

Generalized Low Rank Models

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Abstract

Principal components analysis (PCA) is a well-known technique for approximating a data set represented by a matrix by a low rank matrix. Here, we extend the idea of PCA to handle arbitrary data sets consisting of numerical, Boolean, categorical, ordinal, and other data types. This framework encompasses many well known techniques in data analysis, such as nonnegative matrix factorization, matrix completion, sparse and robust PCA, k -means, k -SVD, and maximum margin matrix factorization. The method handles heterogeneous data sets, and leads to coherent schemes for compressing, denoising, and imputing missing entries across all data types simultaneously. It also admits a number of interesting interpretations of the low rank factors, which allow clustering of examples or of features. We propose several parallel algorithms for fitting generalized low rank models, and describe implementations and numerical results.

This manuscript is a draft. Comments sent to udell@stanford.edu are welcome.

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1 Introduction

In application areas like machine learning and data mining, one is often confronted with large collections of high dimensional data. These data sets consist of many heterogeneous data types, with many missing entries. Exploratory data analysis is often difficult in this setting. To better understand a complex data set, one would like to be able to visualize key archetypes, to cluster examples, to find correlated features, to fill in missing entries, and to remove (or identify) spurious or noisy data points. These tasks are difficult because of the heterogeneity of the underlying data.

If the data sets consists only of numerical (real-valued) data, then a simple and well-known technique which supports these tasks is Principal Components Analysis (PCA). PCA finds a low rank matrix that minimizes the approximation error, in the least-squares sense, to the original data set.

We can extend PCA to approximate an arbitrary data set by extending the notion of approximation, replacing least-squares error with an appropriate loss function. We can also add regularization on the low dimensional factors to improve generalization error and avoid overfitting, or to impose or encourage some structure (such as sparsity) in the low dimensional factors. The resulting low rank representation of the data set then admits all the same interpretations familiar from the PCA context. Many of the problems we must solve to find these low rank representations will be familiar; we recover an optimization formulation of nonnegative matrix factorization, matrix completion, sparse and robust PCA, k -means, k -SVD, and maximum margin matrix factorization, to name just a few. In this paper, we use the term *generalized low rank model* (GLRM) to refer to any low rank approximation of a data set obtained by minimizing a loss function on the approximation error together with regularization of the low dimensional factors.

These low rank approximation problems are not convex, and in general cannot be solved globally and efficiently. There are however a few exceptions, which are known to have convex relaxations that are tight under certain conditions, and hence are efficiently (globally) solvable under these conditions. However, all of these approximation problems can be heuristically (locally) solved by methods that alternate between updating the two factors in the low rank approximation. Each step involves either a convex problem, or a nonconvex problem that is simple enough that we can solve it exactly. While these alternating methods need not find the globally best low rank approximation, they are often very useful and effective for the original data analysis problem.

1.1 Previous work

We are not the first to note that matrix factorization algorithms may be viewed in a unified framework, parametrized by a small number of modeling decisions. The first instance we find in the literature of this unified view appeared in [CDS01], extending PCA to any probabilistic model in the exponential family. Gordon's Generalized² Linear² models [Gor02] further extended the unified framework to loss functions derived from the generalized Bregman divergence of any convex function, which includes models such as Independent Components

Analysis (ICA). Nathan Srebro’s PhD thesis [SRJ04] summarizes a number of models extending the framework to other loss functions (*e.g.*, hinge loss and KL-divergence loss), and adding nuclear norm and max-norm regularization. In [SG08], the authors offer a complete view of the state of the literature on matrix factorization as of 2008 in Table 1 of their paper. They note that by changing the loss function and regularization, one may recover algorithms including PCA, weighted PCA, k -means, k -medians, ℓ_1 SVD, probabilistic latent semantic indexing (pLSI), nonnegative matrix factorization with ℓ_2 or KL-divergence loss, exponential family PCA, and MMMF. GLRMs include all of these models and many more.

Contributions. The present paper differs from previous work in a number of ways. First, we are consistently concerned with the *meaning* of applying these different loss functions and regularizers to approximate a data set. The generality of our view allows us to introduce a number of loss functions and regularizers that have not previously been considered. Moreover, our perspective enables us to extend these ideas to arbitrary data sets, rather than just matrices of real numbers.

A number of new considerations emerge when considering the problem so broadly. First, we must face the problem of comparing incomparable types. For example, we must choose a scaling to trade off the loss due to a misclassification of a categorical value with an error of 0.1 (say) in predicting a real value. Second, we require algorithms that can handle the full gamut of losses and regularizers, which may be smooth or nonsmooth, finite or infinite valued, with arbitrary domain. This work is the first to consider these problems in such generality, and therefore also the first to wrestle with the algorithmic consequences.

Finally, we present some new results on some old problems. For example, in Appendix A, we derive a formula for the solution to quadratically regularized PCA, and show that quadratically regularized PCA has no local nonglobal minima.

1.2 Organization

The organization of this paper is as follows. We first recall some properties of PCA and its common variations to familiarize the reader with our notation. We then generalize the regularization on the low dimensional factors, and the loss function on the approximation error. Returning to the setting of heterogeneous data, we extend these dimensionality reduction techniques to abstract data-types and to multi-dimensional loss functions. Finally, we address algorithms for fitting GLRMs, and describe some implementations of these algorithms that we have developed.

2 PCA and quadratically regularized PCA

Data matrix. In this section, we let $A \in \mathbf{R}^{m \times n}$ be a data matrix consisting of m examples each with n numerical features. Thus, $A_{ij} \in \mathbf{R}$ is the value of the j th feature in the i th example, the i th row of A is the vector of n feature values for the i th example, and the j th column of A is the vector of the j th feature across our set of m examples.

It is also common to represent other kinds of data in a numerical matrix. For example, Boolean data is often encoded as 1 (for true) and 0 (for false); ordinal data is often encoded using consecutive integers to represent the different levels of the variable; and categorical data is often encoded by creating a column for each possible value of the categorical variable, and representing the data using a 1 in the column corresponding to the right value, and 0 in all other columns. We will see more systematic and principled ways to deal with these data types, and others, in §4–6. For now, we assume the entries in the data matrix consist of real numbers.

2.1 PCA

PCA is one of the oldest and most widely used tools in data analysis [Pea01, Hot33]. We review some of its well-known properties here in order to set notation and as a warm-up to the variants presented later. PCA seeks a matrix $Z \in \mathbf{R}^{m \times n}$ of rank $k < \min(m, n)$ that best approximates A in the least-squares sense. The rank constraint can be encoded implicitly by expressing Z in factored form as $Z = XY$, with $X \in \mathbf{R}^{m \times k}$, $Y \in \mathbf{R}^{k \times n}$. The problem then reduces to choosing the matrices X and Y to minimize $\|A - XY\|_F^2$, where $\|\cdot\|_F$ is the Frobenius norm of a matrix, *i.e.*, the square root of the sum of the squares of the entries. We define $x_i \in \mathbf{R}^{1 \times n}$ to be the i th row of X , and $y_j \in \mathbf{R}^m$ to be the j th column of Y , and use this notation throughout this paper. Thus $x_i y_j = (XY)_{ij} \in \mathbf{R}$ denotes a dot or inner product.

The PCA problem can be expressed as

$$\text{minimize } \|A - XY\|_F^2 = \sum_{i=1}^m \sum_{j=1}^n (A_{ij} - x_i y_j)^2 \quad (1)$$

with variables X and Y .

