graphs are often formed for other purposes, and hence their usefulness for MF is uncertain. This leaves room for improving the quality of the graph, leading to a significant reduction in sample complexity Ahn et al. [2018]. In this work we...
will introduce a solution based on contested edges, defined later in the paper.

**Example of Graph Side-Information and Contested Edges** To better understand how graph similarities are not task-specific (are non-specific) to MF, take a common example of a movie-recommendation problem with social network (SN) SI (Ma et al. 2011 and in our experiments on Douban data). Connected users in the SN do not connect based on their similar preference of movies, instead they connect on the basis of a broader social context. Similarly, the demographic information in MovieLens\(^1\) used to form a user-similarity graph, is only very indirectly related to the movie preferences [McPherson et al. 2001]. Nevertheless, more general similarity has been shown to often work well in practice, but some parts of it may turn out to be detrimental as we illustrate below.

Figure 1 (top) shows a small movie-recommendation data matrix with SN SI (bottom-left). Without SI, if row/column observations in the data matrix are similar, latent features will be similar. This can be inaccurate, e.g. users 2 and 3 would be considered similar based on the observations, and thus predictions for user 2 would be similar to ratings of user 3, whereas actually user 2 is similar to user 1. Graph information can help by encouraging latent features of connected users, like user 1 and user 2 here, to be similar, even when there is no observed data in the matrix to indicate they should be. However, for other users such as 4 and 5 the graph may mismatch with the data, indicating similarity whereas 4 and 5 are actually negatively correlated (as seen in their ratings of movies 5 and 6), and using the graph would thus worsen their predictions. We propose using this discrepancy to contest the graph edge between users 4 and 5; removing this edge as in Figure 1 (bottom-right) would improve predictions for users 4 and 5 to be consistent with their observed negative correlation, while the beneficial edge between users 1 and 2 will still remain. In real cases, mismatch between the data matrix and the SI would be detected based on much more data than in this illustration.

We do not propose to identify contested edges directly from the observed data but from correlations between the latent features. We introduce a probabilistic generative model that we call graph-based prior PMF (GPMF). Using the expectation-maximization (EM, Bishop 2006) algorithm we find a maximum a posteriori (MAP) estimate for the latent features and a maximum likelihood estimate (MLE) for the correlations of the latent features. We show in Section 3.3 how using GLASSO approximation we can remove contested edges by simply thresholding a constrained sample covariance matrix (SCM).

There exist a number of approaches to reduce the edges in a labelled graph, graph summarization, Liu et al. 2018 for example. Most of these approaches do not use node attributes (labels) and to the best of our knowledge none use latent features for edge pruning. There are link prediction models that are probabilistic and use node attributes Haghani and Keyvanpour 2017 but none of them can (yet) scale to large data [Li et al. 2014, Nguyen and Mamitsuka 2012, Zhao]...
Figure 1: An illustrative movie recommendation problem. Left: data matrix where entries are user-ratings for movies: observations in black, unseen entries are blank and unseen entries to be predicted are in grey. Middle: Social Network SI; connected users assumed to have similar ratings. The edge shown in red is contested due to negative correlation of $u_4$ and $u_5$ in the data matrix. Right: a graph update with removal of the contested edge to improve prediction accuracy.

This paper introduces GPMF: the generative model in Section 2, the scalable constrained EM algorithm in Section 3, experiments in Section 4 and a conclusion in Section 5.

## 2 GPMF Generative Model and Relations to the Graph Side-Information

We are provided with a partially observed data matrix $R$ with $N$ rows and $M$ columns. $R$ is approximated as the product of two low-rank matrices, $U$ and $V$. The number of latent features $D$ is fixed; $U$ and $V$ have $D$ columns, each row is a latent feature vector for each row / column of $R$ respectively. We use an index set $\Omega$ where $\Omega_{ij}$ is one if the element in row $i$ and column $j$ of $R$ is observed, and zero otherwise. The goal is to learn latent-feature matrices $U$ and $V$ that most accurately represent the full matrix $R$.

$\ell_2$-regularized MF has a scalable probabilistic interpretation: PMF. Each observed entry $R_{ij} : (i, j) \in \{\Omega = 1\}$ is assumed to have Gaussian noise $\sigma^2$; each row of $U$ and $V$ has a zero-mean spherical Gaussian prior. Similar to KPMF Zhou et al. [2012], our model replaces the spherical Gaussian prior with a full-covariance Gaussian over the columns of the latent features.
row-wise dependencies):

\[
p(R \mid U, V, \sigma^2) = \prod_{i=1}^{N} \prod_{j=1}^{M} N(R_{ij} \mid U_i V_j^\top, \sigma^2 \Omega_{ij})
\]

\[
p(U \mid \Lambda_U) = \prod_{d=1}^{D} N(U_d \mid 0, \Lambda_U^{-1})
\]

\[
p(V \mid \Lambda_V) = \prod_{d=1}^{D} N(V_d \mid 0, \Lambda_V^{-1})
\]

Graph SI constrains the structure of the precision matrices (\(\Lambda_U\) or \(\Lambda_V\)) of (2) and (3), discussed next.

