A Unified Algorithm for One-class Structured Matrix Factorization with Side Information

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Abstract

In many applications such as recommender systems and multi-label learning the task is to complete a partially observed binary matrix. Such PU learning (positive-unlabeled) problems can be solved by one-class matrix factorization (MF). In practice side information such as user or item features in recommender systems are often available besides the observed positive user-item connections. In this work we consider a generalization of one-class MF so that two types of side information are incorporated and a general convex loss function can be used. The resulting optimization problem is very challenging, but we derive an efficient and effective alternating minimization procedure. Experiments on large-scale multi-label learning and one-class recommender systems demonstrate the effectiveness of our proposed approach.

1 Introduction

Many practical applications can be modeled in a positive and unlabeled data learning (PU learning) framework. Between two types of objects, some connections between object i of the first type and j of the second type are observed, but for most remaining situations, either i and j are not connected or the connection is not observed. A typical example is the collaborative filtering with one-class information (Pan et al. 2008; Hu, Koren, and Volinsky 2008; Pan and Scholz 2009; Li et al. 2010; Paquet and Koenigstein 2013). Given m users and n items, we observe part of a $0/1$ matrix $Y \in \mathbb{R}^{m\times n}$ with $Y_{ij} = 1$, where $(i,j) \in \Omega^+$. An observed entry indicates that user i likes item j. The goal is to know for any unobserved pair $(i,j) \notin \Omega^+$, whether i likes j or not. Thus, only part of positive-labeled entries are observed, while there are many unknown negative entries. This setting is very different from traditional collaborative filtering, where a real-valued rating (observed or not) is associated with any Y_{ij}. Note that this may be a more common scenario; for example, most people watch the video that interest them, without leaving any rating information.

Another important application that falls into the PU leaning framework is multi-label classification (Kong et al. 2014; Hsieh, Natarajan, and Dhillon 2015). The two types of objects are instances and labels. An entry $Y_{ij} = 1$ indicates that instance i is associated with label j. In practice, only part of instance i's labels have been observed.

PU learning is essentially a matrix completion problem. Given $Y_{ij} = 1,\ \forall (i,j) \in \Omega^+$, we would like to predict if other entries are zero or one. One common approach for matrix completion is through matrix factorization (MF) by finding two low-rank latent matrices

$$W = [\ldots, \boldsymbol{w}_i, \ldots]^\top \in \mathbb{R}^{m\times k} \text{ and } H = [\ldots, \boldsymbol{h}_j, \ldots]^\top \in \mathbb{R}^{n\times k}$$

such that $Y_{ij} = 1 \approx \boldsymbol{w}_i^\top \boldsymbol{h}_j,\ \forall (i,j) \in \Omega^+$. Note that k is a pre-specified number satisfying $k \ll m$ and $k \ll n$. Unlike traditional matrix completion problems where $Y_{ij},\ \forall (i,j) \in \Omega^+$ have different values, here approximating all the observed positive entries will result in the all-one prediction for all $(i,j) \notin \Omega^+$. For such a one-class scenario, in the approximation process one must treat some $(i,j) \notin \Omega^+$ as negative entries so that $Y_{ij} = 0 \approx \boldsymbol{w}_i^\top \boldsymbol{h}_j$. Therefore, existing one-class MF works solve the following optimization problem.

$$\min_{W,H} \sum_{i,j\in\Omega} C_{ij}(Y_{ij} - \boldsymbol{w}_i^T \boldsymbol{h}_j)^2 + \sum_i \lambda_i \|\boldsymbol{w}_i\|^2 + \sum_j \bar{\lambda}_j \|\boldsymbol{h}_j\|^2, \quad (1)$$

where C_{ij} is a cost associated with the loss, and $\lambda_i, \bar{\lambda}_j$ are regularization parameters. The set $\Omega = \Omega^+ \cup \Omega^-$ includes both observed positive and selected negative entries. The rationale of selecting some $(i,j) \notin \Omega^+$ and treating their $Y_{ij} = 0$ is because in general each user likes only a small set of items (or each instance is associated with a small set of labels).

The selection of negative entries in Ω^- is an important issue. Roughly there are two approaches:

- Subsampled: we subsample some unobserved entries to have Ω^- with $|\Omega^-| = O(|\Omega^+|)$.
- Full: $\Omega^- = [m]\times[n]\backslash\Omega^+$. That is, every unobserved entry is considered as negative. Unfortunately, the huge size of Ω^- makes this approach *computationally expensive.*

Recently, Yu, Bilenko, and Lin (2017) successfully developed efficient optimization methods to solve (1) for the Full approach. They show that the Full approach gives *significantly* better results than the Subsampled approach. A shortcoming is that their methods work only with the squared loss $(Y_{ij} - \boldsymbol{w}_i^\top \boldsymbol{h}_j)^2$, which is a real-value regression loss. However Y is a 0/1 matrix in the one-class setting, so a 0/1 classification loss might be more suitable. Yet,

Table 1: Various one-class MF formulations supported by our proposed algorithms. SQ-SQ: we apply the square loss on entries in both Ω^+ and Ω^-. SQ-wSQ: we apply the square loss on entries in Ω^+ and the weighted square loss on Ω^-. General-wSQ: we apply a general loss on entries in Ω^+ and the weighted square loss on Ω^-. For the Full approach of most formulations in this family, our proposed algorithms are the first efficient approach with time complexity linear in $O(|\Omega^+|)$. [1]: (Pan and Scholz 2009), [2]: (Yu, Bilenko, and Lin 2017), [3]: (Yu et al. 2014), and [4]: (Rao et al. 2015).

	SQ-SQ	SQ-wSQ	General-wSQ
loss ℓ_{ij}^+ on Ω^+	square	square	general loss
loss ℓ_{ij}^- on Ω^-	square	weighted square	weighted square
Standard	[1],[2]	[1],[2]	*this paper*
Feature-aware	LEML [3]	*this paper*	*this paper*
Graph-structured	GRALS [4]	*this paper*	*this paper*
Feature+Graph	*this paper*	*this paper*	*this paper*

developing efficient methods for the Full approach with a classification loss remains a challenging problem.

In problem (1), $Y_{ij}, (i,j) \in \Omega^+$ are the only given information. However, for most applications, some "side information" is also available. For example, besides the preference of user i on item j, user or item features may also be known. For multi-label learning, a data instance always comes with a feature vector. Further, relationships among users (items) may be available, which can be represented as a graph. How to effectively incorporate side information into the PU learning framework is thus a crucial research issue.

In this paper, we consider a formulation which unifies and generalizes many existing structured matrix-factorization formulations for PU learning with side information. In Section 2, we introduce the formulation and review related works. Our main contribution in Section 3 is to develop an efficient alternating minimization framework for the Full approach with *any convex loss* function. Experiments in Section 4 consider multi-label classification and recommender systems to illustrate the effectiveness of our approach. Results show a clear performance improvement using a classification loss. A summary showing how we generalize existing works is in Table 1, indicating that our proposed algorithms enable the computational feasibility of the Full approach for many one-class MF formulations with or without side information. The experimental codes and supplementary materials can be found at `http://www.csie.ntu.edu.tw/~cjlin/papers/ocmf-side/`.

2 One-class Structured Matrix Factorization

Assume that two types of side information are available for users (or instances). First, each user is associated with a feature vector, and second, a similarity matrix indicating the relationships between users is available. Our discussion can be easily generalized to the situation that items or both users and items come with side information. The proposed extension of (1) is the following optimization problem.

$$\min_{W,H} \quad f(W,H), \text{ where } f(W,H) = \sum_{(i,j)\in\Omega} C_{ij}\ell(Y_{ij}, \boldsymbol{x}_i^\top W \boldsymbol{h}_j) + \lambda_w \mathcal{R}(W) + \lambda_h \mathcal{R}(H). \tag{2}$$

In (2), λ_w, λ_h and λ_g are regularization parameters;

$$\mathcal{R}(W) = \mathrm{tr}\big(W^\top W + \lambda_g W^\top X^\top L X W\big), \mathcal{R}(H) = \mathrm{tr}\big(H^\top H\big)$$

are regularizers[1]; L is a positive definite matrix;

$$X = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m]^\top \in \mathbb{R}^{m\times d}$$

includes feature vectors corresponding to users; $\ell(a,b)$ is a loss function convex in b. We also use

$$\ell_{ij}(a,b) = C_{ij}\ell(a,b)$$

to denote the loss term for the (i,j) entry. Typically L is in a form of a graph Laplacian matrix with $L = D - S$, where D is a diagonal matrix with $D_{ii} = \sum_{t=1}^m S_{it}$ and $S \in \mathbb{R}^{m\times m}$ is a similarity matrix among users. Then in $\mathcal{R}(W)$ we have

$$\mathrm{tr}\big(W^\top X^\top L X W\big) = \frac{1}{2}\sum_{i_1,i_2} S_{i_1,i_2} \big\| W^\top \boldsymbol{x}_{i_1} - W^\top \boldsymbol{x}_{i_2} \big\|^2.$$

If the relationship between users i_1 and i_2 is strong, the larger S_{i_1,i_2} will make $W^\top \boldsymbol{x}_{i_1}$ closer to $W^\top \boldsymbol{x}_{i_2}$. This use of the graph information in the regularization term has been considered in various learning methods (Smola and Kondor 2003; Li and Yeung 2009; Zhou et al. 2012; Zhao et al. 2015; Rao et al. 2015; Natarajan, Rao, and Dhillon 2015), where Natarajan, Rao, and Dhillon (2015) focus on PU learning. We further note that in the optimization problem (2), $W^\top \boldsymbol{x}_i$ becomes the latent representation of the i-th user (or instance). Thus in contrast to $W \in \mathbb{R}^{m\times k}$ in the standard MF formulation, now we have $W \in \mathbb{R}^{d\times k}$. Then the prediction on unseen instances, such as in multi-label classification, can be done naturally using $W^\top \boldsymbol{x}$ as feature vector $\boldsymbol{x}$'s latent representation. There are other approaches to incorporate side information into MF such as Singh and Gordon (2008), but we focus on the formulation (2) in this paper.

Some past works have considered optimization problems related to (2). In (Rao et al. 2015), for rating-based MF, they consider the same regularization term $\mathcal{R}(W)$ by assuming that pairwise relationships are available via a graph. For squared losses they derive efficient alternating least squares methods to solve the optimization problem. Ours differs from them on: (i) they do not incorporate the side information of feature vectors in X; (ii) we consider one-class rather than rating-based MF; (iii) we consider general losses. Natarajan, Rao, and Dhillon (2015) consider the graph structured one-class MF without feature vectors X and proposes a Frank-Wolf algorithm, which requires $O(mn)$ space and the full eigendecomposition of the graph Laplacian matrix. For multi-label learning, Yu et al. (2014) solve (2) without the graph information for two scenarios:

- the general loss with $C_{ij} = 1$ and $|\Omega| \ll mn$; and
- the squared loss with $C_{ij} = 1$ and $\Omega = [m] \times [n]$.

[1] $\mathrm{tr}(\cdot)$ denotes the trace of a matrix

Theirs does not cover the situation of using a general loss with weighted C_{ij} and $\Omega = [m] \times [n]$.

If side information is not considered, Yu, Bilenko, and Lin (2017) give a detailed study on one-class MF under the Full setting. They consider the squared loss with

$$C_{ij} = \begin{cases} 1 & \text{if } (i,j) \in \Omega^+, \\ p_i q_j & \text{otherwise,} \end{cases} \text{ and } Y_{ij} = \bar{a},\ \forall (i,j) \notin \Omega^+, \quad (3)$$

where $\boldsymbol{p} \in \mathbb{R}^m$ and $\boldsymbol{q} \in \mathbb{R}^n$ are vectors chosen so that $p_i q_j < 1$ because weights for observed entries should be higher and $\bar{a}$ is a real number. A common choice is $\bar{a} = 0$ or -1. This work proposes efficient algorithms, and demonstrates that using $\Omega^- = [m] \times [n] \setminus \Omega^+$ gives much better results than selecting a small set Ω^- with $|\Omega^-| = O(|\Omega^+|)$.

3 Algorithms for One-class Structured MF

We develop efficient optimization algorithms to minimize (2) by considering C_{ij} in (3), *any convex loss*, and $\Omega = [m] \times [n]$ (i.e., the Full approach). We consider an alternating minimization framework to iteratively update

$$W \leftarrow \arg\min_W f(W,H) \text{ and } H \leftarrow \arg\min_H f(W,H),$$

and show that each sub-problem can be efficiently solved. Because $\min_H f(W,H)$ can be treated as a special form of

$$\min_W f(W,H) \text{ with } \lambda_g = 0 \text{ and } X = I,$$

where I is the identity matrix, we focus on the sub-problem when H is fixed. Let

$$\tilde{\boldsymbol{x}}_{ij} = \boldsymbol{h}_j \otimes \boldsymbol{x}_i = \mathrm{vec}\big(\boldsymbol{x}_i \boldsymbol{h}_j^\top\big) \in \mathbb{R}^{dk},\ \tilde{\boldsymbol{w}} = \mathrm{vec}(W) \in \mathbb{R}^{dk},$$

where $\mathrm{vec}(\cdot)$ is the vector by stacking the columns of a matrix. From

$$\boldsymbol{x}_i^\top W \boldsymbol{h}_j = \big(\boldsymbol{h}_j^\top \otimes \boldsymbol{x}_i^\top\big)\,\mathrm{vec}(W) = \tilde{\boldsymbol{x}}_{ij}^\top \tilde{\boldsymbol{w}}, \quad (4)$$

$\min_W\ f(W,H)$ can be reformulated as follows:

$$\min_{\tilde{\boldsymbol{w}}}\ g(\tilde{\boldsymbol{w}}), \text{ where} \quad (5)$$

$$g(\tilde{\boldsymbol{w}}) = \sum\nolimits_{(i,j)\in\Omega} \ell_{ij}\big(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}\big) + \lambda_w R_{\tilde{w}}(\tilde{\boldsymbol{w}}), \text{and}$$

$$R_{\tilde{w}}(\tilde{\boldsymbol{w}}) = \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{w}} + \lambda_g \big((X^\top L X) \otimes I_k\big)\tilde{\boldsymbol{w}}.$$

Because $|\Omega| = mn$ and the number of variables dk can be large, and closed-form solutions may not be available under some loss functions, we may apply iterative optimization methods to solve (5), where the calculations of the function, the gradient, and Hessian-vector product are often needed.

Handling all mn loss values is difficult, so we make the sub-problem easier by restricting the loss function on $(i,j) \in \Omega^-$ to be quadratic. Therefore, with C_{ij} in (3), we have the following two modified loss functions.

$$\ell^+_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}) = \ell_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}) - p_i q_j (\bar{a} - \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})^2$$

$$\ell^-_{ij}(\bar{a}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}) = p_i q_j (\bar{a} - \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})^2. \quad (6)$$

Then, (5) is equivalent to (7).

$$g(\tilde{\boldsymbol{w}}) = \lambda_w \mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}}) + \quad (7)$$

$$\underbrace{\sum_{(i,j)\in\Omega^+} \ell^+_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})}_{L^+(\tilde{\boldsymbol{w}})} + \underbrace{\sum_{(i,j)\in[m]\times[n]} \ell^-_{ij}(\bar{a}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})}_{L^-(\tilde{\boldsymbol{w}})},$$

where $L^+(\tilde{\boldsymbol{w}})$ is the term corresponding to all the entries in Ω^+, and $L^-(\tilde{\boldsymbol{w}})$ is the term considering all mn entries.