We will give several interpretations of the low rank factorization (X, Y) solving (1) in §2.5. But for now we note that (1) can be interpreted as a method for compressing the n features in the original data set to $k < n$ new features. The row vector x_i is associated with example i ; we can think of it as a feature vector for the example using the compressed set of $k < n$ features. The column vector y_j is associated with the original feature j ; it can be interpreted as the mapping from the original feature j into the k new features.

2.2 Quadratically regularized PCA

We can add quadratic regularization on X and Y to the objective. The quadratically regularized PCA problem is

$$\text{minimize } \sum_{i=1}^m \sum_{j=1}^n (A_{ij} - x_i y_j)^2 + \gamma \sum_{i=1}^m \|x_i\|_2^2 + \gamma \sum_{j=1}^n \|y_j\|_2^2, \quad (2)$$

with variables $X \in \mathbf{R}^{m \times d}$ and $Y \in \mathbf{R}^{d \times n}$, and regularization parameter $\gamma \geq 0$. Problem (2) can be written more concisely in matrix form,

$$\text{minimize } \|A - XY\|_F^2 + \gamma \|X\|_F^2 + \gamma \|Y\|_F^2. \quad (3)$$

When $\gamma = 0$, the problem reduces to PCA (1).

2.3 Solution methods

Singular value decomposition. It is well known that a solution to (1) can be obtained from the *singular value decomposition* (SVD) of A . The (compact) SVD of A is given by $A = U\Sigma V^T$, where $U \in \mathbf{R}^{m \times r}$ and $V \in \mathbf{R}^{n \times r}$ have orthonormal columns, and $\Sigma = \mathbf{diag}(\sigma_1, \dots, \sigma_r) \in \mathbf{R}^{r \times r}$, with $\sigma_1 \geq \dots \geq \sigma_r > 0$ and $r = \text{Rank}(A)$. The columns of $U = [u_1 \cdots u_r]$ and $V = [v_1 \cdots v_r]$ are called the left and right singular vectors of A , respectively, and $\sigma_1, \dots, \sigma_r$ are called the singular values of A .

It is less well known that a solution to the quadratically regularized PCA problem can be obtained in the same way. Define

$$\tilde{U} = [u_1 \cdots u_k], \quad \tilde{\Sigma} = \mathbf{diag}((\sigma_1 - \gamma)_+, \dots, (\sigma_k - \gamma)_+), \quad \tilde{V} = [v_1 \cdots v_k], \quad (4)$$

where $(x)_+ = \max(x, 0)$. Here we have both *truncated* the SVD to keep only the top k singular vectors and values, and performed *soft-thresholding* on the singular values to reduce their values by γ . A solution to the quadratically regularized PCA problem (2) is then given by

$$X = \tilde{U}\tilde{\Sigma}^{1/2}, \quad Y = \tilde{\Sigma}^{1/2}\tilde{V}^T. \quad (5)$$

(See Appendix A for a proof.) For $\gamma = 0$, the solution reduces to the familiar solution to PCA (1) obtained by truncating the SVD to the top k singular values.

The solution to (2) is clearly not unique: if X, Y is a solution, then so is $XT, T^{-1}Y$ for any orthogonal matrix $T \in \mathbf{R}^{k \times k}$. For PCA ($\gamma = 0$), the set of solutions is significantly larger: $XG, G^{-1}Y$ is a solution for any invertible matrix $G \in \mathbf{R}^{k \times k}$. If $\sigma_k > \sigma_{k+1}$, then all solutions to (2) have this form.

Alternating minimization. Problem (2) is the only problem we will encounter that has an analytical solution, or, indeed, one that we can compute efficiently. Here we mention an alternative method for solving (2), that can be scaled to large problems using parallel computing, and generalizes to the extensions of PCA that we will discuss below. The *alternating minimization* algorithm simply alternates between minimizing the objective over the variable X , holding Y fixed, and then minimizing over Y , holding X fixed. With initial guesses for the factors X^0 and Y^0 , we repeat the iteration

$$\begin{aligned} X^{l+1} &= \underset{X}{\operatorname{argmin}} \left(\sum_{i=1}^m \sum_{j=1}^n (A_{ij} - x_i y_j^l)^2 + \gamma \sum_{i=1}^m \|x_i\|_2^2 \right) \\ Y^{l+1} &= \underset{Y}{\operatorname{argmin}} \left(\sum_{i=1}^m \sum_{j=1}^n (A_{ij} - x_i^l y_j)^2 + \gamma \sum_{j=1}^n \|y_j\|_2^2 \right) \end{aligned}$$

for $l = 1, \dots$ until a stopping condition is satisfied. (If X and Y are full rank, the minimizers above are unique; when they are not, we can take any minimizer.)

This algorithm does not always work; in particular, it has stationary points that are not solutions of problem (2). But all *stable* stationary points of the iteration are solutions (see

Appendix A), so as a practical matter, the alternating minimization method always works, *i.e.*, the objective converges to the optimal value. The objective function is nonincreasing at each iteration, and therefore bounded. This implies, for $\gamma > 0$, that the iterates X^k and Y^k are bounded.

Parallelizing alternating minimization. The alternating minimization approach parallelizes easily over examples and features. The problem of minimizing over X splits into m independent minimization problems. We can solve the simple quadratic problems

$$\text{minimize } \sum_{j=1}^n (A_{ij} - x_i y_j)^2 + \gamma \|x_i\|_2^2 \quad (6)$$

with variable x_i , in parallel, for $i = 1, \dots, m$. Similarly, the problem of minimizing over Y splits into n independent quadratic problems,

$$\text{minimize } \sum_{i=1}^m (A_{ij} - x_i y_j)^2 + \gamma \|y_j\|_2^2 \quad (7)$$

with variable y_j , which can be solved in parallel for $j = 1, \dots, n$.

Caching factorizations. We can speed up the solution of the quadratic problems using a simple factorization caching technique.

For ease of exposition, we assume here that X and Y have full rank k . Notice that the updates (6) and (7) can be rewritten as

$$X = AY^T(YY^T + \gamma I)^{-1}, \quad Y = (X^T X + \gamma I)^{-1} X^T A.$$

We show below how to efficiently compute $X = AY^T(YY^T + \gamma I)^{-1}$; the Y update admits a similar speedup using the same ideas.

First compute the Gram matrix $G = YY^T$ using an outer product expansion

$$G = \sum_{j=1}^n y_j y_j^T.$$

This sum can be computed on-line by streaming over the index j , or in parallel, split over the index j . This property allows us to scale up to extremely large problems even if we cannot store the entire matrix Y in memory. The computation of the Gram matrix requires $2k^2 n$ floating point operations (flops), but is trivially parallelizable: with r workers, we can expect a speedup on the order of r . We next add the diagonal matrix γI to G in k flops, and form the Cholesky factorization of $G + \gamma I$ in $k^3/3$ flops and cache the factorization.

In parallel over the rows of A , we compute $D = AY^T$ ($2kn$ flops per row), and use the factorization of $G + \gamma I$ to compute $D(G + \gamma I)^{-1}$ with two triangular solves ($2k^2$ flops per row). These computations are also trivially parallelizable: with r workers, we can expect a speedup on the order of r .

Hence the total time required for each update with r workers scales as $\mathcal{O}\left(\frac{k^2(m+n)+kmn}{r}\right)$. For small k , the time is dominated by the computation of AY^T .