### 2.1 Gaussian Markov Random Field (GMRF) relation to Precision matrix

An undirected graph \(G_Z = (V_Z, \mathcal{E}_Z)\) with a set of nodes \(V_Z\), representing a set of random variables \(\{Z_i\}_{i=1}^{P}\), and a set of edges \(\mathcal{E}_Z \subseteq \{(i, j) \mid i, j \in V_Z\}\), defines the conditional independence of the random variables, where the absence of an edge \((i, j) \notin \mathcal{E}_Z\) implies that the two random variables are conditionally independent \([\Lambda_Z]_{ij} = 0\) given the remaining random variables Bishop [2006], Hastie et al. [2009], Lauritzen [1996], Rue and Held [2005]: \(Z_i \perp Z_j \mid \{Z_k : k \in (1, ..., N) \setminus (i, j)\}\). In the remainder of the paper we refer to the adjacency matrix of \(G_Z\): a symmetric matrix where \([A_Z]_{ij} = 1\) if an edge exists between nodes \(i\) and \(j\) and zero otherwise. We can summarize the GMRF relation as \([A_Z]_{ij} = 0 \iff [\Lambda_Z]_{ij} = 0 \mid i \neq j\).

### 2.2 Laplacian Matrix relation to Precision Matrix

The Laplacian matrix of a graph is \(L_Z = D - A_Z\), where \(D_{i,i} = \sum_{j=1}^{N} [A_Z]_{ij}\) is a diagonal degree matrix, and is positive-semi-definite by definition. The regularised Laplacian \(L_Z^+ = L_Z + \gamma I\), \(\gamma > 0\) is a positive-definite matrix; a valid precision matrix retaining the GMRF property Dong et al. [2016], Egilmez et al. [2016, 2017], Hastie et al. [2009], Liu et al. [2014]: \([L_Z^+]_{ij} = 0 \iff [\Lambda_Z]_{ij} = 0 \mid i \neq j\).

**Lemma 1.** If the precision matrix in (2) and (3) is the regularised Laplacian matrix \(L_U^+, L_V^+\), then the MAP estimator of our model has the same objective function as GRALS Rao et al. [2015]. Our GPMF model therefore gives a generalization of the GRALS objective function.

**Proof of Lemma 1.** Our generative model is biconvex, and hence it suffices to prove for \(U\) that the posterior is equivalent to the GRALS objective. Holding
fixed and finding the log posterior of $U$:

$$\ln p(U|R, \sigma^2, V, \Lambda_U) \propto \ln p(R|U, V, \sigma^2)p(U|\Lambda_U)$$

$$\propto -\frac{1}{\sigma^2} \sum_{i=1}^{N} \sum_{j=1}^{M} p_{ij} (R_{ij} - U_i:V_j)^2 - \frac{1}{2} \sum_{d=1}^{D} U_d^T \Lambda_U U_d$$

$$= -\frac{1}{2} \| \Lambda_U (R - UV^T) \|^2_F - \frac{\sigma^2}{2} \text{tr}(U^T \Lambda_U U)$$,

where $U_i$ is row $i$ of matrix $U$ and $U:d$ is column $d$ and noting that $\sum_{i,j} U^2_{ij} = \text{tr}(U^T U) = \| U \|^2_F$. Equation (4) is the GRALS objective function [Rao et al. 2015]. Derivations in the supplementary material.

3 GRAEM: Scalable EM for GPMF

We naturally extend each least-squares sub-problem of GRALS [Rao et al. 2015] with graph-regularised alternating EM (GRAEM), having the same global convergence guarantees as GRALS [Xu and Yin 2013]. We work through optimising $U$ with $V$ fixed, solving for $V$ has the same form.

3.1 The EM Formulation

We have an incomplete data matrix $R$, fixed matrix $V$, latent variable matrix $U$, and graph $\mathcal{G}$. From the graph we derive $L_U$ (see Section 2.2), then set the precision matrix $\Lambda_U = L_U^+$, which we consider our model parameters. We want to maximize the expectation of the joint density of the data and the latent variables, with $U$ as our unknowns and $\Lambda_U$ as our input parameters:

$$Q(\Lambda_U, \Lambda_U^{\text{old}}) = \int_U p(U|R, \Lambda_U^{\text{old}}) \ln p(R|U, \Lambda_U) \, dU$$

$$= \mathbb{E}_{p(U|R, \Lambda_U^{\text{old}})} [ \ln p(R|U, \Lambda_U) ] .$$

3.2 E-step: Expected Value of the Latent Variables

The expected value of our latent variables has a Gaussian posterior distribution (see supplementary material), we can therefore use the MAP, which is equivalent to the GRALS objective function as shown in Lemma [1] $\mathbb{E}_{p(U|R, \Lambda_U^{\text{old}})} [ \ln p(R|U, \Lambda_U) ] = \mu_U^{\text{post.}} \approx \mu_U^{MAP}$.