For the loss function, we do not require them to be differentiable because some optimization methods need just function evaluations. However, if they are, we let

$$\ell'_{ij}(a,b) = \frac{\partial}{\partial b}\ell_{ij}(a,b), \text{ and } \ell''_{ij}(a,b) = \frac{\partial^2}{\partial b^2}\ell_{ij}(a,b),$$

and assume that once a and b are given, these values can be calculated in a constant time.

With the reformulation (7), we can derive efficient procedures to perform function, gradient evaluation and Hessian-vector products. In particular, the $O(mn)$ terms in $L^-(\tilde{\boldsymbol{w}})$ can be efficiently computed with the cost comparable to that for $O(|\Omega^+|)$ terms in $L^+(\tilde{\boldsymbol{w}})$. While Yu et al. (2014) and Yu, Bilenko, and Lin (2017) also achieve such results, their optimization problems are our special cases. The generalization is not trivial. For example, Yu et al. (2014) state that for general losses, the $O(mn)$ term in the overall complexity is inevitable, but here we successfully remove it.

We show details for the function evaluation, but leave most details of gradient evaluation and Hessian-vector products in the supplementary materials. To cover both dense and sparse feature/graph matrices in our complexity analysis we use $\mathrm{nnz}(\cdot)$ to denote the number of nonzeros in a matrix.

3.1 Evaluation of the Objective Value $g(\tilde{\boldsymbol{w}})$

To compute $L^+(\tilde{\boldsymbol{w}})$ in (7), we first compute $B = XW$, where $B = [\ldots, \boldsymbol{b}_i, \ldots]^\top$ in $O(\mathrm{nnz}(X)k)$ time and store it in an $O(mk)$ space. Then for each $(i,j) \in \Omega^+$, from (4), $\tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}$ is a simple inner product $\boldsymbol{b}_i^\top \boldsymbol{h}_j$ that costs only $O(k)$ time. As a result, we can compute the entire $L^+(\tilde{\boldsymbol{w}})$ in $O(\mathrm{nnz}(X)k + |\Omega^+|k)$ time and $O(mk)$ space.

To compute $L^-(\tilde{\boldsymbol{w}})$, we first notice its independence of any Y_{ij} and consider the following equivalent formulation (see a detailed derivation in the supplementary materials).

$$L^-(\mathrm{vec}(W)) = \mathrm{tr}\big(\bar{a}^2 \mathbf{1}_n \mathbf{1}_m^\top \mathrm{diag}(\boldsymbol{p}) \mathbf{1}_m \mathbf{1}_n^\top \mathrm{diag}(\boldsymbol{q})\big) \quad (8)$$

$$+ \mathrm{tr}\big(HW^\top X^\top \mathrm{diag}(\boldsymbol{p}) XWH^\top \mathrm{diag}(\boldsymbol{q})\big) \quad (9)$$

$$- 2\,\mathrm{tr}\big(\bar{a} \mathbf{1}_n \mathbf{1}_m^\top \mathrm{diag}(\boldsymbol{p}) XWH^\top \mathrm{diag}(\boldsymbol{q})\big), \quad (10)$$

where $\mathbf{1}_m \in \mathbb{R}^m$ and $\mathbf{1}_n \in \mathbb{R}^n$ are vectors of ones, respectively. Note that with the availability of

- $B = XW$, obtained from the calculation of $L^+(\tilde{\boldsymbol{w}})$,
- $M = H^\top \mathrm{diag}(\boldsymbol{q}) H$, which can be pre-computed in $O(nk^2)$ time and stored in $O(k^2)$ space,
- $\boldsymbol{d} = X^\top \boldsymbol{p}$, which can be pre-computed in $O(\mathrm{nnz}(X))$ time and stored in $O(d)$ space,
- $\boldsymbol{k} = H^\top \boldsymbol{q}$, which can be pre-computed in $O(nk)$ time and stored in $O(k)$ space, and
- $\boldsymbol{p}^\top \mathbf{1}_m$ and $\boldsymbol{q}^\top \mathbf{1}_n$, which can be pre-computed in $O(m+n)$ time and stored in $O(1)$ spaces,

values in (8)-(10) can be computed efficiently:

$$(8) = \bar{a}^2\,\mathrm{tr}\big(\mathbf{1}_m^\top \mathrm{diag}(\boldsymbol{p}) \mathbf{1}_m \mathbf{1}_n^\top \mathrm{diag}(\boldsymbol{q}) \mathbf{1}_n\big)$$

$$= \bar{a}^2 \big(\boldsymbol{p}^\top \mathbf{1}_m\big)\big(\boldsymbol{q}^\top \mathbf{1}_n\big), \quad (11)$$

$$(9) = \mathrm{tr}\big(\underbrace{(XW)^\top}_{B^\top} \mathrm{diag}(\boldsymbol{p}) \underbrace{(XW)}_{B} \underbrace{\big(H^\top \mathrm{diag}(\boldsymbol{q}) H\big)}_{M}\big)$$

$$= \langle B, \mathrm{diag}(\boldsymbol{p}) BM \rangle, \quad (12)$$

Algorithm 1 Objective value evaluation: $g(\tilde{\boldsymbol{w}})$

- **Pre-processing step:** before any function evaluation
  1 $M = H^\top \operatorname{diag}(\boldsymbol{q}) H$ $\cdots O(nk^2)$
  2 $\boldsymbol{d} = X^\top \boldsymbol{p}$ $\cdots O(\operatorname{nnz}(X))$
  3 $\boldsymbol{k} = H^\top \boldsymbol{q}$ $\cdots O(nk)$
  4 Compute $\boldsymbol{p}^\top \mathbf{1}_m$ and $\boldsymbol{q}^\top \mathbf{1}_n$ $\cdots O(m+n)$
- Each time the function value at $\tilde{\boldsymbol{w}}$ is evaluated:
  1 $B = XW$, where $B = [\cdots \boldsymbol{b}_i \cdots]^\top$ $\cdots O(\operatorname{nnz}(X)k)$
  2 $L^+ = \sum_{(i,j)\in\Omega^+} \ell^+_{ij}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j)$ $\cdots O(|\Omega^+|k)$
  3 $L^- = \bar{a}^2 \big(\boldsymbol{p}^\top \mathbf{1}_m\big)\big(\boldsymbol{q}^\top \mathbf{1}_n\big) + \langle B, \operatorname{diag}(\boldsymbol{p}) BM \rangle$
  $-2\bar{a}\boldsymbol{d}^\top W \boldsymbol{k}$ $\cdots O(mk^2 + dk)$
  4 **Return** $L^+ + L^- + \lambda_w(\|W\|_F^2 + \lambda_g \operatorname{tr}\big(B^\top L B\big))$
  5 $\cdots O(dk + \operatorname{nnz}(L)k)$

$$(10) = -2\bar{a}\operatorname{tr}\big(\underbrace{\mathbf{1}_m^\top \operatorname{diag}(\boldsymbol{p})(X)}_{\boldsymbol{d}^\top} W \underbrace{H^\top \operatorname{diag}(\boldsymbol{q})\mathbf{1}_n}_{\boldsymbol{k}}\big)$$
$$= -2\bar{a}\boldsymbol{d}^\top W \boldsymbol{k}, \tag{13}$$

where $\langle \cdot, \cdot \rangle$ is the element-wise inner product between two same-sized matrices. As a result, computing $L^-(\tilde{\boldsymbol{w}})$ costs $O(mk^2+dk)$ time when $M, \boldsymbol{d}, \boldsymbol{k}, \boldsymbol{p}^\top \mathbf{1}_m$, and $\boldsymbol{q}^\top \mathbf{1}_n$ are pre-computed and B has been obtained in calculating $L^+(\tilde{\boldsymbol{w}})$. In general neither mk nor d is larger than $|\Omega^+|$, so by our setting the cost is comparable to that for $L^+(\tilde{\boldsymbol{w}})$.

To compute $\mathcal{R}_{\tilde{\boldsymbol{w}}}(\tilde{\boldsymbol{w}})$, via $B = XW$ obtained earlier, we calculate $\mathcal{R}_{\tilde{\boldsymbol{w}}}(\tilde{\boldsymbol{w}}) = \operatorname{tr}\big(\tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{w}} + \lambda_g B^\top L B\big)$ in $O(dk + \operatorname{nnz}(L)k)$ time. Details of the description of the function evaluation are given in Algorithm 1.

3.2 Gradient and Hessian-vector Product

Given a current point $\tilde{\boldsymbol{w}}$, calculating gradient $\nabla g(\tilde{\boldsymbol{w}})$ and Hessian-vector product $\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}}$ for a vector $\tilde{\boldsymbol{s}} \in \mathbb{R}^{dk}$ are two common operations in iterative optimization algorithms such as Newton methods. Let $S \in \mathbb{R}^{d\times k}$ be the matrix such that $\tilde{\boldsymbol{s}} = \operatorname{vec}(S)$. With careful derivations (see Section Supp-1.2 and Section Supp-1.3 in the supplementary materials), we show that both operations can be computed by a sequence of matrix-matrix products with a time complexity only linear in $|\Omega^+|$ instead of $|\Omega| = mn$:

$$\nabla g(\tilde{\boldsymbol{w}}) = \operatorname{vec}\big(X^\top\big[D^+ H + 2\operatorname{diag}(\boldsymbol{p})(BM) + 2\lambda_w\lambda_g LB\big] + 2\lambda_w W - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top\big), \tag{14}$$

$$\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} = \operatorname{vec}\big(X^\top\big[U^+ H + 2\operatorname{diag}(\boldsymbol{p})NM + 2\lambda_w\lambda_g LN\big] + 2\lambda_w S\big), \tag{15}$$

where $N = XS$, D^+ and U^+ are sparse matrices with $\forall (i,j) \in \Omega^+$:

$$D^+_{ij} = \ell^{+\prime}_{ij}, \quad U^+_{ij} = \ell^{+\prime\prime}_{ij} \boldsymbol{x}_i^\top S \boldsymbol{h}_j,$$
$$\ell^{+\prime}_{ij} = \ell^{+\prime}_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}), \text{ and } \ell^{+\prime\prime}_{ij} = \ell^{+\prime\prime}_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}).$$

With (14), gradient calculation can be done in

$$O(\operatorname{nnz}(X)k + \big|\Omega^+\big|k + \operatorname{nnz}(L)k + mk^2 + dk) \tag{16}$$

Algorithm 2 Gradient evaluation: $\nabla g(\tilde{\boldsymbol{w}})$

- **Pre-processing step:** before any gradient evaluation
  1 $M = H^\top \operatorname{diag}(\boldsymbol{q}) H$ $\cdots O(nk^2)$
  2 $\boldsymbol{d} = X^\top \boldsymbol{p}$ $\cdots O(\operatorname{nnz}(X))$
  3 $\boldsymbol{k} = H^\top \boldsymbol{q}$ $\cdots O(nk)$
- Each time the gradient at $\tilde{\boldsymbol{w}}$ is evaluated:
  1 $B = XW$, where $B = [\cdots \boldsymbol{b}_i \cdots]^\top$ $\cdots O(\operatorname{nnz}(X)k)$
  2 $D^+_{ij} = \ell^{+\prime}_{ij}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j),\ \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
  3 $G = X^\top(D^+ H + 2\operatorname{diag}(\boldsymbol{p})(BM) + 2\lambda_w\lambda_g LB)$
  4 $\cdots O(|\Omega^+|k + \operatorname{nnz}(X)k + \operatorname{nnz}(L)k + mk^2)$
  5 **Return** $\operatorname{vec}\big(G + 2\lambda_w W - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top\big)$ $\cdots O(dk)$

Algorithm 3 Hessian-vector Product: $\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}}$

- **Pre-processing step:** before any Hessian-vector product
  1 $M = H^\top \operatorname{diag}(\boldsymbol{q}) H$ $\cdots O(nk^2)$
  2 $B = XW$, where $B = [\cdots \boldsymbol{b}_i \cdots]^\top$ $\cdots O(\operatorname{nnz}(X)k)$
  3 $\ell^{+\prime\prime}_{ij} = \ell^{+\prime\prime}_{ij}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j),\ \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
- Each time the Hessian-vector product at $\tilde{\boldsymbol{w}} = \operatorname{vec}(W)$ is required with a given vector $\tilde{\boldsymbol{s}} = \operatorname{vec}(S)$:
  1 $N = XS$, where $N = [\cdots \boldsymbol{n}_i \cdots]^\top$ $\cdots O(\operatorname{nnz}(X)k)$
  2 $U^+_{ij} = \ell^{+\prime\prime}_{ij} \boldsymbol{n}_i^\top \boldsymbol{h}_j,\ \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
  3 $G = X^\top(U^+ H + 2\operatorname{diag}(\boldsymbol{p})(NM) + 2\lambda_w\lambda_g LN)$
  4 $\cdots O(|\Omega^+|k + \operatorname{nnz}(X)k + \operatorname{nnz}(L)k + mk^2)$
  5 **Return** $\operatorname{vec}(G + 2\lambda_w S)$ $\cdots O(dk)$

time. See Algorithm 2 for details. Similarly, with (15), each Hessian-vector products can be done in

$$O(\operatorname{nnz}(X)k + \big|\Omega^+\big|k + \operatorname{nnz}(L)k + mk^2 + dk) \tag{17}$$

time. See details in Algorithm 3. From (16) and (17), clearly the cost is related to $O(|\Omega^+|)$ rather than $O(|\Omega|) = O(mn)$.

3.3 Overall Optimization Procedure

With the efficient procedures proposed in Sections 3.1-3.2, we are able to implement many optimization algorithms to solve (7) such as gradient descent with line search, conjugate gradient, truncated Newton methods with line search, and trust region Newton methods. In Section Supp-1.4 of the supplementary materials, we give an efficient line-search procedure that only costs $O(|\Omega^+|k)$ time to check if the function value is sufficiently decreased.

To illustrate how Algorithms 1-3 are used, in the supplementary materials, we give details of a trust-region Newton method in Algorithm 5 and a gradient descent method with line search in Algorithm 6.

4 Experimental Results

We study one-class MF with various types of side information: standard one-class recommender systems with and without graph information, and multi-label learning by one-class MF with feature vectors as the side information.