2.4 Missing data and matrix completion

Suppose we observe only entries A_{ij} for $(i, j) \in \Omega \subset \{1, \dots, m\} \times \{1, \dots, n\}$ from the matrix A , so the other entries are unknown. Then to find a low rank matrix that fits the data well, we solve the problem

$$\text{minimize } \sum_{(i,j) \in \Omega} (A_{ij} - x_i y_j)^2 + \gamma \|X\|_F^2 + \gamma \|Y\|_F^2, \quad (8)$$

with variables X and Y , with $\gamma > 0$. There are two very different regimes in which solving this problem may be useful.

Imputing missing entries. Consider a matrix A in which very few entries are missing. The typical approach in data analysis is to simply remove those rows with missing entries from the matrix and exclude them from subsequent analysis. If instead we solve the problem above *without* removing these affected rows, we “borrow strength” from the entries that are *not* missing to improve our global understanding of the data matrix A . Furthermore, the solution gives an estimate $x_i y_j$ for the value of those entries $(i, j) \notin \Omega$ that were not observed. In this regime we are imputing the (few) missing entries of A , using the examples that ordinarily we would discard.

Low rank matrix completion. Now consider a matrix A in which most entries are missing, *i.e.*, we only observe relatively few of the mn elements of A , so that by discarding every example with a missing feature or every feature with a missing example, we would discard the *entire* matrix. Then the solution to (8) becomes even more interesting: we are guessing all the entries of a (presumed low rank) matrix, given just a few of them. It is a surprising recent result that this is possible: if at least $|\Omega| = O(nk \log n)$ entries are observed, then the solution to (8) exactly recovers the matrix A with high probability [KMO10].

Alternating minimization. The problem (8) has no known analytical solution, but it is still easy to find a local minimum using alternating minimization. Alternating minimization has been shown to converge geometrically to the global solution when the initial values of X and Y are chosen carefully [JNS13], but in general the method should be considered a heuristic.

2.5 Interpretations and applications

The recovered matrices X and Y in the quadratically regularized PCA problems (2) and (8) admit a number of interesting interpretations. We introduce some of these interpretations now; the terminology we use here will recur throughout the paper.

Feature compression. Quadratically regularized PCA (2) can be interpreted as a method for compressing the n features in the original data set to $k < n$ new features. The row vector x_i is associated with example i ; we can think of it as a feature vector for the example using

the compressed set of $k < n$ features. The column vector y_j is associated with the original feature j ; it can be interpreted as the mapping from the original feature j into the k new features.

Archetypes. We can think of each row of Y as an *archetype* which captures the behavior of one of k idealized and maximally informative examples. These archetypes might also be called profiles, factors, or atoms. Every example $i = 1, \dots, m$ is then represented by row x_i as a linear combination of these archetypes. The coefficient x_{il} gives the resemblance or loading of example i to the l th archetype.

Archotypical representations. We call x_i the *representation* of example i in terms of the archetypes. The rows of X give an embedding of the examples into \mathbf{R}^k , where each coordinate axis corresponds to a different archetype. If the archetypes are simple to understand or interpret, then the representation of an example can provide better intuition about that example.

The examples can be clustered according to their representations in order to determine a group of similar examples. Indeed, one might choose to apply any machine learning algorithm to the representations x_i rather than to the initial data matrix: in contrast to the initial data, which may consist of high dimensional vectors with noisy or missing entries, the representations x_i will be low dimensional, regularized, and complete.

Feature representations. The columns of Y embed the features into \mathbf{R}^k . Here, we think of the columns of X as archotypical features, and represent each feature j as a linear combination of the archotypical features. Just as with the examples, we might choose to apply any machine learning algorithm to the feature representations. For example, we might find clusters of similar features that represent redundant measurements.

Latent variables. Each row of X represents an example by a vector in \mathbf{R}^k . The matrix Y maps these representations back into \mathbf{R}^m . We might think of X as discovering the *latent variables* that best explain the observed data. If the approximation error $\sum_{(i,j) \in \Omega} (A_{ij} - x_i y_j)^2$ is small, then we view these latent variables as providing a good explanation or summary of the full data set.

Probabilistic interpretation. We can give a probabilistic interpretation of X and Y . We suppose that the matrices \bar{X} and \bar{Y} have entries which are generated by taking independent samples from a normal distribution with mean 0 and variance γ^{-1} for $\gamma > 0$. The entries in the matrix $\bar{X}\bar{Y}$ are observed with noise $\eta_{ij} \in \mathbf{R}$,

$$A_{ij} = (\bar{X}\bar{Y})_{ij} + \eta_{ij},$$

where the noise η in the (i, j) th entry is sampled independently from a standard normal distribution. We observe each entry $(i, j) \in \Omega$. Then to find the maximum a posteriori

(MAP) estimator (X, Y) of (\bar{X}, \bar{Y}) , we solve

$$\text{maximize } \exp\left(-\frac{\gamma}{2}\|\bar{X}\|_F^2\right) \exp\left(-\frac{\gamma}{2}\|\bar{Y}\|_F^2\right) \prod_{(i,j) \in \Omega} \exp\left(-(A_{ij} - x_i y_j)^2\right),$$

which is equivalent, by taking logs, to (2).

This interpretation explains the recommendation we gave above for imputing missing observations $(i, j) \notin \Omega$. We simply use the MAP estimator $x_i y_j$ to estimate the missing entry $(\bar{X}\bar{Y})_{ij}$. Similarly, we can interpret $(XY)_{ij}$ for $(i, j) \in \Omega$ as a denoised version of the observation A_{ij} .

Auto-encoder. The matrix X encodes the data; the matrix Y decodes it back into the full space. We can view PCA as providing the best linear auto-encoder for the data; among all bilinear low rank encodings (X) and decodings (Y) of the data, PCA minimizes the squared reconstruction error.

Compression. We impose an *information bottleneck* [TPB00] on the data by using a low rank auto-encoder to fit the data. PCA finds X and Y to maximize the information transmitted through this k -dimensional information bottleneck. We can interpret the solution as a compressed representation of the data, and use it to efficiently store or transmit the information present in the original data.

2.6 Offsets and scaling

For good practical performance of a generalized low rank model, it is critical to ensure that model assumptions match the data. We saw above in §2.5 that quadratically regularized PCA corresponds to a model in which features are observed with $\mathcal{N}(0, 1)$ errors. If instead each column j of XY is observed with $\mathcal{N}(\mu_j, \sigma_j^2)$ errors, our model is no longer unbiased, and may fit very poorly, particularly if some of the column means μ_j are large.

For this reason it is standard practice to *standardize* the data before applying PCA or quadratically regularized PCA: the column means are subtracted from each column, and the columns are normalized by their variances. (This can be done approximately; there is no need to get the scaling and offset exactly right.) Formally, define $n_j = |\{i : (i, j) \in \Omega\}|$, and let

$$\mu_j = \frac{1}{n_j} \sum_{(i,j) \in \Omega} A_{ij} \quad \sigma_j^2 = \frac{1}{n_j - 1} \sum_{(i,j) \in \Omega} (A_{ij} - \mu_j)^2$$

estimate the mean and variance of each column of the data matrix. PCA or quadratically regularized PCA is then applied to the matrix whose (i, j) th entry is $(A_{ij} - \mu_j)/\sigma_j$.