3.3 M-step: Removing Contested Edges

We can remove edges in the graph that correspond to negative correlations between the latent features by simply removing negative covariances from an SCM; this relationship holds for large scale and sparse problems; details follow.
3.3.1 The MLE of the parameters and GLASSO

To find the MLE we maximise the $Q$ function in Equation (5) with respect to $\Lambda_U$. The maximum can be found in closed form by taking the derivative with respect to the parameter $\Lambda_U$ and setting to zero:

$$\arg\max_{\Lambda_U} Q(\Lambda_U, \Lambda_U^{\text{old}}) = \left(\mathbb{E}_{p(U|R, \Lambda_U^{\text{old}})} \left[\frac{1}{D} \sum_{d=1}^{D} U_{:d} U_{:d}^\top \right]\right)^{-1} = \left(\mathbb{E} \left[S_U^U\right]\right)^{-1} = \Lambda^*_U.$$  

(6)

Equation (6) is the inverse of an SCM, where each sample is one of the columns of $U$. Values for $U$ are unknown, so we use the MAP given the previous estimate of the parameters ($\Lambda_U^{\text{old}}$). The solution (if any) is almost surely not sparse. Graphical lasso (GLASSO Mazumder and Hastie [2012]) finds a sparse solution for the MLE of the precision matrix, where samples are assumed to be normally distributed, in line with our model assumptions in Section 2. We therefore propose solving (6) with GLASSO.

3.3.2 Constrained GLASSO and Highly Efficient Approximation

GLASSO finds the MLE of the precision matrix under an $\ell_1$ penalty, given an SCM $S$. Grechkin et al. [2015] showed that the problem space can be reduced with prior knowledge on which pairwise relationships do not exist, forcing them to be zero in the solution:

$$\min_{\Lambda_U \succeq 0} \ tr(S\Lambda_U) - \log |\Lambda_U| + \tau \|\Lambda_U\|_1,$$

subject to $[\Lambda_U]_{ij} = 0, [\Lambda_U^0]_{ij} = 0$.  

(7)

Zhang et al. [2018] uses a relation between the sparsity structure of the $\tau$-thresholded SCM and the GLASSO solution; for large-scale problems, when the solution is very sparse, the connected components are equivalent Mazumder and Hastie [2012], given further assumptions the complete sparsity structure is equivalent Fattahi and Sojoudi [2019], Sojoudi [2016a,b]. However, this solution will locate correlations, positive and negative, with a strong magnitude, greater than $\tau$. Next we detail how to identify edges that correspond to only negative correlations.

3.3.3 Removing a Contested Edge

The sparsity structure of the SCM and the (GLASSO) solution are equivalent under mild assumptions that are found to be true for sufficiently large $\tau$, that result in $\approx 10^N$ non-zeros in the solution Fattahi and Sojoudi [2017] 2019. One of these assumptions is sign-consistency where each non-zero element of the solution has the opposite sign in the SCM. Assuming sign-consistency we can
identify all graph edges that correspond to negative correlations in the latent features, with $\mathbb{E}[\mathbf{S}_U^D]$ from Equation (6) as our SCM:

$$[A_{U}^{\text{new}}]_{ij} = \begin{cases}  
1, & \mathbb{E}\left[\mathbf{S}_U^D\right]_{ij} \geq \tau \\
0, & \mathbb{E}\left[\mathbf{S}_U^D\right]_{ij} < \tau, \ CE \\
0, & \text{otherwise,} \end{cases}$$

(8)

where $A_{U}^{\text{new}}$ is the updated adjacency matrix, the threshold parameter $\tau$ is set to zero (or can be increased for a sparser solution) and $A_{U}^U$ is the adjacency matrix of the graph SI; CE is a contested edge and con-E is a constrained edge. To solve Equation (8) we need to compute $\mathbb{E}[\mathbf{S}_U^D]$, we can decompose the problem:

$$\mathbb{E}[\mathbf{S}_U^D] = \frac{1}{D} \sum_{d=1}^{D} \mathbb{E}\left[\mathbf{U}_{:d}\mathbf{U}_{:d}^T\right]$$

$$\mathbb{E}\left[\mathbf{U}_{:d}\mathbf{U}_{:d}^T\right] = \text{Cov}[\mathbf{U}_{:d}] + \mathbb{E}[\mathbf{U}_{:d}][\mathbf{U}_{:d}^T]$$

$$= \Sigma_{U,d}^{\text{post.}} + [\mu_{U,d}^{\text{post.}}][\mu_{U,d}^{\text{post.}}]^T.$$

The remaining task is to efficiently approximate the posterior covariance $\Sigma_{U,d}^{\text{post.}}$ for each column, $d$, of $\mathbf{U}$, which we discuss next.

### 3.3.4 Posterior Covariance Approximation

The posterior of our GPMF model, in Section 2, is a joint Gaussian distribution, where the likelihood in Equation (1) introduces relations between the columns of the latent features and the prior in Equation (2) introduces relations between the rows. This results in a posterior covariance matrix with an inverse Kronecker sum structure Kalaitzis et al. [2013], Schacke [2004]: $\Sigma_{U}^{\text{post.}} = (I_D \otimes \Lambda_U + \alpha \mathbf{C})^{-1}$ where $\otimes$ is the Kronecker product operator and

$$\mathbf{C} = [c(d,d')]_{d,d'=1}^D,$$

$$c(d,d') = \text{diag}\left(\sum_{j=1}^{M} \Omega_{ij} \mathbf{V}_{jd} \mathbf{V}_{jd'}\right)_{i=1}^N.$$  

**Column-wise independence assumption.** We simplify the Kronecker sum with a column-wise independence assumption, setting all off-diagonals of $\mathbf{C}$ to
\[a^{\text{post.}} \approx I_D \otimes a_U + \alpha \text{ diag} (C)\]
\[= \text{blkdiag} \left( \left\{ a^{\text{post.}}_{U,d} \right\}_{d=1}^{D} \right),\]
\[a^{\text{post.}}_{U,d} = a_U + \alpha \text{ diag} (C_d),\]
\[\text{diag} (C_d) = \text{diag} \left( \sum_{j=1}^{M} \Omega_{i,j} V_{j,d}^2 \right) \left( \sum_{i=1}^{N} \right),\]

where \(\alpha = [\sigma^2]^{-1}\) is the inverse of the observation noise in (1), \text{diag} takes a vector to create a diagonal matrix and \text{blkdiag} takes a sequence of matrices to construct a block-diagonal matrix.