Compared Formulations We consider three one-class MF formulations described in Table 1: SQ-SQ, SQ-wSQ, and General-wSQ. In SQ-SQ, we apply the square loss on

Table 2: Data statistics.

	m	n	$\lvert\Omega^+\rvert$	d	$\text{nnz}(X)$	m_{test}	k
bibtex	4,880	159	11,729	1,836	335,455	2,512	150
mediamill	30,993	101	135,752	120	3,719,160	12,425	100
delicious	12,920	983	245,810	500	234,740	3,182	300
eurlex	17,413	3,993	92,452	5,000	4,121,532	1,933	500
wiki10	14,146	30,938	263,705	101,938	9,526,572	6,616	500

(a) Multi-label learning.

	m	n	$\lvert\Omega^+\rvert$	$\text{nnz}(S)$	$\lvert\Omega^+_{\text{test}}\rvert$	k
ml100k	943	1,682	49,791	29,235	5,584	64
flixster	147,612	48,794	3,619,304	2,538,746	401,917	100
douban	129,490	58,541	9,803,098	1,711,780	1,087,948	128

(b) One-class recommender systems with graph information, S, among m users

entries in both Ω^+ and Ω^-. The difference of SQ-wSQ to SQ-SQ is that we apply the weighted square loss on Ω^-. For General-wSQ, we consider a classification loss: the logistic loss, and denote the formulation as LR-wSQ. Specifically, we apply the logistic loss on entries in Ω^+ and the weighted square loss on Ω^-. We implement the trust region Newton method (Lin, Weng, and Keerthi 2008) with the efficient function/gradient evaluation and Hessian-vector product proposed in Section 3. We also include LR-wLR into the multi-label learning experiments. LR-wLR is a Full approach where we apply the logistic loss on the entries in Ω^+ and apply the weighted logistic loss on entries in $[m] \times [n] \setminus \Omega^+$. It can be used only for small datasets because, without efficient procedures like those in Section 3, each iteration takes $O(mnk)$ cost.

Datasets and Experimental Settings For one-class MF with graph information as the side information, we consider three rating-based recommender system datasets with graph information, S, among m users (see Table 2): ml100k (Rao et al. 2015), flixster (Jamali and Ester 2010), and douban (Ma et al. 2011) and convert them into one-class problems by the same procedure in (Yu, Bilenko, and Lin 2017). Because the feature information is not available, X is the identity matrix. For multi-label learning, we consider five publicly available datasets (see Table 2) and set $\lambda_g = 0$ because the graph information S is not available. All experiments are run on a 20-core machine with 256GB RAM. BLAS operations are used whenever possible for all the implementations. Sparse matrix operations are parallelized using OpenMP. We use precision and nDCG on the top-rank predictions as our evaluation criteria for both recommender systems and multi-label learning. We only show precision@5 in Figures 1-3 and leave figures with other criteria in the supplementary materials. We adopt a held-out validation approach on the training part of each dataset to perform parameter search. See Section Supp-2 in the supplementary materials for more experimental details.

4.1 Full versus Subsampled

We compare Full and Subsampled approaches on multi-label problems, which are special cases of feature-aware one-class MF. An extensive comparison for the standard one-class MF without features has been performed in (Yu, Bilenko, and Lin 2017). Figure 1 shows both training time and test performance on three large datasets.

From Figure 1(a), the three Full approaches: SQ-SQ, SQ-wSQ, and LR-wSQ are highly efficient because with our algorithms in Section 3, the cost per iteration of the trust region Newton method is related to $|\Omega^+|$ rather than $|\Omega| = mn$. Thus the costs of these three Full approaches are similar to the costs of the two Subsampled approaches: SQ-wSQ (S) and LR-wLR (S). Regarding the prediction performance, from Figure 1(b), the Full formulations always outperform the Subsampled formulations. Such observations are consistent with those for one-class MF without side information (Yu, Bilenko, and Lin 2017).

Table 3: Comparison between LR-wLR and LR-wSQ.

		time	p@1	p@2	p@3	p@4	p@5
bibtex	LR-wSQ	22	63.22	48.43	39.89	33.83	29.50
	LR-wLR	85	61.91	46.66	38.21	32.66	28.43
mediamill	LR-wSQ	61	87.77	80.96	70.08	61.48	55.15
	LR-wLR	437	87.78	81.17	70.38	61.85	55.33
delicious	LR-wSQ	23	67.47	64.24	61.85	59.25	56.73
	LR-wLR	446	67.91	65.04	62.27	59.81	57.27

4.2 Comparison on Various Loss Functions

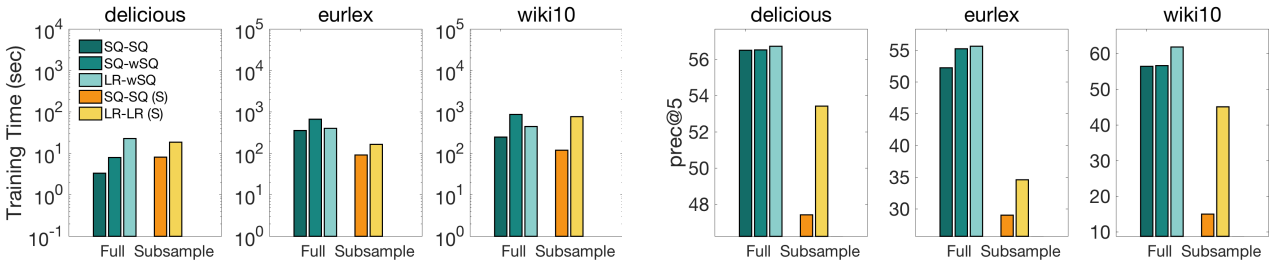
We check various formulations of the Full approach for feature-aware or graph structured one-class MF to study the effectiveness of (i) the use of weighted losses on the entries in Ω^-; and (ii) the use of a classification loss.

LR-wSQ versus LR-wLR To resolve the $O(mnk)$ computational requirement for the Full approach with a general loss function, in Section 3, we propose a technique where the general loss is applied to the observations in Ω^+, while a weighted squared loss is applied to Ω^-. In Table 3, we show the results of LR-wSQ and LR-wLR on three smaller datasets. We observe that LR-wSQ and LR-wLR are similar in terms of prediction performance, while LR-wSQ runs significantly faster. This result indicates that our proposed technique to replace the loss on Ω^- by a weighted loss not only accelerates the training procedure significantly but also yields a similar prediction performance.

SQ-wSQ versus LR-wSQ. By considering three types of one-class problems, in Figure 2, we show the performance improvement of SQ-wSQ and LR-wSQ over SQ-SQ (in percentage) because for recommender systems with graph information, SQ-SQ is equivalent to GRALS (Rao et al. 2015), while for multi-label learning, SQ-SQ is equivalent to LEML (Yu et al. 2014). Clearly LR-wSQ significantly outperforms SQ-wSQ and SQ-SQ. Therefore, the logistic loss seems to be more appropriate for one-class MF problems, and our approach enables its use.

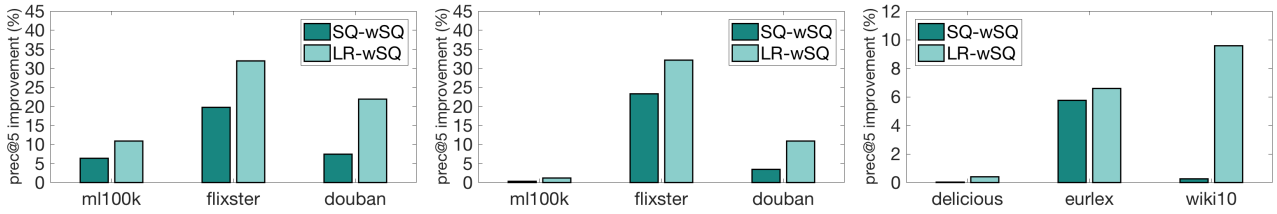
4.3 Non-linear Multi-label Classifiers

Recently, some non-linear methods such as SLEEC (Bhatia et al. 2015) and FastXML (Prabhu and Varma 2014) have



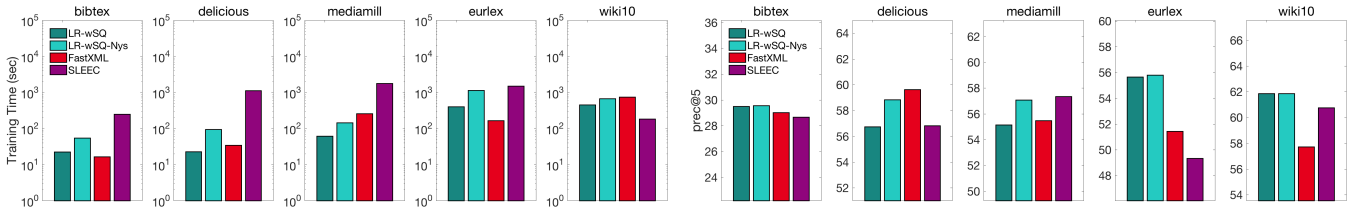
(a) Training Time. (b) Prediction Performance.

Figure 1: Full versus Subsampled on multi-label learning with various loss functions. "(S)" indicates Subsampled.



(a) Standard one-class MF (b) Graph-structured one-class MF (c) Feature-aware one-class MF

Figure 2: Comparison on various loss functions. Y-axis is the improvement over the SQ-SQ formulation in percentage.



(a) Training Time. (b) Prediction Performance.

Figure 3: Comparison on non-linear multi-label classifiers.

been considered state-of-the-art approaches for multi-label learning because they outperform traditional binary relevance approaches. Here we demonstrate that the Full setting considered in this paper yields competitive performances.

Besides directly applying the proposed approach (i.e., LR-wSQ) on feature vectors $\boldsymbol{x}_i$, $\forall i$, we propose a non-linear extension by converting $\boldsymbol{x}_i \in \mathbb{R}^d$ into a new feature vector $\boldsymbol{z}_i \in \mathbb{R}^D$ via a Nyström method. We consider K-means Nyström (Zhang, Tsang, and Kwok 2008) by using $D \ll m$ centers $\{\boldsymbol{c}_t\}$ from the K-means algorithm on $\{\boldsymbol{x}_i\}$ as landmark points. Consider an RBF kernel matrix $K \in \mathbb{R}^{D\times D}$ parameterized by $\gamma > 0$ with

$$K_{ts} = \exp(-\gamma\|\boldsymbol{c}_t - \boldsymbol{c}_s\|^2),\ \forall t, s \in [D] \times [D].$$

Given an $\boldsymbol{x} \in \mathbb{R}^d$, the transformed vector $\boldsymbol{z} \in \mathbb{R}^D$ is obtained by $\boldsymbol{z} = K^{-1/2}\bar{\boldsymbol{z}}$, where $\bar{\boldsymbol{z}} \in \mathbb{R}^D$ is a vector with

$$\bar{z}_t = \exp(-\gamma\|\boldsymbol{c}_t - \boldsymbol{x}\|^2),\ \forall t \in [D].$$

We append the transformed vector $\boldsymbol{z}_i$ to the original $\boldsymbol{x}_i$. See the supplementary materials for details such as the parameters used. We refer tot this approach as LR-wSQ-Nys.

Figure 3 compares LR-wSQ, LR-wSQ-Nys, FastXML, and SLEEC. We can see that LR-wSQ and LR-wSQ-Nys yield competitive prediction performance.

5 Conclusions

In this paper, we consider a generalization of one-class matrix factorization with two types of side information, which has wide applicability to applications with only positive-unlabeled observations such as recommender systems and multi-label learning. We consider the Full approach for one-class MF where all the unlabeled entries are regarded as negative with a lower confidence, and any convex loss function can be used on the observed entries. The resulting optimization problem is very challenging, but we derive an efficient alternating minimization procedure. Experiments demonstrate the effectiveness of our proposed approach.

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Supplementary Materials:

A Unified Algorithm for One-class Structured Matrix Factorization with Side Information

Supp-1 Detailed Derivations of Algorithms

Supp-1.1 Detailed Derivation of $L^-(\mathrm{vec}(W))$

From (4), (6), and (7), we have

$$\begin{aligned}
L^-(\mathrm{vec}(W)) &= \left\| \sqrt{\mathrm{diag}(\boldsymbol{p})}\big(\bar{a}\mathbf{1}_m\mathbf{1}_n^\top - XWH^\top\big)\sqrt{\mathrm{diag}(\boldsymbol{q})} \right\|_F^2 \\
&= \mathrm{tr}\left(\sqrt{\mathrm{diag}(\boldsymbol{q})}\big(\bar{a}\mathbf{1}_n\mathbf{1}_m^\top - HW^\top X^\top\big)\,\mathrm{diag}(\boldsymbol{p})\times \right. \\
&\qquad \left. \big(\bar{a}\mathbf{1}_m\mathbf{1}_n^\top - XWH^\top\big)\sqrt{\mathrm{diag}(\boldsymbol{q})}\right) \\
&= \mathrm{tr}\left(\big(\bar{a}\mathbf{1}_n\mathbf{1}_m^\top - HW^\top X^\top\big)\,\mathrm{diag}(\boldsymbol{p})\times \right. \\
&\qquad \left. \big(\bar{a}\mathbf{1}_m\mathbf{1}_n^\top - XWH^\top\big)\mathrm{diag}(\boldsymbol{q})\right) \\
&= \mathrm{tr}\big(\bar{a}^2\mathbf{1}_n\mathbf{1}_m^\top\,\mathrm{diag}(\boldsymbol{p})\mathbf{1}_m\mathbf{1}_n^\top\,\mathrm{diag}(\boldsymbol{q})\big) \\
&\quad + \mathrm{tr}\big(HW^\top X^\top\,\mathrm{diag}(\boldsymbol{p})XWH^\top\,\mathrm{diag}(\boldsymbol{q})\big) \\
&\quad - 2\,\mathrm{tr}\big(\bar{a}\mathbf{1}_n\mathbf{1}_m^\top\,\mathrm{diag}(\boldsymbol{p})XWH^\top\,\mathrm{diag}(\boldsymbol{q})\big),
\end{aligned}$$

where $\mathbf{1}_m$ and $\mathbf{1}_n$ are vectors of ones with order m and n, respectively, and $\mathrm{tr}(\cdot)$ denotes the trace of a matrix (i.e., the sum of diagonal entries).

Supp-1.2 Gradient Calculation $\nabla g(\tilde{\boldsymbol{w}})$

The following property is useful in subsequent derivations.