3 Generalized regularization

It is easy to see how to extend PCA to allow arbitrary regularization on the rows of X and columns of Y . We form the *regularized PCA problem*

$$\text{minimize } \sum_{(i,j) \in \Omega} (A_{ij} - x_i y_j)^2 + \sum_{i=1}^m r_i(x_i) + \sum_{j=1}^n \tilde{r}_j(y_j), \quad (9)$$

with variables x_i and y_j , with given regularizers $r_i : \mathbf{R}^k \rightarrow \mathbf{R} \cup \{\infty\}$ and $\tilde{r}_j : \mathbf{R}^k \rightarrow \mathbf{R} \cup \{\infty\}$ for $i = 1, \dots, n$ and $j = 1, \dots, m$. Regularized PCA (9) reduces to quadratically regularized PCA (2) when $r_i = \gamma \|\cdot\|_2^2$, $\tilde{r} = \gamma \|\cdot\|_2^2$. We do not restrict the regularizers to be convex.

The objective in problem (9) can be expressed compactly in matrix notation as

$$\|A - XY\|_F^2 + r(X) + \tilde{r}(Y),$$

where $r(X) = \sum_{i=1}^n x_i$ and $\tilde{r}(Y) = \sum_{j=1}^m y_j$. Note that the regularization functions r and \tilde{r} are separable across the rows of X , and the columns of Y , respectively.

Infinite values of r_i and \tilde{r}_j are used to enforce constraints on the values of X and Y . For example, the regularizer

$$r_i(x) = \begin{cases} 0 & x \geq 0 \\ \infty & \text{otherwise,} \end{cases}$$

the indicator function of the nonnegative orthant, imposes the constraint that x_i be nonnegative.

Solutions to (9) need not be unique, depending on the choice of regularizers. If X and Y are a solution, then so are XT and $T^{-1}Y$, where T is any nonsingular matrix that satisfies $r(UT) = r(U)$ for all U and $\tilde{r}(T^{-1}V) = \tilde{r}(V)$ for all V .

By varying our choice of regularizers r and \tilde{r} , we are able to represent a wide range of known models, as well as many new ones. We discuss a number of choices for regularizers below.

3.1 Solution methods

In general, there is no analytical solution for (9). The problem is not convex, even when r and \tilde{r} are convex. However, when r and \tilde{r} are convex, the problem is bi-convex: it is convex in X when Y is fixed, and convex in Y when X is fixed.

Alternating minimization. There is no reason to believe that alternating minimization will always converge to the global minimum of the regularized PCA problem (9); indeed, we will see many cases below in which the problem is known to have many local minima. However, alternating minimization can still be applied in this setting, and it still parallelizes easily over the rows of X and columns of Y . To minimize over X , we solve, in parallel,

$$\text{minimize } \sum_{j:(i,j) \in \Omega} (A_{ij} - x_i y_j)^2 + r_i(x_i) \quad (10)$$

with variable x_i , for $i = 1, \dots, m$. Similarly, to minimize over Y , we solve, in parallel,

$$\text{minimize } \sum_{i:(i,j) \in \Omega} (A_{ij} - x_i y_j)^2 + \tilde{r}_i(y_j) \quad (11)$$

with variable y_j , for $j = 1, \dots, n$.

When the regularizers are convex, these problems are convex. When the regularizers are not convex, there are still many cases in which we can find analytical solutions to the nonconvex subproblems (10) and (11), as we will see below. A number of concrete algorithms, in which these subproblems are solved explicitly, are given in §7.

Caching factorizations. Often, the X and Y updates (10) and (11) reduce to convex quadratic programs. For example, this is the case for nonnegative matrix factorization, sparse PCA, and quadratic mixtures (which we define and discuss below in §3.2). The same factorization caching of the Gram matrix that was described above in the case of PCA can be used here to speed up the solution of these updates. Variations on this idea are described in detail in §7.3.

3.2 Examples

Here and throughout the paper, we present a set of examples chosen for pedagogical clarity, not for completeness. In all of the examples below, $\gamma > 0$ is a parameter that controls the strength of the regularization, and we drop the subscripts from r (or \tilde{r}) to lighten the notation. Of course, it is possible to mix and match these regularizers, *i.e.*, to choose different r_i for different i , and choose different \tilde{r}_j for different j .

Nonnegative matrix factorization. Consider the regularized PCA problem (9) with $r = I_+$ and $\tilde{r} = I_+$, where I_+ is the indicator function of the nonnegative reals. (Here, and throughout the paper, we define the indicator function of a set C , to be 0 when its argument is in C and ∞ otherwise.) Then a solution to problem (9) gives the matrix best approximating A that has a nonnegative factorization (*i.e.*, a factorization into elementwise nonnegative matrices) [LS99]. The nonnegative matrix factorization problem has a rich analytical structure [BRRT12, DS14] and a wide range of uses in practice [LS99, SBPP06, BBL⁺07, Vir07, KP07, FBD09]; hence the literature on it is extensive, and a number of specialized algorithms and codes for it are available [LS01, Lin07, KP08a, KP08b, BDKP14, KHP14, KP11].

We can also replace the nonnegativity constraint with any interval constraint; for example, r and \tilde{r} can be 0 if all entries of X and Y , respectively, are between 0 and 1, and infinite otherwise.

Sparse PCA. If very few of the coefficients of X and Y are nonzero, it can be easier to interpret the archetypes and representations. We can understand each archetype using only a small number of features, and can understand each example as a combination of only a small number of archetypes. To get a sparse version of PCA, we use a sparsifying penalty as the regularization. Many variants on this basic idea have been proposed [dEGJL04, ZHT06, SH08, Mac09, RTA12].

For example, we could enforce that no entry A_{ij} depend on more than s columns of X or of Y by setting r to be the indicator function of a s -sparse vector, *i.e.*,

$$r(x) = \begin{cases} 0 & \mathbf{card}(x) \leq s \\ \infty & \text{otherwise.} \end{cases}$$

and defining $\tilde{r}(y)$ similarly, where $\mathbf{card}(x)$ denotes the cardinality (number of nonzeros) in the vector x . The updates (10) and (11) are not convex, but one can find approximate

solutions using a pursuit algorithm (see, *e.g.*, [CDS98, TG07]), or exact solutions (for small s) using the branch and bound method [LW66, BM03].

This regularization can be relaxed to a convex, but still sparsifying, penalty by letting $r(x) = \gamma\|x\|_1$, $\tilde{r}(y) = \gamma\|y\|_1$ [ZHT06].

Orthogonal nonnegative matrix factorization. One well known property of PCA is that the principal components obtained (*i.e.*, the columns of X and rows of Y) are orthogonal (*i.e.*, $X^T X$ and $Y Y^T$ are both diagonal). When performing nonnegative matrix factorization, we might also want to obtain orthogonal factors. However, due to the nonnegativity of the matrix, two columns of X cannot be orthogonal if they both have a nonzero in the same row. Conversely, if X has only one nonzero per row, then its columns are mutually orthogonal. That is, orthogonal nonnegative matrix factorization requires X to be 1-sparse and nonnegative. Hence orthogonal nonnegative matrix factorization can be achieved by using the regularizer

$$r(x) = \begin{cases} 0 & \mathbf{card}(x) = 1, \quad x \geq 0 \\ \infty & \text{otherwise,} \end{cases}$$

and letting $\tilde{r}(y)$ be the indicator of the nonnegative orthant, as in NNMF.

Geometrically, we can interpret this problem as modeling the data A as a union of rays. Each row of Y , interpreted as a point in \mathbf{R}^n , defines a ray from the origin passing through that point. Orthogonal nonnegative matrix factorization models each row of X as a point along one of these rays.

Some authors [DLPP06] have also considered how to obtain a *bi-orthogonal* nonnegative matrix factorization, in which both X and Y^T have orthogonal columns. By the same argument as above, we see this is equivalent to requiring both X and Y^T to have only one positive entry per row, with the other entries equal to 0.