Sparse Cholesky factorisation: Each \(\hat{a}^{\text{post.}}_{U,d}\) is still too large to invert. Assuming the high-dimensional matrix is sparse, as in [Zhang et al., 2018], its Cholesky factorisation is computable in \(O(N)\) time [Davis et al., 2004]. We compute \(K\) samples as an unbiased estimate for the approximate posterior covariance:

\[\hat{\Sigma}^{\text{post.}}_{U,d} = \left[ a^{\text{post.}}_{U,d} \right]^{-1} \approx \frac{1}{K} \sum_{k=1}^{K} x_k x_k^\top\]
\[x_k \sim \mathcal{N} \left( 0, \left[ a^{\text{post.}}_{U,d} \right]^{-1} \right).\]

3.4 The Algorithm

The EM algorithm iterates between E-step and M-step until convergence. We initialize the latent feature matrices \((U, V)\) by finding the MAP with no graph SI using PMF, to learn latent features that reflect the observed entries of the data matrix. In practise any method to learn the latent features with no SI can be used. The M step uses the relations between the latent features to identify negative correlations and remove them from the graph SI. The E-step then finds the MAP of the latent features given the updated graph. In theory the E and M step could be continued until some convergence criterion was met, but this would be less efficient and we get good results with just one step. So the three steps of our algorithm are lines 1, 3 and 4:

3.5 Scalability: Computational Complexity

The algorithm has three steps: lines 1,3,4 in Algorithm 1. Line 1 is linear in the number of non-zero \(\text{nz}\) in the data matrix \(O(nz(\Omega))\) per conjugate gradient (CG) iteration. Line 3 comprises sparse Cholesky factorisation, linear in time
with respect to the dimension size $O(N + M)$, constrained SCM computation and thresholding, $O(nz(A_U) + nz(A_V))$ both converge in one time step. Line 4 uses GRALS with the sparsified graphs: $O(nz(\Omega) + nz(A_U^+ + nz(A_V^+))$ per CG iteration. Line 4 is initialised with $U, V$ values from the PMF run, largely reducing the number of iterations required. Our algorithm remains linear with respect to the number of non-zeros. The additional M-step is a trivial additional cost, and if $A_U^+, A_V^+$ are much sparser, reducing iteration costs in Line 3, the overall computational load can be less than GRALS using the original graphs.

4 Experiments

We compare our algorithm to a baseline with no graph SI (PMF, Mnih and Salakhutdinov [2008]), the current most scalable method, GRALS Rao et al. [2015], and for accuracy less scalable methods KPMF Zhou et al. [2012] and sRMGCNN Monti et al. [2017]. For sRMGCNN we used their published code, ran it on a (NVIDIA Tesla P100) GPU and used cross validation to find a
Algorithm 1 Graph-regularised alternating EM (GRAEM)

Input: $A^0_U, A^0_V$
Output: $U, V, A^+_U, A^+_V$
1: $U^0, V^0 \leftarrow$ Initialise with PMF (GRALS with no graphs)
2: while not converged do
3: $A^t_U, A^t_V \leftarrow$ Run M-step Equation (8) with $U^{t-1}, V^{t-1}$ and $A^0_U, A^0_V$ as structural constraints
4: $U^t, V^t \leftarrow$ Run E-step with regularized Laplacians given $A^t_U, A^t_V$
5: end while

good T value; note that this model took several orders of magnitude more time than the other methods: on Flixster data GPMF and GRALS converged in 20 seconds, PMF in 0.2 seconds, sRMGCNN took 30 minutes. We also ran KBMF Gönen et al. [2013] but with an extremely long computational time on even the smallest dataset, and a large number of parameters, we failed to achieve reasonable results.

4.1 Experiments on Synthetic Data

To analyze the behaviour of our algorithm we generate a data matrix with a known underlying graph. Therefore we can replace true edges in the graph with corrupted edges (CEs) that contest the true underlying structure, controlling the accuracy of the graph SI. We use a block-diagonal regularised-Laplacian precision matrix. We generate a $400 \times 400$ data matrix by Equations (1)-(3), with proportion of corrupted edges 0.3, observation noise 0.01, 7% observed values, and 40 latent dimensions; we vary these settings in the experiments below. See supplementary material for further details.

Graph Fidelity. In Figure 2 (a) we vary the number of CEs. A graph with no CEs has fidelity one ($F = 1$), with all CEs $F = 0$. GPMF consistently improves prediction accuracy over methods with graph SI for $F > 0$, and performance is equal for $F = 0$. PMF with no graph performs better below $F = 0.3$, showing that a graph of low quality can make prediction accuracy worse.

Observation Noise. Figure 2 (b) shows the benefit of GPMF diminishes as noise increases; learning negative correlations requires learning from the observations. However, at worst GPMF is only as bad as using the original corrupted graph.