Property 1. *Let $X = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m]^\top$, $H = [\boldsymbol{h}_1, \ldots, \boldsymbol{h}_n]^\top$, and $D \in \mathbb{R}^{m\times n}$. We have*

$$X^\top DH = \sum_{ij} \boldsymbol{x}_i D_{ij} \boldsymbol{h}_j^\top \tag{1.1}$$

From (7), the gradient of $g(\tilde{\boldsymbol{w}})$ is

$$\nabla g(\tilde{\boldsymbol{w}}) = \nabla L^+(\tilde{\boldsymbol{w}}) + \nabla L^-(\tilde{\boldsymbol{w}}) + \lambda_w \nabla \mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}}),$$

where

$$\begin{aligned}
\nabla L^+(\tilde{\boldsymbol{w}}) &= \sum_{(i,j)\in\Omega^+} \ell_{ij}^{+\prime}\tilde{\boldsymbol{x}}_{ij} = \sum_{(i,j)\in\Omega^+} \mathrm{vec}\Big(\ell_{ij}^{+\prime}\boldsymbol{x}_i\boldsymbol{h}_j^\top\Big) \\
&= \mathrm{vec}\big(X^\top D^+ H\big). \qquad (1.2)
\end{aligned}$$

The last equality follows from (1.1), $\ell_{ij}^{+\prime}$ is the abbreviation of $\ell_{ij}^{+\prime}(Y_{ij}, \tilde{\boldsymbol{w}}^\top\tilde{\boldsymbol{x}}_{ij})$ and,

$$D_{ij}^+ = \begin{cases} \ell_{ij}^{+\prime}, & \forall (i,j)\in\Omega^+, \\ 0, & \text{otherwise.} \end{cases}$$

Similar to the situation of computing $L^+(\tilde{\boldsymbol{w}})$ in Section 3.1, if $B = XW$ has been calculated, then constructing a sparse matrix D^+ requires only $O(|\Omega^+|k)$ operations and $O(|\Omega^+|)$ space. With a similar derivation in (1.2), we have

$$\nabla L^-(\tilde{\boldsymbol{w}}) = \mathrm{vec}\big(X^\top D^- H\big),$$

where D^- is a dense $m \times n$ matrix with $D_{ij}^- = \ell_{ij}^{-\prime}$, $\forall (i,j) \in [m]\times[n]$. From the definition of $\ell^-(\cdot,\cdot)$ in (6),

$$\begin{aligned}
&\frac{\partial}{\partial b}\ell^-(\bar{a}, b) = 2p_iq_j(b - \bar{a}) \\
\Rightarrow\quad & \ell_{ij}^{-\prime} = 2p_iq_j\big(\tilde{\boldsymbol{w}}^\top\tilde{\boldsymbol{x}}_{ij} - \bar{a}\big) = 2p_iq_j\Big(\big(XWH^\top\big)_{ij} - \bar{a}\Big).
\end{aligned}$$

Thus, we have

$$D^- = 2\,\mathrm{diag}(\boldsymbol{p})\big(XWH^\top - \bar{a}\mathbf{1}_m\mathbf{1}_n^\top\big)\,\mathrm{diag}(\boldsymbol{q}).$$

Straightforward computation of entire D^- requires $O(mnk + \mathrm{nnz}(X)k)$ time and $O(mn)$ space; both requirements are infeasible for large values of m and n. Fortunately, $\nabla L^-(\tilde{\boldsymbol{w}}) = \mathrm{vec}\big(X^\top D^- H\big)$ can be computed without explicitly forming D^- as follows:

$$\begin{aligned}
&X^\top D^- H \\
=&2X^\top\,\mathrm{diag}(\boldsymbol{p})XWH^\top\,\mathrm{diag}(\boldsymbol{q})H \\
&\quad - 2\bar{a}X^\top\,\mathrm{diag}(\boldsymbol{p})\mathbf{1}_m\mathbf{1}_n^\top\,\mathrm{diag}(\boldsymbol{q})H \qquad (1.3) \\
=&2X^\top\,\mathrm{diag}(\boldsymbol{p})\underbrace{(XW)}_{B}\underbrace{\big(H^\top\,\mathrm{diag}(\boldsymbol{q})H\big)}_{M} - 2\bar{a}\,\underbrace{\big(X^\top\boldsymbol{p}\big)}_{\boldsymbol{d}}\underbrace{\big(\boldsymbol{q}^\top H\big)}_{\boldsymbol{k}^\top},
\end{aligned}$$

where B, M, $\boldsymbol{d}$, and $\boldsymbol{k}$ are the same matrices/vectors used in the objective value evaluation introduced in Algorithm 1. Combining (1.2), (1.3), and $\tilde{\boldsymbol{w}} = \mathrm{vec}(W)$, $\nabla g(\tilde{\boldsymbol{w}})$ can be computed using the following sequence of matrix-matrix products:

$$\begin{aligned}
\nabla g(\tilde{\boldsymbol{w}}) &= \mathrm{vec}\big(X^\top D^+ H + X^\top D^- H + \lambda_w\nabla\mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}})\big) \\
&= \mathrm{vec}\left(X^\top\big[D^+H + 2\,\mathrm{diag}(\boldsymbol{p})(BM) + 2\lambda_w\lambda_g LB\big]\right. \\
&\qquad \left. + 2\lambda_w W - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top\right),
\end{aligned}$$

where the last equality follows from (1.3) and

$$\begin{aligned}
\nabla\mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}}) &= 2\,\mathrm{vec}\big((I + \lambda_g X^\top LX)W\big) \\
&= 2\,\mathrm{vec}\big(W + \lambda_g X^\top LB\big).
\end{aligned}$$

Thus, the cost is

$$O(\mathrm{nnz}(X)k + \big|\Omega^+\big|k + \mathrm{nnz}(L)k + mk^2 + dk) \tag{1.4}$$

time. A detailed procedure is shown in Algorithm 2. Note that if the computation of $\nabla g(\tilde{\boldsymbol{w}})$ follows immediately after the objective value evaluation of the same $\tilde{\boldsymbol{w}}$, then M, $\boldsymbol{d}$, $\boldsymbol{q}$, $\boldsymbol{k}$, and B can be re-used to save additional computation.[2]

Note that we may use a different sequence of matrix-matrix products for (1.3) if the number of features d is very small such that

$$d^2 + dk < mk. \tag{1.5}$$

By pre-computing $\bar{M} = X^\top\,\mathrm{diag}(\boldsymbol{p})X$ in $O(\mathrm{nnz}(X)d)$ time and storing it in $O(d^2)$ space, the following sequence to compute $\nabla g(\tilde{\boldsymbol{w}})$,

$$\begin{aligned}
\nabla g(\tilde{\boldsymbol{w}}) &= \mathrm{vec}\big(X^\top D^+ H + X^\top D^- H + \lambda_w\nabla\mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}})\big) \\
&= \mathrm{vec}\left(X^\top\big(D^+H + 2\lambda_w\lambda_g LB\big) + 2\bar{M}WM\right. \\
&\qquad \left. + 2\lambda_w W - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top\right),
\end{aligned}$$

costs

$$O(\mathrm{nnz}(X)k + \big|\Omega^+\big|k + \mathrm{nnz}(L)k + d^2k + dk^2)$$

time, which is smaller than that in (1.4) because of (1.5).

[2] $\mathrm{diag}(\boldsymbol{p})(BM)$ can also be re-used.

Supp-1.3 Hessian-vector Multiplication $\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}}$

Given a current point $\tilde{\boldsymbol{w}}$ and a vector $\tilde{\boldsymbol{s}} \in \mathbb{R}^{dk}$, computing $\nabla^2 g(\tilde{\boldsymbol{w}})\boldsymbol{s}$ is a common operation required in many iterative optimization algorithms such as conjugate gradient. Let $S \in \mathbb{R}^{d\times k}$ be the matrix such that $\tilde{\boldsymbol{s}} = \mathrm{vec}(S)$. From (7), we have

$$\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} = \nabla^2 L^+(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} + \nabla^2 L^-(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} + \lambda_w \nabla^2 \mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}},$$

where

$$\begin{aligned}
\nabla^2 L^+(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} &= \sum_{(i,j)\in\Omega^+} \ell_{ij}^{+\prime\prime} \tilde{\boldsymbol{x}}_{ij}\tilde{\boldsymbol{x}}_{ij}^\top \tilde{\boldsymbol{s}} \\
&= \sum_{(i,j)\in\Omega^+} \ell_{ij}^{+\prime\prime} \big((\boldsymbol{h}_j \boldsymbol{h}_j^\top) \otimes (\boldsymbol{x}_i \boldsymbol{x}_i^\top) \big) \,\mathrm{vec}(S) \\
&= \sum_{(i,j)\in\Omega^+} \mathrm{vec}\Big(\ell_{ij}^{+\prime\prime} \boldsymbol{x}_i \boldsymbol{x}_i^\top S \boldsymbol{h}_j \boldsymbol{h}_j^\top \Big) \qquad (1.6) \\
&= \sum_{(i,j)\in\Omega^+} \mathrm{vec}\big(\boldsymbol{x}_i \underbrace{\ell_{ij}^{+\prime\prime} \boldsymbol{x}_i^\top S \boldsymbol{h}_j}_{U_{ij}^+} \boldsymbol{h}_j^\top \big) \\
&= \mathrm{vec}\big(X^\top U^+ H \big). \qquad (1.7)
\end{aligned}$$

Note that (1.6) is from (4), (1.7) is from (1.1), U^+ is a sparse matrix with

$$U_{ij}^+ = \begin{cases} \ell_{ij}^{+\prime\prime} \boldsymbol{x}_i^\top S \boldsymbol{h}_j, & \forall (i,j) \in \Omega^+, \\ 0 & \text{otherwise}, \end{cases}$$

and $\ell_{ij}^{+\prime\prime} = \ell_{ij}^{+\prime\prime}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})$, $\forall (i,j) \in \Omega^+$. Similar to the gradient computation, $\ell_{ij}^{+\prime\prime}$ can be computed in $O(k)$ time if $B = XW$ is pre-computed. To efficiently compute U_{ij}^+, $\forall (i,j) \in \Omega^+$, we first compute a matrix-matrix product XS in $O(\mathrm{nnz}(X)k)$ time and store it in an $m \times k$ matrix $N = [\ldots, \boldsymbol{n}_i, \ldots]^\top$ such that $\boldsymbol{n}_i = S^\top \boldsymbol{x}_i$. Then the entire sparse matrix U^+ can be constructed in $O(|\Omega^+|k + \mathrm{nnz}(X)k)$ time.

With a similar derivation as above, we have

$$\nabla^2 L^-(\tilde{\boldsymbol{w}})\boldsymbol{s} = \mathrm{vec}\big(X^\top U^- H \big),$$

where U^- is a dense $m \times n$ matrix with

$$U_{ij}^- = \ell_{ij}^{-\prime\prime} \boldsymbol{x}_i^\top S \boldsymbol{h}_j, \ \forall (i,j) \in [m] \times [n].$$

From the definition of $\ell^-(\cdot,\cdot)$ in (6),

$$\frac{\partial^2}{\partial b^2} \ell_{ij}^-(\bar{a}, b) = 2 p_i q_j, \ \forall b \quad \Rightarrow \quad \ell_{ij}^{-\prime\prime} = 2 p_i q_j.$$

Thus, we have

$$U^- = 2\,\mathrm{diag}(\boldsymbol{p}) X S H^\top \,\mathrm{diag}(\boldsymbol{q}).$$

Similar to the situation in the gradient computation, computing $\nabla^2 L^-(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} = \mathrm{vec}\big(X^\top U^- H\big)$ can be done without forming the entire U^- explicitly as follows:

$$X^\top U^- H = 2 X^\top \,\mathrm{diag}(\boldsymbol{p}) \underbrace{(XS)}_{N} \underbrace{H^\top \,\mathrm{diag}(\boldsymbol{q}) H}_{M}, \qquad (1.8)$$

where N is available when we construct the sparse matrix U^+, and M can be pre-computed and stored (same M in the objective value evaluation and gradient computation). Combining (1.7), (1.8), and $\tilde{\boldsymbol{w}} = \mathrm{vec}(W)$, $\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}}$ can be computed using the following sequence of matrix-matrix products:

$$\begin{aligned}
&\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} = \mathrm{vec}\big(X^\top U^+ H + X^\top U^- H + \lambda_w \nabla^2 \mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} \big) \\
&= \mathrm{vec}\big(X^\top \big[U^+ H + 2\,\mathrm{diag}(\boldsymbol{p}) N M \big] + \lambda_w \nabla^2 \mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} \big) \\
&= \mathrm{vec}\big(X^\top \big[U^+ H + 2\,\mathrm{diag}(\boldsymbol{p}) N M + 2\lambda_w \lambda_g L N \big] + 2\lambda_w S \big),
\end{aligned}$$

where the last equality follows from

$$\begin{aligned}
\nabla^2 \mathcal{R}_{\tilde{w}}(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}} &= 2\,\mathrm{vec}\big(S + \lambda_g X^\top L X S \big) \\
&= 2\,\mathrm{vec}\big(S + \lambda_g X^\top L N \big).
\end{aligned}$$

Thus, the cost is

$$O(\mathrm{nnz}(X)k + |\Omega^+|k + \mathrm{nnz}(L)k + mk^2 + dk)$$

time. Note that we can move the computation of $\ell_{ij}^{+\prime\prime}$, $\forall (i,j) \in \Omega^+$ into the pre-processing phase to save some repeated operations when the Hessian-vector products are performed many times with the same $\tilde{\boldsymbol{w}}$, a common situation in iterative optimization algorithms such as conjugate gradient. Further, when the squared loss $\ell(a,b) = (a-b)^2$ is used, for entries in Ω^+, $\ell_{ij}^{+\prime\prime} = 2(1 - p_i q_j)$ is independent of the choice of $\tilde{\boldsymbol{w}}$ and can be pre-computed in the beginning of the entire optimization procedure. A detailed procedure is presented in Algorithm 3.

Similar to the gradient calculation, when $d^2 + dk < mk$, we can reduce the cost by using another sequence of matrix-matrix products to compute $\nabla^2 g(\tilde{\boldsymbol{w}})\tilde{\boldsymbol{s}}$ in

$$O(|\Omega^+|k + \mathrm{nnz}(X)k + \mathrm{nnz}(L)k + d^2 k + dk^2)$$

time with $\bar{M} = X^\top \,\mathrm{diag}(\boldsymbol{p}) X$ as follows:

$$X^\top \big(U^+ H + 2\lambda_w \lambda_g L N \big) + 2\bar{M} S M + 2\lambda_w S.$$

Supp-1.4 Line Search Procedure and Trust Region Method

Line search procedures and trust region methods are two common techniques to determine a step size and guarantee the asymptotic convergence for an optimization algorithm. In this section, we briefly introduce how to apply these two techniques to (7).

Line Search Procedure A line search procedure is used to ensure the sufficient decrease of the objective function value after a search direction ΔW is given. Common choices for the search direction include the negative gradient direction and the Newton direction. However, even if ΔW is a descent direction, $g(W + \Delta W)$ is not necessary smaller than $g(W)$. Thus, in a backward line search procedure, we try a sequence of step size $\alpha = 1, \beta, \beta^2, \ldots$, with $\beta < 1$ such that

$$g(W + \alpha \Delta W) < g(W) + \sigma \alpha \langle \nabla g(W), \Delta W \rangle, \qquad (1.9)$$

where $\sigma < 1/2$. Note that even with our proposed efficient function value evaluation procedure (Algorithm 1), recalculating function value at $W + \alpha \Delta W$ for each α can still be expensive.