Max-norm matrix factorization. We take $r = \tilde{r} = \phi$ with

$$\phi(x) = \begin{cases} 0 & \|x\|_2^2 \leq \mu \\ \infty & \text{otherwise.} \end{cases}$$

This penalty enforces that

$$\|X\|_{2,\infty}^2 \leq \mu, \quad \|Y^T\|_{2,\infty}^2 \leq \mu,$$

where the $(2, \infty)$ norm of a matrix X with rows x_i is defined as $\max_i \|x_i\|_2$. This is equivalent to requiring the *max-norm* (sometimes called the γ_2 -norm) of $Z = XY$, which is defined as

$$\|Z\|_{\max} = \inf\{\|X\|_{2,\infty}\|Y^T\|_{2,\infty} : XY = Z\},$$

to be bounded by μ . This penalty has been proposed by [LRS⁺10] as a heuristic for low rank matrix completion, which can perform better than Frobenius norm regularization when the low rank factors are known to have bounded entries.

Quadratic clustering. Consider (9) with $\tilde{r} = 0$. Let r be the indicator function of a selection, *i.e.*,

$$r(x) = \begin{cases} 0 & x = e_l \text{ for some } l \in \{1, \dots, k\} \\ \infty & \text{otherwise,} \end{cases}$$

where e_l is the l -th standard basis vector. Thus x_i encodes the cluster (one of k) to which the data vector (A_{i1}, \dots, A_{im}) is assigned.

Alternating minimization on this problem reproduces the well-known k -means algorithm. The x update (10) is not a convex problem, but is easily solved. The solution is given by assigning x_i to the closest archetype (often called a *cluster centroid* in the context of k -means): $x_i = e_{l^*}$ for $l^* = \operatorname{argmin}_l \left(\sum_{j=1}^n (A_{ij} - Y_{lj})^2 \right)$. The y update (11) is a least squares problem with the simple solution

$$Y_{lj} = \frac{\sum_{i:(i,j) \in \Omega} A_{ij} X_{il}}{\sum_{i:(i,j) \in \Omega} X_{il}},$$

i.e., each row of Y is updated to be the mean of the rows of A assigned to that archetype.

Quadratic mixtures. We can also implement partial assignment of data vectors to clusters. Take $\tilde{r} = 0$, and let r be the indicator function of the set of probability vectors, *i.e.*,

$$r(x) = \begin{cases} 0 & \sum_{l=1}^k x_l = 1, \quad x_l \geq 0 \\ \infty & \text{otherwise.} \end{cases}$$

Subspace clustering. PCA approximates a data set by a single low dimensional subspace. We may also be interested in approximating a data set as a *union* of low dimensional subspaces. This problem is known as *subspace clustering* (see [Vid10] and references therein). Subspace clustering may also be thought of as generalizing quadratic clustering to assign each data vector to a low dimensional subspace rather than to a single cluster centroid.

To frame subspace clustering as a regularized PCA problem (9), partition the columns of X into k blocks. Then let r be the indicator function of block sparsity (*i.e.*, $r(x) = 0$ if only one block of x has nonzero entries, and otherwise $r(x) = \infty$).

It is easy to perform alternating minimization on this objective function; this method is sometimes called the *k-planes* algorithm [Vid10, Tse00, AM04], which alternates over assigning examples to subspaces, and fitting the subspaces to the examples. Once again, the X update (10) is not a convex problem, but can be easily solved. Each block of the columns of X defines a subspace spanned by the corresponding rows of Y . We compute the distance from example i (the i th row of A) to each subspace (by solving a least squares problem), and assign example i to the subspace that minimizes the least squares error by setting x_i to be the solution to the corresponding least squares problem.

Many other algorithms for this problem have also been proposed, such as the k -SVD [AEB06] and sparse subspace clustering [EV09], some with provable guarantees on the quality of the recovered solution [SC12].

Supervised learning. Sometimes we want to understand the variation that a certain set of features can explain, and the variance that remains unexplainable. To this end, one natural strategy would be to regress the labels in the dataset on the features; to subtract the predicted values from the data; and to use PCA to understand the remaining variance. This procedure gives the same answer as the solution to a single regularized PCA problem. Here we present the case in which the features we wish to use in the regression are present in the data as the first column of A . To construct the regularizers, we make sure the first column of A appears as a feature in the supervised learning problem by setting

$$r_i(x) = \begin{cases} r_0(x_2, \dots, x_{k+1}) & x_1 = A_{i1} \\ \infty & \text{else,} \end{cases}$$

where $r_0 = 0$ can be chosen as in any regularized PCA model. The regularization on the first row of Y is the regularization used in the supervised regression, and the regularization on the other rows will be that used in regularized PCA.

Thus we see that regularized PCA can naturally combine supervised and unsupervised learning into a single problem.

Feature selection. We can use regularized PCA to perform feature selection. Consider (9) with $r(x) = \|x\|_2^2$ and $\tilde{r}(y) = \|y\|_2$. (Notice that we are *not* using $\|y\|_2^2$.) The regularizer \tilde{r} encourages the matrix \tilde{Y} to be column-sparse, so many columns are all zero. If $\tilde{y}_j = 0$, it means that feature j was uninformative, in the sense that its values do not help much in predicting any feature in the matrix A (including feature j itself). In this case we say that feature j was not selected. For this approach to make sense, it is important that the columns of the matrix A should have mean zero. Alternatively, one can use the de-biasing regularizers r' and \tilde{r}' introduced in §3.3 along with the feature selection regularizer introduced here.

Dictionary learning. Dictionary learning (also sometimes called *sparse coding*) has become a popular method to design concise representations for very high dimensional data [OF97, LBRN06, MBPS09, MPS⁺09]. These representations have been shown to perform well when used as features in subsequent (supervised) machine learning tasks [RBL⁺07]. In dictionary learning, each row of A is modeled as a linear combination of dictionary atoms, represented by rows of Y . The total size of the dictionary used is often very large ($k \gg \max(m, n)$), but each example is represented using a very small number of atoms. To fit the model, one solves the regularized PCA problem (9) with $r(x) = \|x\|_1$, to induce sparsity in the number of atoms used to represent any given example, and with $\tilde{r}(y) = \|y\|_2^2$ or $\tilde{r}(y) = I_+(c - \|y\|_2)$ for some $c > 0 \in \mathbf{R}$, in order to ensure the problem is well posed. (Note that our notation transposes the usual notation in the literature on dictionary learning.)

Mix and match. It is possible to combine these regularizers to obtain a factorization with any combination of the above properties. As an example, one may require that both X and Y be simultaneously sparse and nonnegative by choosing

$$r(x) = \|x\|_1 + I_+(x) = \mathbf{1}^T x + I_+(x),$$

and similarly for $\tilde{r}(y)$. Similarly, [KP07] show how to obtain a nonnegative matrix factorization in which one factor is sparse by using $r(x) = \|x\|_1^2 + I_+(x)$ and $\tilde{r}(y) = \|y\|_2^2 + I_+(y)$; they go on to use this factorization as a clustering technique.

3.3 Offsets and scaling

In our discussion of the quadratically regularized PCA problem (2), we saw that it can often be quite important to standardize the data before applying PCA. Conversely, in regularized PCA problems such as nonnegative matrix factorization, it can be disastrous to standardize the data, since subtracting column means may introduce negative entries into the matrix or otherwise worsen the fit of the model.