Proportion of Observations. In Figure 2 (c) with just 10% of observed entries our algorithm can almost attain the same prediction accuracy as using the true graph. GRALS requires 30% to achieve a similar accuracy. At 40% of observed entries the graph is no longer beneficial. Note that most large scale matrix completion problems have fewer than 10% observed entries.

Model Capacity. Figure 2 (d) shows that with too few latent features all models are negatively effected, but overall GPMF attains the best prediction
accuracy.

GLASSO accuracy We analyse the accuracy of removing CEs over several simulations. With 7% of observed entries, 31.7% of CEs are correctly removed and 19% of true edges (TEs) are wrongly removed; increasing observed entries to 40%, 44.3% of CEs are removed and 0.3% of TEs. Fixing observed entries at 20%, with noise $\sigma^2 = 0.01$, 39% of CEs and 2.7% of TEs are removed, and with $\sigma^2 = 1$, 34.3% CEs and 42.7% TEs are removed. We see clearly that observation noise strongly effects the ability to identify contested edges, as shown in Figure 2 (b). Accuracy improves with more observed entries, but even with low levels of noise and a reasonable amount of observations successful removal of CEs is only moderate. Regardless of this moderate accuracy, experiments show this is enough to attain significant improvements in prediciton accuracy.

4.2 Experiments on Real Data

In Table 1 GPMF using GRAEM (our method) gives improved accuracy over GRALS on all small datasets: 3000 (3k) by 3k subsets of Flixter and Douban (Monti et al. 2017) (full datasets not attainable) and MovieLens100k (Harper and Konstan 2015)); the bottom rows of the table show the size and number of observations for each data matrix and the number of edges in each side-information graph. In Figure 3 our method is shown to add no computational cost on large data: MovieLens 20 million (Harper and Konstan 2015), Epinions (Tang et al. 2012) and Yahoo Music (Rao et al. 2015, Dror et al. 2011), note that proportion of edges used by GPMF is reported in figure title. Figure 3 (a) is an example of poor quality graph side-information, we see this as PMF outperforms GRALS with the side-information; our method (GPMF using GRAEM) estimates over half the edges as contested, removing them seem to improve the quality.
We believe that there were no gains in Figure 3 (b) as the graph is extremely sparse and removing some edges has little effect. We test this hypothesis with MovieLens 20M in Table 1 by increasing the number of nearest neighbours from 10 to 40, we see that GRALS with the original graph decreases in performance while our algorithm continues to improve, we plot the best results in Figure 3 (c); the computational time to estimate contested edges (between the two vertical broken lines) is a fraction of the running time of the algorithm.

We also tested general usefulness of the updated graph: We get a small improvement for Douban with KPMF using with 77 % of edges, we also get the same accuracy for Flixster with almost half the edges.

Table 1: Result summary on real datasets (RMSE), $A^+$ is the graph updated with GRAEM (our method). Bold = best result.

| Algo.            | Flixster (3k) | Douban (3k) | MovieLens 100k | Epinions | Yahoo Music | MovieLens 20M (10-20-/40-NN) |
|------------------|---------------|-------------|-----------------|----------|-------------|-----------------------------|
| PMF              | 0.9809        | 0.7492      | 0.9728          | 0.31     | 22.991      | 0.7980 / 0.7980 / 0.7980    |
| GRALS            | 0.9152        | 0.7504      | 0.9178          | 0.32     | 22.760      | 0.7898 / 0.7925 / 0.7922    |
| GPMF / GRAEM (ours) | **0.8857**    | 0.7497      | **0.9174**      | **0.28** | **22.795**  | 0.7894 / 0.7895 / **0.7887** |
| KPMF             | 0.9212        | 0.7324      | 0.9336          | -        | -           | -                           |
| KPMF ($A^+$)     | 0.9212        | **0.7323**  | 0.9374          | -        | -           | -                           |
| sRMGCNN          | 0.9108        | 0.7915      | 0.9263          | -        | -           | -                           |

| Data dims.       | 3k x 3k       | 3k x 3k     | 1k x 1.5k       | 22k x 296k | 250k x 300k | 138k x 27k                 |
|------------------|---------------|-------------|-----------------|------------|-------------|-----------------------------|
| Num. of obs.     | 2.6k          | 137k        | 100k            | 824k       | 6M          | 138k x 27k                 |
| Edges ($A_U/A_V$)| 59k / 51k     | 2.7k / 0    | 12.6k / 29k     | 574k / 0   | 0 / 3M      | 0 / 493k - 0 / 963k - 0 / 1.9M |
| Prop. ($A_U/A_V$)| 0.57 / 0.63   | 0.77 / 0    | 0.63 / 0.61     | 0.45 / 0   | 0 / 0.8     | 0 / 0.88 - 0 / 0.71 - 0 / 0.65 |

5 Conclusion

We present a highly efficient method to improve the quality of graph side-information for matrix factorisation. Of the three steps in the algorithm, the initialisation of the latent features and the estimation of the latent features with the updated graph (the E-step) can be performed with any method for matrix completion without SI and with graph SI respectively. With such a small computational cost a graph update (the M-step) to improve quality seems like a valuable step when including graph side-information into matrix factorisation. Furthermore, we demonstrated the added robustness using our algorithm on real graph side-information. By increasing the number of nearest neighbours for generating graphs from feature side-information our algorithm, GRAEM, improved while GRALS worsened. Our graph update step allows for more noisy graphs to improve the matrix completion accuracy.