We propose an effective trick to reduce the cost for line search by taking that $\tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}$ is a linear function of $\tilde{\boldsymbol{w}}$, $\ell^-_{ij}(\bar{a}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})$ is a quadratic function of $\tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}$, and $\mathcal{R}(\tilde{\boldsymbol{w}})$ is a quadratic function of $\tilde{\boldsymbol{w}}$. The idea is to have

$$\begin{aligned}
&g(W+\alpha\Delta W)\\
=&L^+(W+\alpha\Delta W)+L^-(W+\alpha\Delta W)+\lambda_w\mathcal{R}(W+\alpha\Delta W)\\
=&g(W)-L^+(W)+L^+(W+\alpha\Delta W)+\alpha\text{Val_1}+\alpha^2\text{Val_2},
\end{aligned}$$

where Val_1 and Val_2 can be calculated with the cost of one function evaluation. If these two values are available, then the sufficient decrease condition in (1.9) can be easily checked as follows.

$$\begin{aligned}
&g(W+\alpha\Delta W)-g(W)\\
=&-L^+(W)+L^+(W+\alpha\Delta W)+\alpha\text{Val_1}+\alpha^2\text{Val_2}\\
<&\sigma\alpha\langle\nabla g(W),\Delta W\rangle.
\end{aligned}$$

Moreover, when the line-search procedure terminates, we have the next iterate $W+\alpha\Delta W$ and the new function value. From (8)-(13) in the main text,

$$\begin{aligned}
&L^-(W+\alpha\Delta W)\\
=&\bar{a}^2(\boldsymbol{p}^\top\mathbf{1}_m)(\boldsymbol{q}^\top\mathbf{1}_n)+\langle B+\alpha\Delta B,\operatorname{diag}(\boldsymbol{p})(B+\alpha\Delta B)M\rangle\\
&\qquad-2\bar{a}\boldsymbol{d}^\top(W+\alpha\Delta W)\boldsymbol{k}\\
=&L^-(W)+\alpha^2\langle\Delta B,\operatorname{diag}(\boldsymbol{p})\Delta BM\rangle+\\
&\alpha\big(\langle\Delta B,\operatorname{diag}(\boldsymbol{p})BM\rangle+\langle B,\operatorname{diag}(\boldsymbol{p})\Delta BM\rangle-2\bar{a}\boldsymbol{d}^\top\Delta W\boldsymbol{k}\big)
\end{aligned}$$

and

$$\begin{aligned}
&\mathcal{R}(W+\alpha\Delta W)\\
=&\operatorname{tr}\Big((W+\alpha\Delta W)^\top(W+\alpha\Delta W)\Big)\\
&+\lambda_g\operatorname{tr}\Big((B+\alpha\Delta B)^\top L(B+\alpha\Delta B)\Big)\\
=&\mathcal{R}(W)+\alpha\big(2\operatorname{tr}\big(W^\top\Delta W+\lambda_g B^\top L\Delta B\big)\big)\\
&+\alpha^2\operatorname{tr}\big(\Delta W^\top\Delta W+\lambda_g\Delta B^\top L\Delta B\big),\\
=&\mathcal{R}(W)+\alpha(2\langle W,\Delta W\rangle+2\lambda_g\langle B,L\Delta B\rangle)\\
&+\alpha^2\Big(\|\Delta W\|_F^2+\lambda_g\langle\Delta B,L\Delta B\rangle\Big),
\end{aligned}$$

where

$$\Delta B = X\Delta W.$$

The above calculation shows that in addition to the matrix B, we can maintain

$$\hat{M}=\operatorname{diag}(\boldsymbol{p})BM,\text{ and }\hat{L}=LB.$$

Before the line-search procedure,

$$\Delta B = X\Delta W, \tag{1.10}$$

$$\Delta\hat{M}=\operatorname{diag}(\boldsymbol{p})\Delta BM, \tag{1.11}$$

$$\Delta\delta=\boldsymbol{d}^\top\Delta W\boldsymbol{k},\text{ and} \tag{1.12}$$

$$\Delta\hat{L}=L\Delta B \tag{1.13}$$

are calculated. Then

$$\begin{aligned}
\text{Val_1}=&\Big\langle\Delta B,\hat{M}\Big\rangle+\Big\langle B,\Delta\hat{M}\Big\rangle-2\bar{a}\Delta\delta\\
&+2\lambda_w\Big(\langle W,\Delta W\rangle+\lambda_g\Big\langle B,\Delta\hat{L}\Big\rangle\Big),\\
\text{Val_2}=&\Big\langle\Delta B,\Delta\hat{M}\Big\rangle\\
&+\lambda_w\Big(\|\Delta W\|_F^2+\lambda_g\Big\langle\Delta B,\Delta\hat{L}\Big\rangle\Big).
\end{aligned}$$

Clearly, the computation for (1.10)-(1.13) costs

$$O(\operatorname{nnz}(X)k+mk^2+dk+\operatorname{nnz}(L)k),$$

which is the same as the cost of one function evaluation. For Val_1 and Val_2, the cost $O(dk+mk)$ is much smaller. To check the sufficient decrease condition (1.9), we precalculate $\nabla g(W)^\top\Delta W$ before the line-search procedure, so the calculation under an α is $O(|\Omega^+|k)$ for calculating $L^+(W+\alpha\Delta W)$.

If the squared loss is considered on entries in Ω^+, the same technique for calculating $L^-(W+\alpha\Delta W)$ can be applied for calculating $L^+(W+\alpha\Delta W)$. Then the $O(|\Omega^+|k)$ cost is needed only before the line-search procedure rather than at each step of checking an α value.

Trust Region Methods Trust region method is an alternative technique of line search to guarantee asymptotic convergence, which is also widely used in many machine learning applications (Lin, Weng, and Keerthi 2008). At the t-th iteration of a trust region method, we have the current iterate $\tilde{\boldsymbol{w}}^t$, a size Δ^t of trust region, and a quadratic model $q_t(\tilde{\boldsymbol{s}})$ as the approximation of the value $g(\tilde{\boldsymbol{w}}^t+\tilde{\boldsymbol{s}})-g(\tilde{\boldsymbol{w}}^t)$. Two common choices for $q_t(\tilde{\boldsymbol{s}})$ are the first-order approximation

$$q_t(\tilde{\boldsymbol{s}})=\nabla g(\tilde{\boldsymbol{w}}^t)^\top\tilde{\boldsymbol{s}}+\frac{1}{2}\tilde{\boldsymbol{s}}^\top\tilde{\boldsymbol{s}} \tag{1.14}$$

and the second-order approximation

$$q_t(\tilde{\boldsymbol{s}})=\nabla g(\tilde{\boldsymbol{w}}^t)^\top\tilde{\boldsymbol{s}}+\frac{1}{2}\tilde{\boldsymbol{s}}^\top\nabla^2 g(\tilde{\boldsymbol{w}}^t)\tilde{\boldsymbol{s}}. \tag{1.15}$$

Next we find $\tilde{\boldsymbol{s}}^t$ to approximately solve

$$\min_{\|\tilde{\boldsymbol{s}}\|\le\Delta^t} q_t(\tilde{\boldsymbol{s}}). \tag{1.16}$$

If (1.16) is the choice, we can apply conjugate gradient to obtain $\tilde{\boldsymbol{s}}^t$ with our efficient Hessian-vector product procedure in Algorithm 3. In Algorithm 4, we present a detailed conjugate gradient procedure to solve (1.16). See Lin, Weng, and Keerthi (2008) for more details about the convergence property and the implementation issues of Algorithm 4.

We then update $\tilde{\boldsymbol{w}}^t$ and Δ^t as follows:

$$\tilde{\boldsymbol{w}}^{t+1}=\begin{cases}\tilde{\boldsymbol{w}}^t+\tilde{\boldsymbol{s}} & \text{if } \rho^t>\eta_0,\\ \tilde{\boldsymbol{w}}^t & \text{otherwise,}\end{cases} \tag{1.17}$$

$$\Delta^{t+1}\in\begin{cases}[\sigma_1\min(\|\tilde{\boldsymbol{s}}^t\|,\Delta^t),\sigma_2\Delta^t] & \text{if } \rho^t\le\eta_1,\\ [\sigma_1\Delta^t,\sigma_3\Delta^t] & \text{if } \rho^t\in(\eta_1,\eta_2),\\ [\Delta^t,\sigma_3\Delta^t] & \text{if } \rho^t\ge\eta_2,\end{cases} \tag{1.18}$$

where ρ^t is the ratio of the actual reduction in the function to the predicted reduction in the quadratic model:

$$\rho^t = \frac{g(\tilde{\boldsymbol{w}}^t + \tilde{\boldsymbol{s}}^t) - g(\tilde{\boldsymbol{w}}^t)}{q_t(\tilde{\boldsymbol{s}}^t)},$$

and η_0, η_1, η_2, and $\sigma_1, \sigma_2, \sigma_3$ are pre-specified positive constants such that $\eta_1 < \eta_2 < 1$ and $\sigma_1 < \sigma_2 < 1 < \sigma_3$. The idea behind a trust region method is that if the ratio ρ^t is large enough, we can accept the current step $\tilde{\boldsymbol{s}}^t$ and enlarge the size of trust region Δ^t; otherwise, we reject the current step and shrink the size of trust region. More details can be found in Lin, Weng, and Keerthi (2008).

We can see that the computation of the ratio ρ^t requires a function value evaluation at $g(\tilde{\boldsymbol{w}}^t + \tilde{\boldsymbol{s}}^t)$ and $q_t(\tilde{\boldsymbol{s}}^t)$. To compute $g(\tilde{\boldsymbol{w}}^t + \tilde{\boldsymbol{s}}^t)$, we can apply Algorithm 1. To compute $q_t(\tilde{\boldsymbol{s}}^t)$, we can utilize our proposed algorithms as subroutines to perform a straightforward computation. For example, assume the second-order approximation in (1.15) is considered and the conjugate gradient described in Algorithm 4 is applied to solve (1.16). In the procedure in Algorithm 4, $\nabla g(\tilde{\boldsymbol{w}}^t)$ is required as an input. Further, we have the final residual vector

$$\boldsymbol{r}^{i^*} = -\nabla q_t(\bar{\boldsymbol{s}}^{i^*}) = -\nabla g(\tilde{\boldsymbol{w}}^t) - \nabla^2 g(\tilde{\boldsymbol{w}}^t)\bar{\boldsymbol{s}}^{i^*}$$

available when Algorithm 4 terminates, where i^* is the number of CG iterations performed, and $\tilde{\boldsymbol{s}}^t = \bar{\boldsymbol{s}}^{i^*}$. Then, we can compute

$$q_t(\tilde{\boldsymbol{s}}^t) = -\frac{1}{2}\Big(\big(-\nabla g(\tilde{\boldsymbol{w}}^t)\big)^\top \tilde{\boldsymbol{s}}^t - \big(\tilde{\boldsymbol{s}}^t\big)^\top \boldsymbol{r}^{i^*}\Big)$$

in $O(dk)$ time.

Supp-1.5 Complete Optimization Procedures

With the efficient procedures proposed in Section 3, we are able to implement many optimization algorithms to solve (7) such as gradient descent with line search, nonlinear conjugate gradient, truncated Newton methods with line search, and trust region Newton methods. To illustrate how Algorithms 1-3 are used in practice, in Algorithm 5, we use a trust region Newton method (TRON) (Lin, Weng, and Keerthi 2008) as an example to show the complete optimization procedure.

We give another Algorithm 6 to demonstrate the use of line search in a gradient descent method for solving (7). Note that we use a Newton direction in Algorithm 5 and a negative gradient direction in Algorithm 6, respectively, though in either algorithm any descent direction can be considered.

Algorithm 4 Conjugate gradient procedure to approximately solve the trust-region subproblem (1.16).

Input: $\nabla g(\tilde{\boldsymbol{w}}^t)$, a relative stopping parameter $\xi < 1$, and a size of trust region $\Delta^t > 0$

Output: $\tilde{\boldsymbol{s}}^t = \bar{\boldsymbol{s}}^{i^*}$ and $\boldsymbol{r}^{i^*} = -\nabla g(\tilde{\boldsymbol{w}}^t) - \nabla^2 g(\tilde{\boldsymbol{w}}^t)\tilde{\boldsymbol{s}}^t$

// Initialization
$\bar{\boldsymbol{s}}^0 = \underline{0}$ *// initial point*
$\boldsymbol{r}^0 = -\nabla g(\tilde{\boldsymbol{w}}^t)$ *// initial residual*
$\boldsymbol{d}^0 = \boldsymbol{r}^0$ *// initial direction*
for $i = 0, 1, 2, 3, \ldots$ (CG iterations) **do**
  if $\|\boldsymbol{r}^i\| \leq \xi\|\boldsymbol{r}^0\|$ **then**
    Stop the **for** loop and return $\tilde{\boldsymbol{s}}^t = \bar{\boldsymbol{s}}^i$ and $\boldsymbol{r}^i$
  Compute and store $\nabla^2 g(\tilde{\boldsymbol{w}}^t)\boldsymbol{d}^i$ by Algorithm 3
  $\alpha^i = \|\boldsymbol{r}^i\|^2 / \langle \boldsymbol{d}^i, \nabla^2 g(\tilde{\boldsymbol{w}}^t)\boldsymbol{d}^i \rangle$
  $\bar{\boldsymbol{s}}^{i+1} = \bar{\boldsymbol{s}}^i + \alpha^i \boldsymbol{d}^i$
  if $\|\bar{\boldsymbol{s}}^{i+1}\| \geq \Delta^t$ **then**
    Compute τ such that $\|\bar{\boldsymbol{s}}^i + \tau \boldsymbol{d}^i\| = \Delta^t$
    $\bar{\boldsymbol{s}}^{i+1} = \bar{\boldsymbol{s}}^i + \tau \boldsymbol{d}^i$
    $\boldsymbol{r}^{i+1} = \boldsymbol{r}^i - \tau \nabla^2 g(\tilde{\boldsymbol{w}}^t)\boldsymbol{d}^i$
    Stop the **for** loop and return $\tilde{\boldsymbol{s}}^t = \bar{\boldsymbol{s}}^{i+1}$ and $\boldsymbol{r}^{i+1}$
  $\boldsymbol{r}^{i+1} = \boldsymbol{r}^i - \alpha^i \nabla^2 g(\tilde{\boldsymbol{w}}^t)\boldsymbol{d}^i$
  $\beta^i = \|\boldsymbol{r}^{i+1}\|^2 / \|\boldsymbol{r}^i\|^2$
  $\boldsymbol{d}^{i+1} = \boldsymbol{r}^{i+1} + \beta^i \boldsymbol{d}^i$

Algorithm 5 A trust-region Newton method for (7).

Input: feature matrix $X = [\boldsymbol{x}_1, \dots, \boldsymbol{x}_m]^\top \in \mathbb{R}^{m\times d}$, label matrix $Y = [\boldsymbol{y}_1, \dots, \boldsymbol{y}_m]^\top \in \mathbb{R}^{m\times n}$, $H \in \mathbb{R}^{n\times k}$, and parameters k, λ_w, λ_g, $\boldsymbol{p}$, $\boldsymbol{q}$, $\bar{a}$, and an initial size $\Delta > 0$ of trust region. Choose positive constants $\eta_0, \eta_1 < \eta_2 < 1$ and $\sigma_1 < \sigma_2 < 1 < \sigma_3$.