A flexible approach is to allow an offset in the model: we solve

$$\text{minimize } \sum_{(i,j) \in \Omega} (A_{ij} - x_i y_j - \mu_j)^2 + \sum_{i=1}^m r_i(x_i) + \sum_{j=1}^n \tilde{r}_j(y_j), \quad (12)$$

with variables x_i , y_j , and μ_j . Here, μ_j takes the role of the column mean, and in fact will be equal to the column mean in the trivial case $k = 0$.

An offset may be included in the standard form regularized PCA problem (9) by augmenting the problem slightly. Suppose we are given an instance of the problem (9), *i.e.*, we are given k , r , and \tilde{r} . We can fit an offset term μ_j by letting $k' = k + 1$ and modifying the regularizers. Extend the regularization $r : \mathbf{R}^k \rightarrow \mathbf{R}$ and $\tilde{r} : \mathbf{R}^k \rightarrow \mathbf{R}$ to new regularizers $r' : \mathbf{R}^{k+1} \rightarrow \mathbf{R}$ and $\tilde{r}' : \mathbf{R}^{k+1} \rightarrow \mathbf{R}$ which enforce that the first column of X is constant and the first row of Y is not penalized. Using this scheme, the first row of the optimal Y will be equal to the optimal μ in (12).

Explicitly, let

$$r'(x) = \begin{cases} r(x_2, \dots, x_{k+1}) & x_1 = 1 \\ \infty & \text{else,} \end{cases}$$

and $\tilde{r}'(y) = \tilde{r}(y_2, \dots, y_{k+1})$. (Here, we identify $r(x) = r(x_1, \dots, x_k)$ to explicitly show the dependence on each coordinate of the vector x , and similarly for \tilde{r} .)

It is also possible to introduce row offsets in the same way.

4 Generalized loss functions

We may also generalize the *loss* function in PCA to form a *generalized low rank model*,

$$\text{minimize } \sum_{(i,j) \in \Omega} L_{ij}(x_i y_j, A_{ij}) + \sum_{i=1}^m r_i(x_i) + \sum_{j=1}^n \tilde{r}_j(y_j), \quad (13)$$

where $L_{ij} : \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}_+$ are given loss functions for $i = 1, \dots, m$ and $j = 1, \dots, n$. Problem (13) reduces to PCA with generalized regularization when $L_{ij}(u, a) = (a - u)^2$. However, the loss function L_{ij} can now depend on the data A_{ij} in a more complex way.

4.1 Solution methods

As before, problem (13) is not convex, even when L_{ij} , r_i and \tilde{r}_j are convex; but if all these functions are convex, then the problem is bi-convex.

Alternating minimization. Alternating minimization can still be used to find a local minimum, and it is still often possible to use factorization caching to speed up the solution of the subproblems that arise in alternating minimization. We defer a discussion of how to solve these subproblems explicitly to §7.

Stochastic proximal gradient method. For use with extremely large scale problems, we discuss fast variants of the basic alternating minimization algorithm in §7. For example, we present an alternating directions stochastic proximal gradient method. This algorithm accesses the functions L_{ij} , r_i , and \tilde{r}_j only through a subgradient or proximal interface, allowing it to generalize trivially to nearly any loss function and regularizer. We defer a more detailed discussion of this method to §7.

4.2 Examples

Weighted PCA. A simple modification of the PCA objective is to weight the importance of fitting each element in the matrix A . In the generalized low rank model, we let $L_{ij}(u-a) = w_{ij}(a-u)^2$, where w_{ij} is a weight, and take $r = \tilde{r} = 0$. Unlike PCA, the weighted PCA problem has no known analytical solution [SJ03]; in fact, it is NP-hard to find an exact solution to weighted PCA [GG11], although it is not known whether approximate solutions of moderate accuracy may always be efficiently obtained.

Robust PCA. Despite its widespread use, PCA is very sensitive to outliers. Many authors have proposed a robust version of PCA obtained by replacing least-squares loss with ℓ_1 loss, which is less sensitive to large outliers [CLMW11, WGR⁺09, XCS12]. They propose to solve the problem

$$\begin{aligned} & \text{minimize} && \|S\|_1 + \|Z\|_* \\ & \text{subject to} && S + Z = A, \end{aligned} \tag{14}$$

where the *nuclear norm* $\|Z\|_*$ is defined to be the sum of the singular values of Z . The authors interpret Z as a robust version of the principal components of the data matrix A , and S as the sparse, possibly large noise corrupting the observations.

We can frame robust PCA as a generalized low rank model problem in the following way. If $L_{ij}(u, a) = |a - u|$, and $r(x) = \frac{\gamma}{2}\|x\|_2^2$, $\tilde{r}(y) = \frac{\gamma}{2}\|y\|_2^2$, then (13) becomes

$$\text{minimize} \quad \|A - XY\|_1 + \frac{\gamma}{2}\|X\|_F^2 + \frac{\gamma}{2}\|Y\|_F^2.$$

We can rewrite the problem by introducing a new variable Z as

$$\begin{aligned} & \text{minimize} && \|A - Z\|_1 + \frac{\gamma}{2}\|X\|_F^2 + \frac{\gamma}{2}\|Y\|_F^2 \\ & \text{subject to} && Z = XY. \end{aligned} \tag{15}$$

Now we use the fact that

$$\|Z\|_* = \inf \left\{ (1/2)\|X\|_F^2 + (1/2)\|Y\|_F^2 : XY = Z \right\}$$

to partially minimize over the variables X and Y holding Z constant. This results in the rank-constrained robust PCA problem

$$\begin{aligned} & \text{minimize} && \|S\|_1 + \gamma \|Z\|_* \\ & \text{subject to} && S + Z = A \\ & && \text{Rank}(Z) \leq k, \end{aligned}$$

where we have introduced the new variable $S = A - Z$.

Huber PCA. The Huber function is defined as

$$\mathbf{huber}(x) = \begin{cases} (1/2)x^2 & |x| \leq 1 \\ |x| - (1/2) & |x| > 1. \end{cases}$$

Using Huber loss,

$$L_{ij}(u, a) = \mathbf{huber}(u - a),$$

in place of ℓ_1 loss also yields an estimator robust to occasionally large outliers [Hub11]. The Huber function is less sensitive to small errors $|u - a|$ than the ℓ_1 norm, but becomes linear in the error for large errors. This choice of loss function results in a generalized low rank model formulation that is robust both to large outliers and to small Gaussian perturbations in the data.

Previously, the problem of Gaussian noise in robust PCA has been treated by decomposing the matrix $A = L + S + N$ into a low rank matrix L , a sparse matrix S , and a matrix with small Gaussian entries N by minimizing the loss

$$\|L\|_* + \|S\|_1 + (1/2)\|N\|_F^2$$

over all decompositions $A = L + S + N$ of A [XCS12].

In fact, this formulation is equivalent to Huber PCA with quadratic regularization on the factors X and Y . The argument showing this is very similar to the one we made above for robust PCA. The only added ingredient is the observation that

$$\mathbf{huber}(x) = \inf\{|s| + (1/2)n^2 : x = n + s\}.$$

Robust regularized PCA. We can design robust versions of all the regularized PCA problems above by the same transformation we used to design robust PCA. Simply replace the quadratic loss function with an ℓ_1 or Huber loss function. For example, k -medioids [KR09, PJ09] is obtained by using ℓ_1 loss in place of quadratic loss in the quadratic clustering problem. Similarly, robust subspace clustering [SEC13] can be obtained by using an ℓ_1 or Huber penalty in the subspace clustering problem.