Future work on improving the graph update could further improve this method; we showed with simulated data the GLASSO approximation is only moderately successful.
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7 Appendix

A Posterior of GPMF model

We derive the posterior of $U$, fixing $V$, given the data $\{R, \Omega\}$ and parameters $\Lambda_U$ for the Graph-based prior probabilistic matrix factoriation (GPMF) model. The posterior for $V$ follows the same steps with $U$ fixed. We start by breaking down the likelihood and prior into scalar operations:

$$
\log p(R \mid U, V, \alpha, \Lambda_U) \propto - \sum_{i=1}^{N} \sum_{j=1}^{M} \Omega_{ij} \left[ \frac{\alpha}{2} \left( R_{ij} - U_i V_j^\top \right)^2 \right] - \sum_{d=1}^{D} \frac{1}{2} U_{id} \Lambda_U U_{id} \quad (10)
$$

$$
= - \frac{\alpha}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} \Omega_{ij} \left[ \left( R_{ij}^2 - 2 R_{ij} \sum_{d=1}^{D} U_{id} V_{jd} + \sum_{d=1}^{D} \sum_{d'=1}^{D} V_{jd} U_{id} V_{jd'} \right) \right] \quad (11)
$$

$$
- \frac{1}{2} \sum_{d=1}^{D} \sum_{i=1}^{N} \sum_{i'=1}^{N} U_{id} \Lambda_{ii'} U_{i'd} \quad (12)
$$

$$
= - \frac{\alpha}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} \Omega_{ij} R_{ij}^2 - \frac{1}{2} \sum_{i=1}^{N} \left( \alpha \sum_{j=1}^{M} \Omega_{ij} \sum_{d=1}^{D} \sum_{d'=1}^{D} V_{jd} U_{id} V_{jd'} \right) \quad (13)
$$

$$
- 2 U_{id} V_{jd} R_{ij} + \sum_{d=1}^{D} \sum_{i'=1}^{N} U_{id} \Lambda_{ii'} U_{i'd} \quad (14)
$$

Using the scalar expansion we recombine to form the full posterior in scalar form in Equation (20), with respect to the vectorization of $U$ Equation (22) and w.r.t.
the vectorization of $U^\top$.

The vectorization of Equation (23):

$$
\log p(U \mid R, \alpha, V, \Lambda_U)
\propto -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{d=1}^{D} \left( \alpha \Omega_{ij} \left[ \sum_{d'=1}^{D} V_{jd} U_{id} V_{jd'} - 2 U_{id} V_{jd} R_{ij} \right] + \sum_{i'=1}^{N} [\Lambda_U]_{ii'} U_{i'd} \right)
$$

(17)

$$
= -\frac{1}{2} \sum_{i=1}^{N} \sum_{d=1}^{D} U_{id} \left( \alpha \sum_{j=1}^{M} \Omega_{ij} \left[ \sum_{d'=1}^{D} V_{jd} U_{id} V_{jd'} - 2 V_{jd} R_{ij} \right] + \sum_{i'=1}^{N} [\Lambda_U]_{ii'} U_{i'd} \right)
$$

(18)

$$
= -\frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} \sum_{d=1}^{D} \sum_{d'=1}^{D} \left[ U_{id} \left( \alpha \sum_{j=1}^{M} \Omega_{ij} \left[ \sum_{d'=1}^{D} V_{jd} V_{jd'} - 2 V_{jd} R_{ij} \right] + \sum_{i'=1}^{N} [\Lambda_U]_{ii'} \right) U_{i'd'} \right]
$$

(19)

$$
= -\frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} \sum_{d=1}^{D} \sum_{d'=1}^{D} \left( -2 \alpha U_{id} V_{jd} R_{ij} \right)
$$

(20)

$$
= -\frac{1}{2} \text{vec}(U^\top) \left( I_D \otimes \Lambda_U + \alpha C \right) \text{vec}(U) - 2 \alpha \text{Tr}(U^\top R V)
$$

(21)

$$
= -\frac{1}{2} \text{vec}(U^\top)^\top \left( \Lambda_U \otimes I_D + \alpha \text{blkdiag} \left( \{B_i\}_{i=1}^{N} \right) \right) \text{vec}(U^\top) - 2 \alpha \text{Tr}(U V^\top R^\top),
$$

(22)

where $[i = j]$ is Iverson bracket notation where the value is one if the proposition is satisfied and zero otherwise, $\otimes$ is the Kronecker product, vec$(X)$ stacks the columns of matrix $X$ to produce a vector, Tr$(X)$ is the trace of matrix $X$ and finally $I_N$ is an $N \times N$ identity matrix and:

$$
C = \begin{bmatrix}
  c(1,1) & c(1,2) & \cdots & c(1,D) \\
  c(2,1) & c(2,2) & \cdots & c(2,D) \\
  \vdots & \vdots & \ddots & \vdots \\
  c(D,1) & c(D,2) & \cdots & c(D,D)
\end{bmatrix}
$$

(24)

$$
c(d,d') = \text{diag} \left( \left\{ \sum_{j=1}^{M} \Omega_{ij} V_{jd} V_{jd'} \right\}_{i=1}^{N} \right)
$$

(25)

$$
B_i = \sum_{\{j:(i,j)\} \in \{\Omega = 1\}} V_{j}^\top V_{j}:
$$

(26)