$M = H^\top \operatorname{diag}(\boldsymbol{q}) H$ $\cdots O(nk^2)$
$\boldsymbol{d} = X^\top \boldsymbol{p}$ $\cdots O(\operatorname{nnz}(X))$
$\boldsymbol{k} = H^\top \boldsymbol{q}$ $\cdots O(nk)$
Compute $\boldsymbol{p}^\top \mathbf{1}_m$ and $\boldsymbol{q}^\top \mathbf{1}_n$ $\cdots O(m+n)$
$B = XW$, where $B = [\cdots, \boldsymbol{b}_i, \cdots]^\top$ $\cdots O(\operatorname{nnz}(X)k)$
$\hat{M} = \operatorname{diag}(\boldsymbol{p}) B M$ $\cdots O(mk^2)$
$\delta = \boldsymbol{d}^\top W \boldsymbol{k}$ $\cdots O(dk)$
$\hat{L} = LB$ $\cdots O(\operatorname{nnz}(L)k)$
$L^+ = \sum_{(i,j)\in\Omega^+} \ell_{ij}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j)$ $O(|\Omega^+|k)$
$L^- = \bar{a}^2(\boldsymbol{p}^\top \mathbf{1}_m)(\boldsymbol{q}^\top \mathbf{1}_n) + \left\langle B, \hat{M}\right\rangle - 2\bar{a}\delta$ $\cdots O(mk)$
obj $= L^+ + L^- + \lambda_w\left(\|W\|_F^2 + \lambda_g \left\langle B, \hat{L}\right\rangle\right)$
$\cdots O(dk + mk)$
// Compute gradient
$D_{ij}^+ = \ell_{ij}^{+\prime}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j), \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
$G = X^\top(D^+ H + 2\hat{M})$ $\cdots O(|\Omega^+|k + \operatorname{nnz}(X)k + mk^2)$
$G = G - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top + 2\lambda_w\lambda_g X^\top \hat{L}$
$\cdots O(dk + \operatorname{nnz}(X)k)$
// Pre-processing for Hessian-vector products
$\ell_{ij}^{+\prime\prime} = \ell_{ij}^{+\prime\prime}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j), \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
for $t = 1, 2, 3, \dots$ **do**
  // Solve (1.16) *approximately*
  Get $\tilde{\boldsymbol{s}} = \operatorname{vec}(S)$ and $\boldsymbol{r}^{i^*} = \operatorname{vec}(R)$ by Algorithm 4 with Δ
  // Compute $q_t(\tilde{\boldsymbol{s}})$
  $q_t(\tilde{\boldsymbol{s}}) = -\frac{1}{2}(-\langle G, S\rangle - \langle R, S\rangle)$ $\cdots O(dk)$
  // Compute $g(\tilde{\boldsymbol{w}}^t + \tilde{\boldsymbol{s}})$
  $W_{\text{new}} = W + S$ $\cdots O(dk)$
  $B_{\text{new}} = XW_{\text{new}}$ $\cdots O(\operatorname{nnz}(X)k)$
  $\hat{M} = \operatorname{diag}(\boldsymbol{p}) B_{\text{new}} M$ $O(mk^2)$
  $\delta = \boldsymbol{d}^\top W_{\text{new}} \boldsymbol{k}$ $\cdots O(dk)$
  $\hat{L} = LB_{\text{new}}$ $\cdots O(\operatorname{nnz}(L)k)$
  $L^+ = \sum_{(i,j)\in\Omega^+} \ell_{ij}(Y_{ij}, (\boldsymbol{w}_{\text{new}})_i^\top \boldsymbol{h}_j)$ $\cdots O(|\Omega^+|k)$
  $L^- = \bar{a}^2(\boldsymbol{p}^\top \mathbf{1}_m)(\boldsymbol{q}^\top \mathbf{1}_n) + \left\langle B_{\text{new}}, \hat{M}\right\rangle - 2\bar{a}\delta$
  $\cdots O(mk)$
  $\text{obj}_{\text{new}} = L^+ + L^- + \lambda_w\left(\|W_{\text{new}}\|_F^2 + \lambda_g \left\langle B_{\text{new}}, \hat{L}\right\rangle\right)$
  $\cdots O(mk + dk)$
  $\rho = (\text{obj}_{\text{new}} - \text{obj})/q_t(\tilde{\boldsymbol{s}})$ $\cdots O(1)$
  Update Δ based on ρ and (1.18) $\cdots O(1)$
  if $\rho > \eta_0$ **then**
    $\text{obj} = \text{obj}_{\text{new}}$ $\cdots O(1)$
    $W = W_{\text{new}}$ $\cdots O(dk)$
    $B = B_{\text{new}}$ $\cdots O(mk)$
    // Compute gradient
    $D_{ij}^+ = \ell_{ij}^{+\prime}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j), \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
    $G = X^\top(D^+ H + 2\hat{M})$
    $\cdots O(|\Omega^+|k + \operatorname{nnz}(X)k + mk^2)$
    $G = G - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top + 2\lambda_w\lambda_g X^\top \hat{L}$
    $\cdots O(dk + \operatorname{nnz}(X)k)$
    // Pre-processing for Hessian-vector products
    $\ell_{ij}^{+\prime\prime} = \ell_{ij}^{+\prime\prime}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j), \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$

Algorithm 6 A gradient-descent method with backtracking line search to minimize (7).

Input: feature matrix $X = [\boldsymbol{x}_1, \dots, \boldsymbol{x}_m]^\top \in \mathbb{R}^{m\times d}$, label matrix $Y = [\boldsymbol{y}_1, \dots, \boldsymbol{y}_m]^\top \in \mathbb{R}^{m\times n}$, $H \in \mathbb{R}^{n\times k}$, and parameters k, λ_w, λ_g, $\boldsymbol{p}$, $\boldsymbol{q}$, and $\bar{a}$. Choose $\beta < 1$ and $\sigma < 1/2$.

$M = H^\top \operatorname{diag}(\boldsymbol{q}) H$ $\cdots O(nk^2)$
$\boldsymbol{d} = X^\top \boldsymbol{p}$ $\cdots O(\operatorname{nnz}(X))$
$\boldsymbol{k} = H^\top \boldsymbol{q}$ $\cdots O(nk)$
Compute $\boldsymbol{p}^\top \mathbf{1}_m$ and $\boldsymbol{q}^\top \mathbf{1}_n$ $\cdots O(m+n)$
$B = XW$, where $B = [\cdots, \boldsymbol{b}_i, \cdots]^\top$ $\cdots O(mk^2)$
$\hat{M} = \operatorname{diag}(\boldsymbol{p}) B M$ $\cdots O(mk^2)$
$\hat{L} = LB$ $\cdots O(\operatorname{nnz}(L)k)$
$L^+ = \sum_{(i,j)\in\Omega^+} \ell_{ij}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j)$ $O(|\Omega^+|k)$
for $t = 1, 2, 3, \dots$ **do**
  // Compute gradient
  $D_{ij}^+ = \ell_{ij}^{+\prime}(Y_{ij}, \boldsymbol{b}_i^\top \boldsymbol{h}_j), \forall (i,j) \in \Omega^+$ $\cdots O(|\Omega^+|k)$
  $G = X^\top(D^+ H + 2\hat{M})$ $\cdots O(|\Omega^+|k + \operatorname{nnz}(X)k + mk^2)$
  $G = G - 2\bar{a}\boldsymbol{d}\boldsymbol{k}^\top + 2\lambda_w\lambda_g X^\top \hat{L}$ $\cdots O(dk + \operatorname{nnz}(X)k)$

  // Obtain a descent direction ΔW
  $\Delta W = -G$

  // Perform backtracking line search
  $\Delta B = X\Delta W$ $\cdots O(\operatorname{nnz}(X)k)$
  $\Delta\hat{M} = \operatorname{diag}(\boldsymbol{p})\Delta B M$ $\cdots O(mk^2)$
  $\Delta\delta = \boldsymbol{d}^\top \Delta W \boldsymbol{k}$ $\cdots O(dk)$
  $\Delta\hat{L} = L\Delta B$ $\cdots O(\operatorname{nnz}(L)k)$
  $\text{Val\_1} = \left\langle \Delta B, \hat{M}\right\rangle + \left\langle B, \Delta\hat{M}\right\rangle - 2\bar{a}\Delta\delta$
  $+2\lambda_w\left(\langle W, \Delta W\rangle + \lambda_g\left\langle B, \Delta\hat{L}\right\rangle\right) \cdots O(dk + mk)$
  $\text{Val\_2} = \left\langle \Delta B, \Delta\hat{M}\right\rangle$
  $+\lambda_w\left(\|\Delta W\|_F^2 + \lambda_g\left\langle \Delta B, \Delta\hat{L}\right\rangle\right) \cdots O(dk + mk)$
  $c = \langle G, \Delta W\rangle$ $\cdots O(dk)$
  for $\alpha = 1, \beta, \beta^2, \dots$ **do**
    $B_{\text{new}} = B + \alpha\Delta B$ $\cdots O(mk)$
    $L_{\text{new}}^+ = \sum_{(i,j)\in\Omega^+} \ell_{ij}(Y_{ij}, \boldsymbol{b}_i^{\text{new}\top} \boldsymbol{h}_j)$ $O(|\Omega^+|k)$
    if $-L^+ + L_{\text{new}}^+ + \alpha\text{Val\_1} + \alpha^2\text{Val\_2} < \alpha\sigma c$ **then**
      $W = W + \alpha\Delta W$ $\cdots O(dk)$
      $B = B_{\text{new}}$ $\cdots O(mk)$
      $\hat{M} = \hat{M} + \alpha\Delta\hat{M}$ $\cdots O(mk)$
      $\hat{L} = \hat{L} + \alpha\Delta\hat{L}$ $\cdots O(mk)$
      $L^+ = L_{\text{new}}^+$ $\cdots O(1)$
      Break the line-search **for**-loop

Supp-2 Experimental Details

Supp-2.1 Evaluation Criteria and Data Sources

We used Precision@k and nDCG@k as evaluation criteria. For a predicted score vector $\hat{\boldsymbol{y}} \in \mathbb{R}^L$ and the true label vector $\boldsymbol{y} \in \{0,1\}^L$, Precision@$k$ is defined as

$$p@k \equiv \frac{1}{k} \sum_{l \in \text{toprank}_k(\hat{\boldsymbol{y}})} y_l,$$

and nDCG@k is defined as

$$\text{DCG@}k \equiv \sum_{l \in \text{toprank}_k(\hat{\boldsymbol{y}})} \frac{y_l}{\log(l+1)},$$

$$\text{nDCG@}k \equiv \frac{\text{DCG@}k}{\sum_{l=1}^{\min(k, \|\boldsymbol{y}\|_0)} \frac{1}{\log(l+1)}}.$$

For multi-label learning, the data sets are downloaded from *Mulan: A Java Library for Multi-Label Learning*[3] and *The Extreme Classification Repository*.[4] To avoid the $0/0$ situation in the calculation of nDCG, data instances in the test set without any active labels (i.e., $\|\boldsymbol{y}\|_0 = 0$) are removed. For recommender systems with graph information, the data sources have been mentioned in the main text.

Supp-2.2 Parameter Selection

To select a suitable set of parameters, we hold out 1/5 of the training instances for multi-label problems. Similarly, we hold out 1/5 of the observed entries for graph structured one-class MF. The chosen parameters are those that give the highest validation performance on the hold out set. Since the best parameter for different measures ($p@1$ to $p@5$) may slightly vary, we used the one corresponding to the highest $p@5$. However, if the best parameter for $p@5$ has a very bad performance for other measures on the hold out set, we will choose the second best parameter for $p@5$.

For our methods, we fix $\bar{a}$ in (3) to -1 because of the following reasons. First, for LR-wLR, we have

$$\ell^+_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}) = \ell^-_{ij}(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})$$
$$= \log\Big(1 + e^{-Y_{ij} \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}}\Big),$$

where $Y_{ij} = \pm 1$. Therefore, for $(i,j) \in \Omega^-$, its $Y_{ij} = \bar{a}$ should be -1. For other formulations such as LR-wSQ, we have

$$\ell^-(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij}) = (\bar{a} - \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})^2.$$

The logistic loss $\ell^+(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})$ intends to have

$$(i,j) \in \Omega^+ \quad \text{if } \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij} \geq 0,$$

but for the squared loss $\ell^-(Y_{ij}, \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij})$, it intends to have

$$(i,j) \in \Omega^- \quad \text{if } \tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij} \approx 0.$$

Clearly, a conflict occurs when $\tilde{\boldsymbol{w}}^\top \tilde{\boldsymbol{x}}_{ij} > 0$ but ≈ 0. On the other hand, for LEML (Yu et al. 2014), which is SQ-SQ, we use $\bar{a} = 0$ in order be consistent with their experiment setting. For our methods that include a weighted loss (SQ-wSQ, LR-wSQ and LR-wLR), $p_i q_j$ in assumption (3) is set to a constant ρ. We perform a grid search for $\log_2(\rho) \in \{-9, -7, -5, -3, -1, 0\}$. For Subsampled approaches, we fix $\rho = 1$ and perform the grid search on the ratio $|\Omega^-|/|\Omega^+| \in \{0.25, 0.5, 1, 2\}$.

For regularization parameters λ_w and λ_h, we set $\lambda_w = \lambda_h$ and perform a grid search on $\log_2(\lambda_w) \in \{-6, -4, -2, 0, 2, 4, 6\}$. For problems without graph information, we set $\lambda_g = 0$. For problems with graph information, λ_g is non-zero and is obtained by a grid search on $\log_2(\lambda_g \lambda_w) \in \{-6, -3, 0, 3, 6, 8, 10\}$. We consider the same setting for LEML.

For the kernel Nyström method in the last experiment, we use the same regularization and weight-loss parameters selected earlier for the setting without the Nyström method. For the Gaussian kernel $K(\boldsymbol{x}, \boldsymbol{y}) = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{y}\|^2)$, we check $\gamma \in \{0.5/\sigma^2, 1/\sigma^2, 2/\sigma^2\}$, where σ^2 is the variance of all feature values in the entire training data set. We also conduct a grid search on the number of columns using $D \in \{500, 1000\}$.

For all one-class MF formulations, we run 15 alternating iterations in our validation process and obtain the validation performance at each iteration. We then use the iteration index yielding the best validation performance as the number of iterations to be run in training a model for predicting the test set. Note that the held-out validation set is included so we use the whole training set for generating the final model.

For the non-linear method SLEEC, since it includes 8 hyper-parameters, a grid search on this high dimensional space is not easy. Therefore we first fix the number of clusters to 1. Then the number of learners also becomes 1 because the use of several learners is due to the randomness in clustering. Next we conduct a grid search on the two most sensitive parameters: the k in kNN and the number of neighbors considered during the singular value projection method as suggested by the paper. For all other parameters we use the suggested values given by the authors.

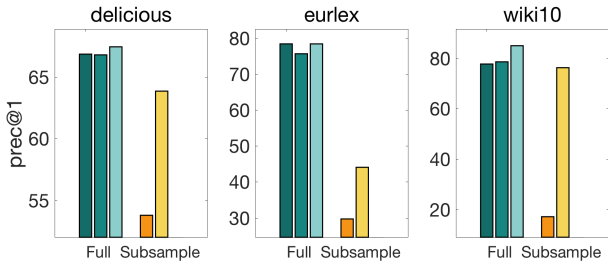
Supp-2.3 More Experimental Results

The results are shown in both tables and figures.