Quantile PCA. For some applications, it can be much worse to *overestimate* the entries of A than to *underestimate* them, or vice versa. One can capture this asymmetry by using the loss function

$$L_{ij}(u, a) = \alpha(u - a)_+ + (1 - \alpha)(u - a)_-$$

and choosing $\alpha \in (0, 1)$ appropriately, where we define $(x)_- = \min(x, 0)$. This loss function can also be interpreted as performing *quantile regression*, e.g., fitting the 20th percentile [KB78, Koe05].

Fractional PCA. For other applications, we may be interested in finding an approximation of the matrix A whose entries are close to the original matrix on a relative, rather than an absolute, scale. Here, we assume the entries A_{ij} are all positive. The loss function

$$L_{ij}(u, a) = \max\left(\frac{a - u}{u}, \frac{u - a}{a}\right)$$

can capture this objective. A solution (X, Y) to the resulting generalized low rank model with optimal value less than $0.10mn$ would allow one to claim that XY is a low rank matrix that is on average within 10% of the original matrix.

Exponential family PCA. It is easy to formulate a version of PCA corresponding to any loss in the exponential family. Here we give some interesting loss functions generated by exponential families when all the entries A_{ij} are positive. (See [CDS01] for a general treatment of exponential family PCA.) One popular loss function in the exponential family is the KL-divergence loss,

$$L(u, a) = a \log\left(\frac{a}{u}\right) - a + u.$$

which corresponds to a Poisson generative model [CDS01]. Another interesting loss function is the Itakura-Saito (IS) loss,

$$L(u, a) = \log\left(\frac{a}{u}\right) - 1 + \frac{a}{u},$$

which has the property that it is scale invariant, so scaling a and u by the same factor produces the same loss. The β -divergence,

$$L(u, a) = \frac{a^\beta}{\beta(\beta - 1)} + \frac{u^\beta}{\beta} - \frac{au^{\beta-1}}{\beta - 1},$$

generalizes both of these losses. With $\beta = 2$, we recover quadratic loss; in the limit as $\beta \rightarrow 1$, we recover the KL-divergence loss; and in the limit as $\beta \rightarrow 0$, we recover the IS loss.

4.3 Offsets and scaling

In PCA, standardization rescales the data in order to compensate for unequal scaling in different features. It is possible to instead rescale the *loss functions* in order to compensate for unequal scaling. A savvy user may be able to select loss functions L_{ij} that are already appropriately scaled to reflect the importance of fitting different columns. However, it is useful to have a default automatic scaling for use in other cases. The scaling proposed here generalizes the idea of standardization to a setting with heterogeneous loss functions.

Given initial loss functions L_{ij} , for each feature j let

$$\begin{aligned}\mu_j &= \operatorname{argmin}_{\mu} \sum_{i:(i,j) \in \Omega} L_{ij}(\mu, A_{ij}) \\ \sigma_j &= \frac{1}{n_j - 1} \sum_{i:(i,j) \in \Omega} L_{ij}(\mu_j, A_{ij}).\end{aligned}$$

It is easy to see that μ_j generalizes the mean of column j , while σ_j generalizes the variance. For example, if $L_{ij}(u, a) = (u - a)^2$ for every $i = 1, \dots, m$, $j = 1, \dots, n$, then μ_j will be the mean of the j th column of A ; but if $L_{ij}(u, a) = |u - a|$ for every $i = 1, \dots, m$, $j = 1, \dots, n$, then μ_j will be the median of the j th column of A .

We rescale the loss functions by σ_j and solve

$$\text{minimize } \sum_{(i,j) \in \Omega} L_{ij}(A_{ij}, x_i y_j + \mu_j) / \sigma_j + \sum_{i=1}^m r_i(x_i) + \sum_{j=1}^n \tilde{r}_j(y_j). \quad (16)$$

Note that this problem can be recast in the standard form for a generalized low rank model (13). For the offset, we may use the same trick described in §3.3 to encode the offset in the regularization; and for the scaling, we simply replace the original loss function L_{ij} by L_{ij}/σ_j .

5 Loss functions for abstract data types

We began our study of generalized low rank modeling by considering the best way to approximate a matrix by another matrix of lower rank. In this section, we apply the same procedure to approximate a data table with data that may not consist of real numbers, by choosing a loss function that respects the data type.

We now consider our data A to be a *database* or *table* consisting of m examples (*i.e.*, rows, samples) and n features (*i.e.*, columns, attributes), with entries A_{ij} drawn from a feature set \mathcal{F}_j . The feature set \mathcal{F}_j may be discrete or continuous. So far, we have only considered numerical data ($\mathcal{F}_j = \mathbf{R}$ for $j = 1, \dots, n$), but now \mathcal{F}_j can represent more abstract data types. For example, entries of A can take on Boolean values ($\mathcal{F}_j = \{T, F\}$), integral values ($\mathcal{F}_j = 1, 2, 3, \dots$), ordinal values ($\mathcal{F}_j = \{\text{very much, a little, not at all}\}$), or consist of a tuple of these types ($\mathcal{F}_j = \{(a, b) : a \in \mathbf{R}\}$).

We are given a loss function $L_{ij} : \mathbf{R} \times \mathcal{F}_j \rightarrow \mathbf{R}$. The loss $L_{ij}(u, a)$ describes the approximation error incurred when we represent a feature value $a \in \mathcal{F}_j$ by the number $u \in \mathbf{R}$. We give a number of examples of these loss functions below.

We now formulate a generalized low rank model on the database A as

$$\text{minimize } \sum_{(i,j) \in \Omega} L_{ij}(x_i y_j, A_{ij}) + \sum_{i=1}^m r_i(x_i) + \sum_{j=1}^n \tilde{r}_j(y_j), \quad (17)$$

with variables $X \in \mathbf{R}^{n \times k}$ and $Y \in \mathbf{R}^{k \times m}$, and with loss L_{ij} as above and regularizers $r_i(x_i) : \mathbf{R}^{1 \times k} \rightarrow \mathbf{R}$ and $\tilde{r}_j(y_j) : \mathbf{R}^{k \times 1} \rightarrow \mathbf{R}$ (as before). When the domain of each loss function is $\mathbf{R} \times \mathbf{R}$, we recover the generalized low rank model on a matrix (13).

5.1 Solution methods

As before, this problem is not convex, but it is bi-convex if r_i , and \tilde{r}_j are convex, and L_{ij} is convex in its first argument. The problem is also separable across samples $i = 1, \dots, m$ and features $j = 1, \dots, m$. These properties makes it easy to perform alternating minimization on this objective. Once again, we defer a discussion of how to solve these subproblems explicitly to §7.

5.2 Examples

Boolean PCA. Suppose $A_{ij} \in \{-1, 1\}^{m \times n}$, and we wish to approximate this Boolean matrix. We may take the loss to be

$$L(u, a) = (1 - au)_+,$$

which is the hinge loss [BV04], and solve the problem (17) with or without regularization. When the regularization is sum of squares ($r(x) = \lambda \|x\|_2^2$, $\tilde{r}(y) = \lambda \|y\|_2^2$), fixing X and minimizing over y_j is equivalent to training a support vector machine (SVM) on a data set consisting of m examples with features x_i and labels A_{ij} . Hence alternating minimization for the problem (13) reduces to repeatedly training an SVM. This model has been previously considered under the name Maximum Margin Matrix Factorization (MMMMF) [SRJ04, RS05].