Notice that in the posterior when stacking the columns vec$(U)$ in Equation (22) the prior precision matrix is a block diagonal matrix and the evidence matrix is a partitioned matrix with each block being diagonal, when stacking the rows vec$(U^\top)$ the structural pattern is the other way around: the prior is a partitioned matrix of diagonal blocks and the evidence matrix is a block diagonal matrix. It is worth noting that Equation (22) and Equation (23) both have the structure of a Kronecker sum, $A \oplus D = A \otimes I + I \otimes D$. We look more closely at Equation (23).
showing the relation with the scalar summations and the final notation in more detail. Firstly the linear term:

\[-2\alpha \sum_{i=1}^{N} \sum_{d=1}^{D} U_{id} \sum_{j=1}^{M} \Omega_{ij} V_{jd} R_{ij} = -2\alpha \sum_{i=1}^{N} \sum_{d=1}^{D} U_{id} \sum_{j=1}^{M} V_{jd} R_{ij} \]

\[
= -2\alpha \sum_{d=1}^{D} U_{d}^{T} R V_{d} 
\]

\[
= -2\alpha \text{vec}(U)^{T} \text{vec}(RV) 
\]

\[
= -2\alpha \text{Tr}(U^{T}RV) 
\]

\[
= -2\alpha \sum_{i=1}^{N} U_{i} V^{T} [R_{i}]^{T} 
\]

\[
= -2\alpha \text{vec}(U^{T})^{T} \text{vec}(V^{T}R^{T}) 
\]

\[
= -2\alpha \text{Tr}(UV^{T}R^{T}),
\]

and the quadratic term:

\[
\sum_{i=1}^{N} \sum_{i'=1}^{N} \sum_{d=1}^{D} \sum_{d'=1}^{D} U_{id} \sum_{j=1}^{M} [i'=i] [V_{jd} V_{jd'}] U_{i'd'} = \text{vec}(U)^{T} \left[ \sum_{j=1}^{M} V_{j} V_{j}^{T} \otimes I_{N} \right] \text{vec}(U) 
\]

\[
= \text{vec}(U)^{T} \left[ \text{diag} \left\{ \sum_{j=1}^{M} V_{j} V_{j}^{T} \right\} \right] \text{vec}(U) 
\]

\[
\sum_{i=1}^{N} \sum_{i'=1}^{N} \sum_{d=1}^{D} \sum_{d'=1}^{D} U_{id} [d = d'] [A_{i}]_{ii'} U_{i'd'} = \text{vec}(U)^{T} [A_{U} \otimes I_{D}] \text{vec}(U) 
\]

\[
= \text{vec}(U)^{T} [I_{D} \otimes A_{U}] \text{vec}(U^{T}) .
\]

Having organized the posterior, with respect to $U$, into a quadratic and a linear term we can complete the square to find the mean $\mu_{U}^{(n)}$ and precision matrix $\Lambda_{U}^{(n)}$ of the conditional posterior distribution for the matrix $U$:

\[
\Lambda_{U}^{(n)} = [A_{U} \otimes I_{D}] + \alpha \text{blkdiag} \left( \{ B_{i} \}_{i=1}^{N} \right) 
\]

\[
\mu_{U}^{(n)} = [\Lambda_{U}^{(n)}]^{-1} \text{vec}(V^{T}R^{T}) 
\]

or the mean and covariance can be represented as different formulations with scalar sums [21], or vectorization of the matrix without transposing [22].
B Experiments: further details

We compare our GPMF method to GRALS\textsuperscript{2} [Rao et al. 2015], PMF (GRALS with no graph side-information) [Mnih and Salakhutdinov 2008], KPMF\textsuperscript{3} [Zhou et al. 2012] and sRMGCNN\textsuperscript{4} [Monti et al. 2017]. KPMF uses the regularised Laplacian graph kernel. We also tested KBMF\textsuperscript{5} [Gonen et al. 2013], but with many tuning parameters and a slow learning speed, making parameter tuning costly and complex, making a similar effort as made for tuning the other algorithms we were not able to attain good results. GRALS, PMF, GPMF (GRAEM, our method), KPMF and KBMF experiments were run on a regular laptop computer: Hewlett Packard EliteBook 840 G3 notebook with Intel Core i5 and 16 GiB memory. sRMGCNN was run on a GPU (NVIDIA Tesla P100, running on a 2x12 core Xeon Dell PowerEdge C4130). For model learning and evaluation we use the same training and validation set for all models. We use the same systematic search procedure (similar effort for tuning) for each model for a fair comparison.

B.1 Synthetic Data

Default settings for the experiments, if no other details are mentioned, are a 400 × 400 data matrix with 7 percent observed values, a graph fidelity of 0.7, observation noise \(\sigma^2 = 0.01\), 40 latent feature dimensions and noise between similar latent features 0.0001. We use the graphs to create the latent feature matrices \(U\) and \(V\) according to the GPMF model. Sampling of observed entries for training and validation is according to a non-uniform distribution; to avoid rows and columns having similar numbers of observations, we use a multinomial distribution with Dirichlet prior). Each experiment setting is run five times for each model and an average is reported with the standard deviation as the height of the error bar.