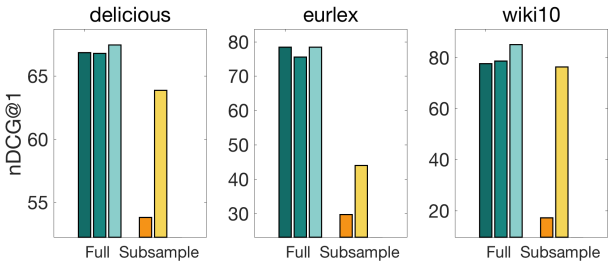
- In Figure Supp-1, we show the results of Full versus Subsampled for multi-label learning in bar charts.
- In Figure Supp-2 and Figure Supp-3, we show the results of various loss functions for three types of one-class MF problems in bar charts.
- In Figure Supp-4, we show the results of the comparison of non-linear multi-label classifiers in bar charts.
- In Table Supp-1, we show the detailed results of recommender systems with and without graph information in terms of precision@1 to precisions@5 and nDCG@1 to nDCG@5.
- In Table Supp-2, we show the detailed results of the comparison among non-linear multi-label classifiers in terms of precision@1 to precisions@5 and nDCG@1 to nDCG@5.
- In Table Supp-3, we show the detailed results of the multi-label learning in terms of precision@1 to precisions@5 and nDCG@1 to nDCG@5.

[3] http://mulan.sourceforge.net/datasets-mlc.html

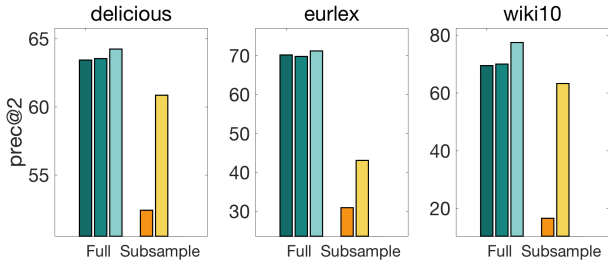
[4] https://manikvarma.github.io/downloads/XC/XMLRepository.html



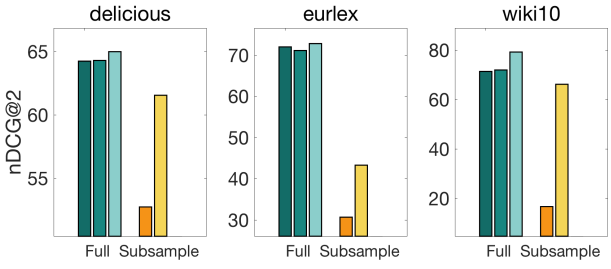
(a) Prediction Performance (precision).



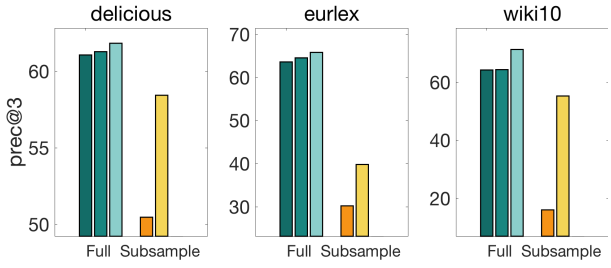
(b) Prediction Performance (nDCG).



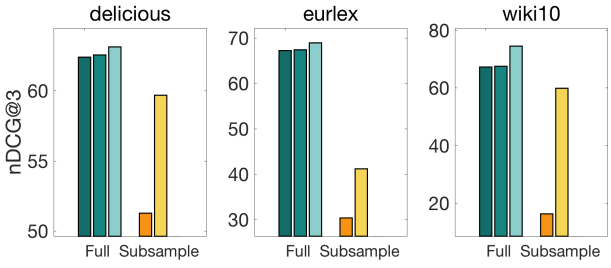
(c) Prediction Performance (precision).



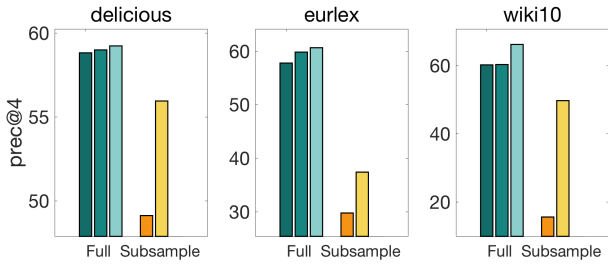
(d) Prediction Performance (nDCG).



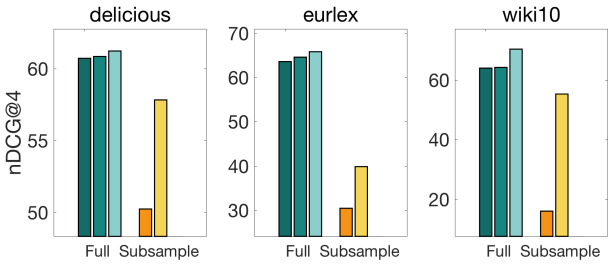
(e) Prediction Performance (precision).



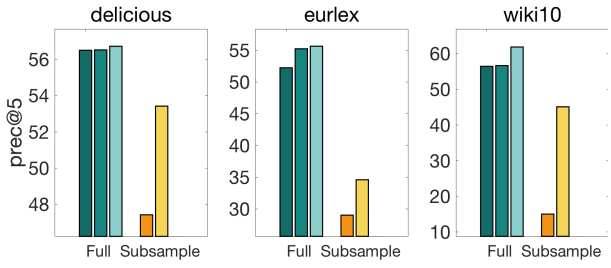
(f) Prediction Performance (nDCG).



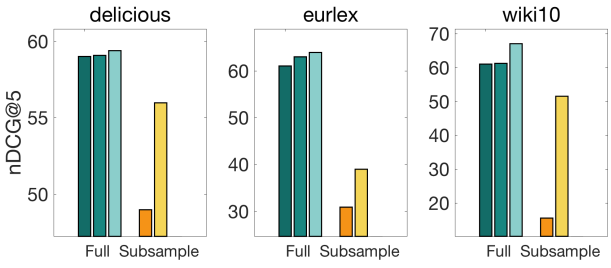
(g) Prediction Performance (precision).



(h) Prediction Performance (nDCG).

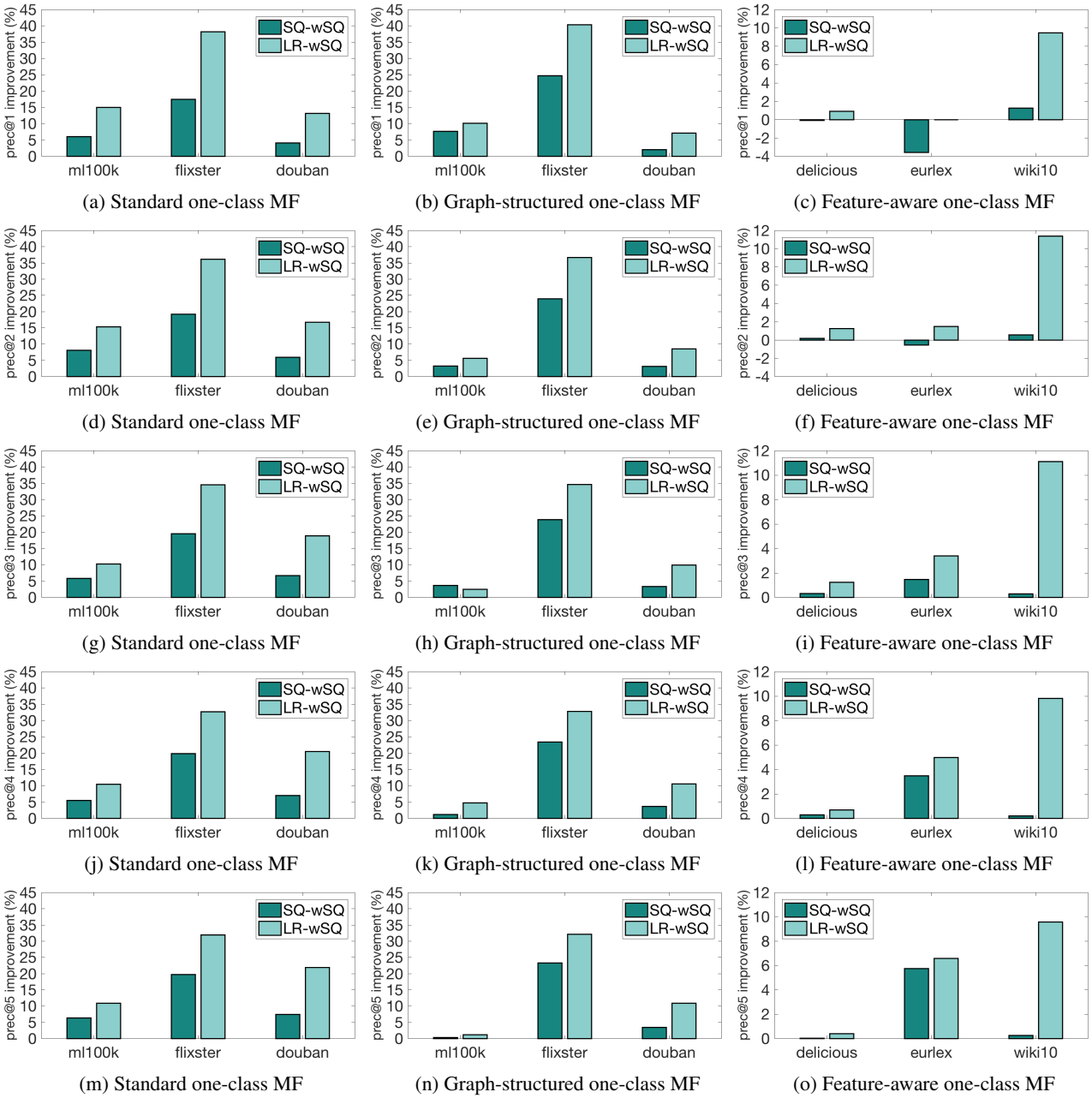


(i) Prediction Performance (precision).



(j) Prediction Performance (nDCG).

Figure Supp-1: Full v.s. Subsampled on multi-label learning with various loss functions. See Figure 1 for the legend information.



(a) Standard one-class MF (b) Graph-structured one-class MF (c) Feature-aware one-class MF

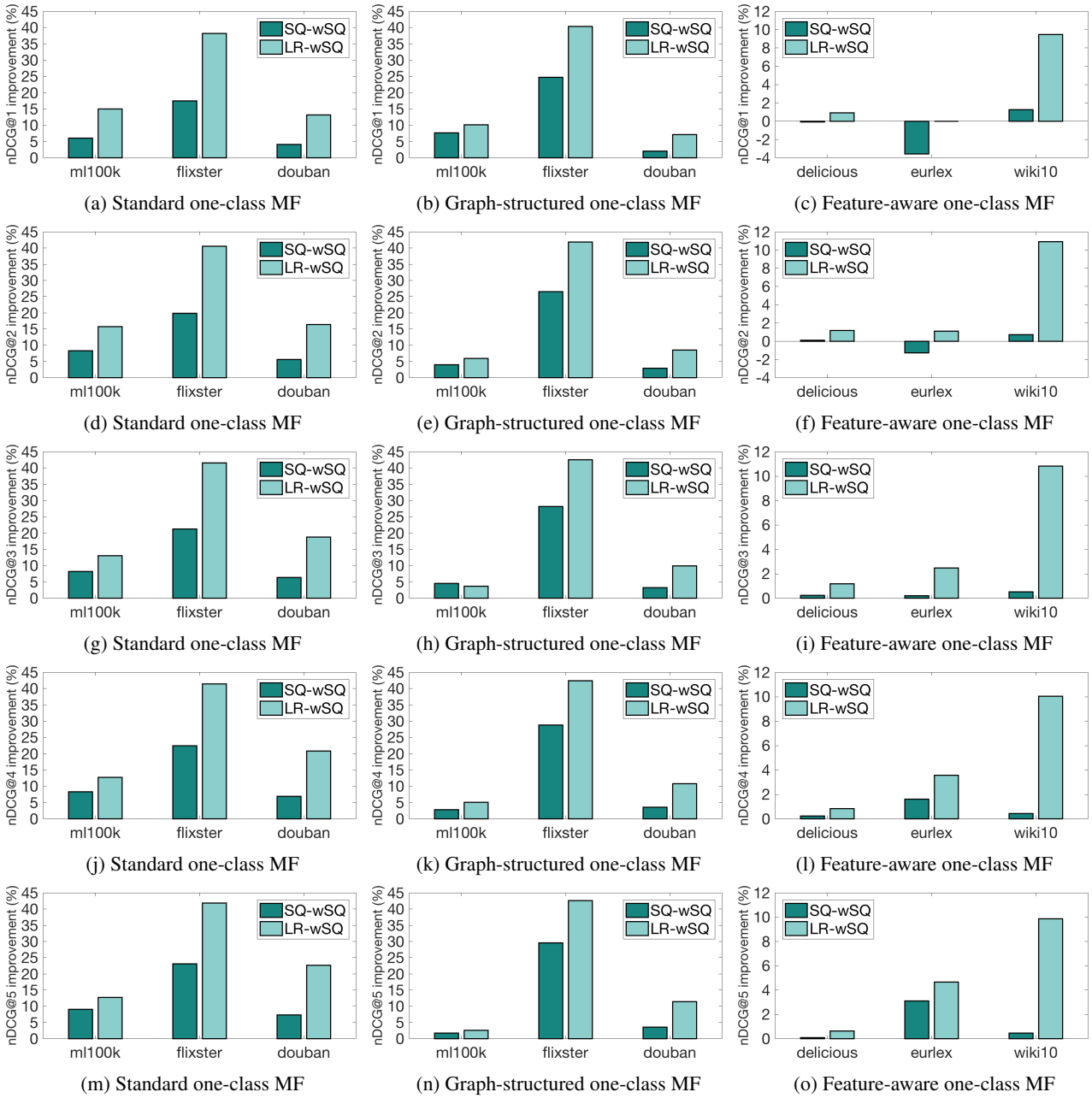
(d) Standard one-class MF (e) Graph-structured one-class MF (f) Feature-aware one-class MF

(g) Standard one-class MF (h) Graph-structured one-class MF (i) Feature-aware one-class MF

(j) Standard one-class MF (k) Graph-structured one-class MF (l) Feature-aware one-class MF

(m) Standard one-class MF (n) Graph-structured one-class MF (o) Feature-aware one-class MF

Figure Supp-2: Comparison on various loss functions. Y-axis is the improvement of Precision@k over the SQ-SQ formulation in percentage.



(a) Standard one-class MF (b) Graph-structured one-class MF (c) Feature-aware one-class MF

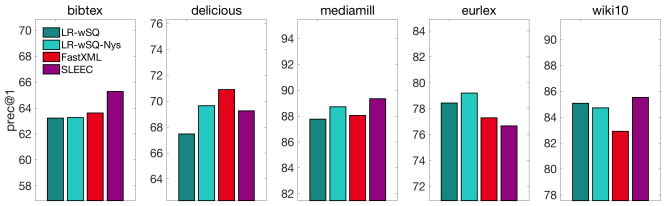
(d) Standard one-class MF (e) Graph-structured one-class MF (f) Feature-aware one-class MF

(g) Standard one-class MF (h) Graph-structured one-class MF (i) Feature-aware one-class MF

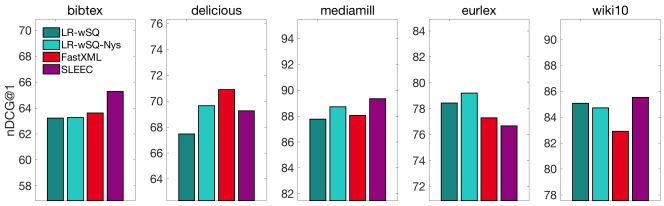
(j) Standard one-class MF (k) Graph-structured one-class MF (l) Feature-aware one-class MF

(m) Standard one-class MF (n) Graph-structured one-class MF (o) Feature-aware one-class MF

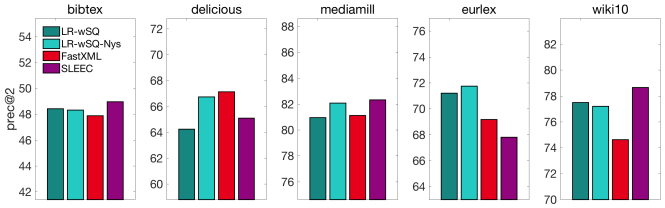
Figure Supp-3: Comparison on various loss functions. Y-axis is the improvement of nDCG@k over the SQ-SQ formulation in percentage.