B.2 Real data experiments

**Flixster (3k).** A three thousand dimensional subset matrix from the original Flixster dataset\textsuperscript{6} as in Monti et al. [2017]. Where graph side information is constructed from the scores of the original matrix: \(G_U\) with 59354 edges and \(G_V\) 50918 edges.

**Douban (3k).** A three thousand dimensional subset matrix from the original Douban dataset\textsuperscript{7} as in Monti et al. [2017]. Where user graph side-information is a social network with 2688 edges.

\footnote{GRALS code: https://github.com/rofuyu/exp-grmf-nips15}
\footnote{KPMF code: https://people.eecs.berkeley.edu/~tinghuiz/}
\footnote{Recurrent Multi-Graph Neural Networks code: https://github.com/fmonti/mgc}
\footnote{Software: https://github.com/mehmetgonen/kbfm}
\footnote{https://github.com/fmonti/mgcnn}
\footnote{See footnote 1}
**MovieLens 100k and 20M.** The GroupLens official MovieLens\(^8\) 100k and 20M datasets [Harper and Konstan 2015]. For MovieLens 100k graph side-information is constructed for users, based on user demographic information using k-nearest neighbour (kNN) algorithm with ten neighbours. For MoveLens 20M graph side-information is constructed using kNN with k={10,20,40} based on movie genre data with 492956, 962644 and 1870508 edges respectively.

**Epinions.** We take the Epinions\(^9\) dataset as described in KPMF, but we use a much larger data size\(^10\) (22164 x 296277) with user trust network data (22164 x 22164) [Tang et al. 2012]. The dataset is extremely sparse (9.8312e-05 proportion of observed entries), and distributed un-uniformly, making this a difficult problem.

**YahooMusic** The official Yahoo Music ratings data from the KDD cup [Dror et al. 2011] as used in [Rao et al. 2015] to demonstrate scalability. We construct the graph with exact kNN on the music covariate data (artist,genre,album) with ten neighbours. This results in a very sparse graph, likely connecting many music tracks from the same artist and in the same album only.

**Model tuning** Data is split into test and validation. We use a procedure of parameter searching that we repeat for each model. PMF observation noise is fixed at \(\sigma^2 = 1\). PMF, GRALS and GPMF use the same CG iterations configuration (CG). GPMF uses \(\tau = 0\) for thresholding. KPMF uses the regularised Laplacian graph kernel with graph strength \(\gamma\) and learning rate \(\epsilon\). KBMF is trained with uninformative priors: \((\alpha = 1, \beta = 1)\), changing these values we saw no improvments; with at most one graph for each kernel multi-kernel parameters do not require tuning.

**General use of updated graph** We believe that removing the contested edges improves the graph for this task in general for any model, not just for GPMF. To this end we tested this by using the full graph vs. updated graph for KPMF [Zhou et al. 2012]. We plot an example of improved covergence speed and accuracy for KPMF in Figure 4.

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\(^8\)https://grouplens.org/datasets/movielens/
\(^9\)www.epinions.com
\(^10\)https://www.cse.msu.edu/~tangjili/trust.html, https://www.cse.msu.edu/~tangjili/datasetcode/epinions.zip
Table 2: Model parameter tuning for real world experiments

|                  | Flixster (3k) | Douban (3k) | MovieLens 100k | Epinions |
|------------------|---------------|-------------|----------------|----------|
| **D**=            | 10            | 10          | 10             | 10       |
| **PMF** (σ_u, σ_v, CG) | 0.1,0.1,1.1   | 5.5,1       | 1.2,1.2,2      | 0.75,0.2,3 |
| **GRALS** (λ_L, λ_u, λ_v) | 3,0.5,0.5     | 8,2.5       | 0.1,0.01,0.01  | 0.01,0.01,0.02 |
| **GPMF** (σ_2, λ_L, λ_u, λ_v) | 1.5,1.1       | 0.5,5,2.5   | 0.05,1,0.05,0.05 | 0.1,0.1,0.1,0.1 |
| **KPMF** (σ_2^2, ε, γ_u, γ_v) | 0.1,10^{-6},1.1,0.1 | 0.07,10^{-6},100,100 | 0.2,10^{-5},1.1,1.1 | N/A       |
| **KBMF** (γ_u, γ_v, σ_g, σ_y) | 1,1,0.1,1     | 1,1,0.2,1   | 0.35,0.3,0.1,0.15 | N/A       |

|                  | Yahoo Music 10M | MovieLens 20M 10NN | 20NN | 40NN |
|------------------|-----------------|---------------------|------|------|
| **D**=            | 20              | 10                  | 10   | 10   |
| **PMF** (σ_u, σ_v, CG) | 10,10           | 1.25,12.5,10        | 1.25,12.5,10 | 1.25,12.5,10 |
| **GRALS** (λ_L, λ_u, λ_v) | 100,200         | 5,0.5,0.01          | 1,1,10 | 1,1,10 |
| **GPMF** (σ_2, λ_L, λ_u, λ_v) | 10,10,100,200   | 0.05,5,0.1,0.01     | 0.5,5,0.1,0.1 | 0.5,2.5,0.01,0.01 |

Figure 4: Convergence time on MovieLens 100k. We provide an updated graph with 65% of the edges learnt with GPMF to another graph-regularised matrix factorisation method (KPMF Zhou et al. [2012]), to show that the optimised graph improves the convergence speed and precision of arbitrary algorithms for the graph regularised matrix completion problem.