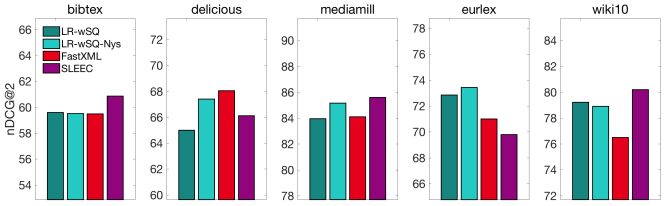
(a) Prediction Performance (precision).



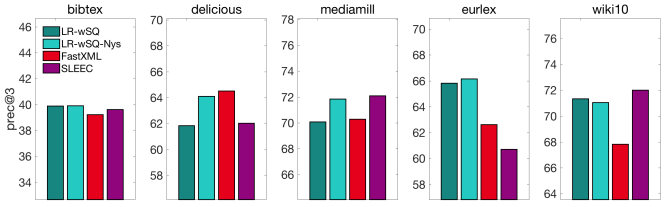
(b) Prediction Performance (nDCG).



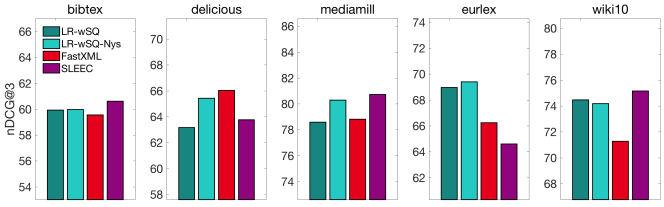
(c) Prediction Performance (precision).



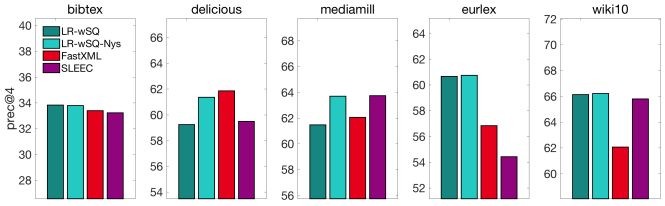
(d) Prediction Performance (nDCG).



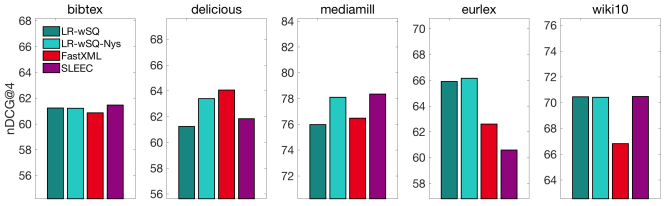
(e) Prediction Performance (precision).



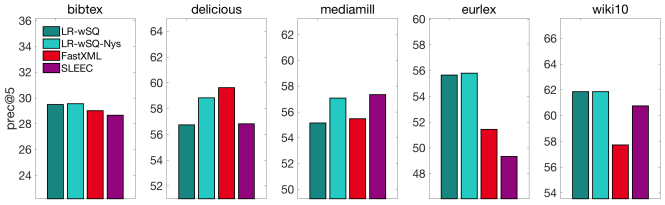
(f) Prediction Performance (nDCG).



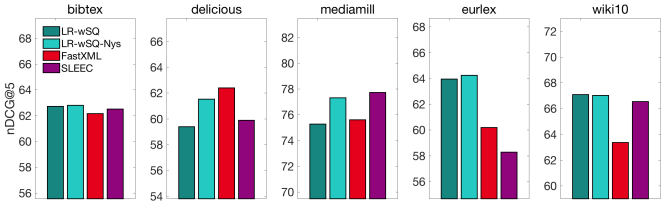
(g) Prediction Performance (precision).



(h) Prediction Performance (nDCG).



(i) Prediction Performance (precision).



(j) Prediction Performance (nDCG).

Figure Supp-4: Comparison on non-linear multi-label classifiers.

Table Supp-1: Comparison on graph structured one-class MF. Loss1-Loss2 denotes the formulation with the Loss1 on entries in Ω^+ and Loss2 on entries in Ω^-. wSQ/wLR denote the weighted square/logistic loss functions respectively. Note that the SQ-SQ formulation for the *graph structured one-class MF* part is equivalent to the formulation considered in Rao et al. (2015).

(a) Precision@k (b) nDCG@k

		time	p@1	p@2	p@3	p@4	p@5	n@1	n@2	n@3	n@4	n@5
					Standard one-class MF						*Standard one-class MF*	
ml100k	SQ-SQ	1.2	26.93	22.20	20.00	18.47	16.95	26.93	23.99	23.00	22.84	22.54
	SQ-wSQ	0.9	28.56	23.99	21.16	19.48	18.04	28.56	25.98	24.88	24.72	24.59
	LR-wSQ	1.8	30.98	25.61	22.04	20.41	18.80	30.98	27.76	26.00	25.75	25.42
					Graph structured one-class MF						*Graph structured one-class MF*	
	SQ-SQ	1.3	28.55	24.62	22.04	20.26	19.05	28.55	26.54	25.57	25.28	25.38
	SQ-wSQ	0.9	30.75	25.43	22.85	20.49	19.12	30.75	27.59	26.73	25.99	25.82
	LR-wSQ	7.0	31.45	26.01	22.58	21.21	19.28	31.45	28.12	26.50	26.55	26.04
					Standard one-class MF						*Standard one-class MF*	
flixster	SQ-SQ	23.7	14.87	12.41	10.96	10.06	9.35	14.87	14.46	14.44	14.64	14.84
	SQ-wSQ	51.2	17.46	14.79	13.09	12.05	11.19	17.46	17.33	17.51	17.94	18.26
	LR-wSQ	161.3	20.54	16.89	14.74	13.34	12.34	20.54	20.33	20.44	20.72	21.04
					Graph structured one-class MF						*Graph structured one-class MF*	
	SQ-SQ	27.4	14.66	12.37	10.97	10.06	9.35	14.66	14.35	14.38	14.59	14.78
	SQ-wSQ	54.0	18.28	15.34	13.60	12.42	11.53	18.28	18.16	18.43	18.80	19.15
	LR-wSQ	180.6	20.58	16.91	14.77	13.36	12.36	20.58	20.36	20.50	20.77	21.08
					Standard one-class MF						*Standard one-class MF*	
douban	SQ-SQ	64.8	17.42	15.07	13.56	12.47	11.62	17.42	15.84	14.97	14.44	14.09
	SQ-wSQ	100.3	18.13	15.97	14.47	13.35	12.48	18.13	16.74	15.93	15.43	15.13
	LR-wSQ	514.3	19.71	17.59	16.12	15.03	14.16	19.71	18.44	17.78	17.45	17.29
					Graph structured one-class MF						*Graph structured one-class MF*	
	SQ-SQ	58.3	18.89	16.61	15.07	13.97	13.11	18.89	17.41	16.60	16.14	15.89
	SQ-wSQ	75.0	19.27	17.12	15.58	14.47	13.56	19.27	17.93	17.14	16.71	16.45
	LR-wSQ	571.4	20.23	18.02	16.57	15.44	14.53	20.23	18.89	18.24	17.88	17.70

Table Supp-2: Comparison of state-of-the-art approaches on multi-label learning.

(a) Precision@k (b) nDCG@k

		time	p@1	p@2	p@3	p@4	p@5	n@1	n@2	n@3	n@4	n@5
bibtex	LR-wSQ	22	63.22	48.43	39.89	33.83	29.50	63.22	59.59	59.93	61.24	62.73
	LR-wSQ-Nys	54	63.26	48.33	39.91	33.80	29.55	63.26	59.53	59.97	61.21	62.81
	FastXML	17	63.62	47.89	39.22	33.39	29.01	63.62	59.49	59.55	60.87	62.16
	SLEEC	249	65.29	48.97	39.63	33.24	28.76	65.29	60.87	60.62	61.46	62.52
delicious	LR-wSQ	23	67.47	64.24	61.85	59.25	56.73	67.47	64.99	63.16	61.23	59.40
	LR-wSQ-Nys	94	69.64	66.74	64.11	61.35	58.84	69.64	67.41	65.43	63.39	61.54
	FastXML	34	70.90	67.14	64.52	61.87	59.63	70.90	68.05	66.04	64.06	62.40
	SLEEC	1,124	69.27	65.10	62.03	59.49	56.82	69.27	66.11	63.78	61.84	59.89
mediamill	LR-wSQ	61	87.77	80.96	70.08	61.48	55.15	87.77	83.96	78.60	75.97	75.28
	LR-wSQ-Nys	144	88.72	82.08	71.85	63.70	57.08	88.72	85.17	80.29	78.10	77.32
	FastXML	256	88.04	81.12	70.29	62.06	55.48	88.04	84.10	78.81	76.48	75.61
	SLEEC	1,764	89.34	82.33	72.09	63.73	57.34	89.34	85.60	80.73	78.36	77.73
eurlex	LR-wSQ	404	78.43	71.21	65.82	60.67	55.64	78.43	72.84	68.97	65.91	63.96
	LR-wSQ-Nys	1,134	79.20	71.75	66.15	60.75	55.80	79.20	73.44	69.41	66.15	64.25
	FastXML	164	77.29	69.17	62.63	56.84	51.44	77.29	71.00	66.25	62.60	60.19
	SLEEC	1,497	76.67	67.80	60.71	54.45	49.34	76.67	69.80	64.61	60.58	58.28
wiki10	LR-wSQ	449	85.07	77.50	71.33	66.14	61.85	85.07	79.21	74.47	70.46	67.10
	LR-wSQ-Nys	666	84.72	77.20	71.05	66.22	61.86	84.72	78.90	74.18	70.41	67.02
	FastXML	744	82.91	74.63	67.82	62.06	57.73	82.91	76.50	71.27	66.83	63.37
	SLEEC	183	85.52	78.65	72.00	65.81	60.75	85.52	80.20	75.16	70.48	66.55

Table Supp-3: Comparison of various Full and Subsampled formulations on multi-label learning. Loss1-Loss2 denotes the formulation with the Loss1 on entries in Ω^+ and Loss2 on entries in Ω^-. wSQ/wLR denote the weighted square/logistic loss functions respectively. Note that the Full approach with SQ-SQ is equivalent to the LEML (Yu et al. 2014) formulation.

		(a) Precision@k						(b) nDCG@k				
		time	p@1	p@2	p@3	p@4	p@5	n@1	n@2	n@3	n@4	n@5
bibtex	*the* Subsampled *approach*											
	SQ-SQ	12	46.04	23.16	31.31	27.59	24.63	46.04	45.47	46.71	48.87	50.66
	LR-LR	9	52.92	39.42	32.63	28.27	25.08	52.92	49.17	49.59	51.32	52.94
	the Full *approach*											
	SQ-SQ	13	63.14	47.58	38.77	33.09	28.81	63.14	58.99	58.95	60.34	61.71
	SQ-wSQ	12	63.30	48.35	39.78	33.74	29.37	63.30	59.61	59.96	61.26	62.65
	LR-wSQ	22	63.22	48.43	39.89	33.83	29.50	63.22	59.59	59.93	61.24	62.73
	LR-wLR	85	61.91	46.66	38.21	32.66	28.43	61.91	57.75	57.91	59.40	60.76
delicious	*the* Subsampled *approach*											
	SQ-SQ	8	53.80	52.42	50.46	49.13	47.41	53.80	52.73	51.28	50.26	49.02
	LR-LR	19	63.89	60.86	58.44	55.95	53.43	63.89	61.56	59.71	57.84	55.99
	the Full *approach*											
	SQ-SQ	3	66.88	63.44	61.09	58.84	56.51	66.88	64.24	62.42	60.72	59.03
	SQ-wSQ	8	66.81	63.55	61.29	59.01	56.52	66.81	64.31	62.57	60.86	59.07
	LR-wSQ	23	67.47	64.24	61.85	59.25	56.73	67.47	64.99	63.16	61.23	59.40
	LR-wLR	446	67.91	65.04	62.27	59.81	57.27	67.91	65.74	63.68	61.85	59.99
mediamill	*the* Subsampled *approach*											
	SQ-SQ	83	83.20	79.21	69.62	61.66	55.50	83.20	81.59	77.17	75.10	74.60
	LR-LR	93	87.62	80.72	69.87	61.37	55.08	87.62	83.74	78.39	75.82	75.15
	the Full *approach*											
	SQ-SQ	8	87.70	81.05	69.89	61.23	54.72	87.70	83.99	78.43	75.75	74.88
	SQ-wSQ	41	84.85	79.82	69.92	61.79	55.47	84.85	82.41	77.75	75.57	74.92
	LR-wSQ	61	87.77	80.96	70.08	61.48	55.15	87.77	83.96	78.60	75.97	75.28
	LR-wLR	437	87.78	81.17	70.38	61.85	55.33	87.78	84.17	78.87	76.33	75.50
eurlex	*the* Subsampled *approach*											
	SQ-SQ	93	29.75	30.94	30.23	29.75	29.04	29.75	30.67	30.38	30.47	30.92
	LR-LR	166	44.08	43.09	39.83	37.39	34.58	44.08	43.32	41.17	39.90	38.99
	the Full *approach*											
	SQ-SQ	335	78.43	70.18	63.67	57.80	52.21	78.43	72.04	67.30	63.63	61.12
	SQ-wSQ	672	75.63	69.79	64.60	59.82	55.21	75.63	71.11	67.45	64.66	63.02
	LR-wSQ	404	78.43	71.21	65.82	60.67	55.64	78.43	72.84	68.97	65.91	63.96
wiki10	*the* Subsampled *approach*											
	SQ-SQ	121	17.23	16.58	16.14	15.59	15.04	17.23	16.73	16.38	15.98	15.56
	LR-LR	764	76.30	63.29	55.28	49.72	45.09	76.30	66.23	59.91	55.40	51.62
	the Full *approach*											
	SQ-SQ	247	77.71	69.58	64.20	60.23	56.45	77.71	71.42	67.20	64.04	61.07
	SQ-wSQ	872	78.69	69.97	64.39	60.35	56.59	78.69	71.94	67.55	64.31	61.34
	LR-wSQ	449	85.07	77.50	71.33	66.14	61.85	85.07	79.21	74.47	70.46	67.10