Logistic PCA. Again supposing $A_{ij} \in \{-1, 1\}^{m \times n}$, we can also use a logistic loss to measure the approximation quality. Let

$$L(u, a) = \log(1 + \exp(-au)).$$

With this loss, fixing X and minimizing over y_j is equivalent to using logistic regression to predict the labels A_{ij} . This model has been previously considered under the name logistic PCA [SSU03].

Poisson PCA. Now suppose the data A_{ij} are nonnegative integers. We can use any loss function that might be used in a regression framework to predict integral data to construct a generalized low rank model for Poisson PCA. For example, we can take

$$L(u, a) = \exp(u) - au + a \log a - a.$$

This is the exponential family loss corresponding to Poisson data. (It differs from the KL-divergence loss from §4.2 only in that u has been replaced by $\exp(u)$, which allows u to take negative values.)

Ordinal PCA. Suppose the data A_{ij} denote the levels of some ordinal variable, encoded as $\{1, 2, \dots, d\}$. We wish to penalize the entries of the low rank matrix XY which deviate by many levels from the encoded ordinal value. A convex version of this penalty is given by the function

$$L(u, a) = \sum_{a' < a} (1 - u + a')_+ + \sum_{a' > a} (1 + u - a')_+,$$

which generalizes the hinge loss to ordinal data.

This loss function may be useful for encoding Likert-scale data indicating degrees of agreement with a question [Lik32]. For example, we might have

$$\mathcal{F}_j = \{\text{strongly disagree, disagree, neither agree nor disagree, agree, strongly agree}\}.$$

Interval PCA. Suppose that the data $A_{ij} \in \mathbf{R}^2$ are tuples denoting the endpoints of an interval, and we wish to find a low rank matrix whose entries lie inside these intervals. We can capture this objective using, for example, the deadzone-linear loss

$$L(u, a) = \max((a_1 - u)_+, (u - a_2)_+).$$

5.3 Missing data and data imputation

We can use the solution (X, Y) to a low rank model to impute values corresponding to missing data $(i, j) \notin \Omega$. This process is sometimes also called *inference*. Above, we saw that the MAP estimator for the missing entry A_{ij} was equal to $x_i y_j$. This is still true for many of the loss functions above, such as the Huber function or ℓ_1 loss, for which it makes sense for the data to take on any real value.

However, to approximate abstract data types we must consider a more nuanced view. While we can still think of the solution (X, Y) to the generalized low rank model (13) in Boolean PCA as approximating the Boolean matrix A , the solution is not a Boolean matrix. Instead we say that we have *encoded* the original Boolean matrix as a real-valued low rank matrix XY , or that we have *embedded* the original Boolean matrix into the space of real valued matrices.

To fill in missing entries in the original matrix A , we compute the value \hat{A}_{ij} that minimizes the loss for $x_i y_j$:

$$\hat{A}_{ij} = \operatorname{argmin}_a L_{ij}(x_i y_j, a).$$

This implicitly constrains \hat{A}_{ij} to lie in the domain \mathcal{F}_j of L_{ij} . When $L_{ij} : \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}$, as is the case for the losses in §4 above (including ℓ_2 , ℓ_1 , and Huber loss), then $\hat{A}_{ij} = x_i y_j$. But when the data is of an abstract type, the minimum $\operatorname{argmin}_a L_{ij}(u, a)$ will not in general be equal to u .

For example, when the data is Boolean, $L_{ij} : \{0, 1\} \times \mathbf{R} \rightarrow \mathbf{R}$, we compute the Boolean matrix \hat{A} implied by our low rank model by solving

$$\hat{A}_{ij} = \operatorname{argmin}_{a \in \{0, 1\}} (a(XY)_{ij} - 1)_+$$

for MMMF, or

$$\hat{A}_{ij} = \operatorname{argmin}_{a \in \{0,1\}} \log(1 + \exp(-a(XY)_{ij}))$$

for logistic PCA. These problems both have the simple solution

$$\hat{A}_{ij} = \mathbf{sign}(x_i y_j).$$

When \mathcal{F}_j is finite, inference *partitions* the real numbers into regions

$$\mathcal{R}_a = \{x \in \mathbf{R} : L_{ij}(u, x) = \min_a L_{ij}(u, a)\}$$

corresponding to different values $a \in \mathcal{F}_j$. When L_{ij} is convex, these regions are intervals.

We can use the estimate \hat{A}_{ij} even when $(i, j) \in \Omega$ was observed. If the original observations have been corrupted by noise, we can view \hat{A}_{ij} as a denoised version of the original data. This is an unusual kind of denoising: both the noisy (A_{ij}) and denoised (\hat{A}_{ij}) versions of the data lie in the *abstract* space \mathcal{F}_j .

5.4 Interpretations and applications

We have already discussed some interpretations of X and Y in the PCA setting. Now we reconsider those interpretations in the context of approximating these abstract data types.

Archetypes. As before, we can think of each row of Y as an *archetype* which captures the behavior of an idealized example. However, the rows of Y are real numbers. To represent each archetype $l = 1, \dots, k$ in the abstract space as \mathcal{Y}_l with $(\mathcal{Y}_l)_j \in \mathcal{F}_j$, we solve

$$(\mathcal{Y}_l)_j = \operatorname{argmin}_{a \in \mathcal{F}_j} L_j(y_{lj}, a).$$

(Here, we assume that the loss $L_{ij} = L_j$ is independent of the example i .)

Archetypical representations. As before, we call x_i the *representation* of example i in terms of the archetypes. The rows of X give an embedding of the examples into \mathbf{R}^k , where each coordinate axis corresponds to a different archetype. If the archetypes are simple to understand or interpret, then the representation of an example can provide better intuition about that example.

In contrast to the initial data, which may consist of arbitrarily complex data types, the representations x_i will be low dimensional vectors, and can easily be used in a machine learning algorithm. Using the generalized low rank model, we have converted an abstract feature space into a vector space.

Feature representations. The columns of Y embed the features into \mathbf{R}^k . Here, we think of the columns of X as archetypical features, and represent each feature j as a linear combination of the archetypical features. Just as with the examples, we might choose to apply any machine learning algorithm to the feature representations.

This procedure allows us to compare non-numeric features using their representation in \mathbf{R}^l . For example, if the features \mathcal{F} are Likert variables giving the extent to which respondents on a questionnaire agree with statements $1, \dots, n$, we might be able to say that questions i and j are similar if $\|y_i - y_j\|$ is small; or that question i is a more polarizing form of question j if $y_i = \alpha y_j$, with $\alpha > 1$.

Even more interesting, it allows us to compare features of different types; we could say that the real-valued feature i is similar to Likert-valued question j if $\|y_i - y_j\|$ is small.

Latent variables. Each row of X represents an example by a vector in \mathbf{R}^k . The matrix Y maps these representations back into the original feature space (now nonlinearly) as described in the discussion on data imputation in §5.3. We might think of X as discovering the *latent variables* that best explain the observed data, with the added benefit that these latent variables lie in the vector space \mathbf{R}^k . If the approximation error $\sum_{(i,j) \in \Omega} L_{ij}(x_i y_j, A_{ij})$ is small, then we view these latent variables as providing a good explanation or summary of the full data set.

Probabilistic interpretation. We can give a probabilistic interpretation of X and Y . We suppose that the matrices \bar{X} and \bar{Y} are generated according to a probability distribution with probability proportional to $\exp(-r(\bar{X}))$ and $\exp(-\tilde{r}(\bar{Y}))$, respectively. Our observations A of the entries in the matrix $\bar{Z} = \bar{X}\bar{Y}$ are given by

$$A_{ij} = \psi_{ij}((\bar{X}\bar{Y})_{ij}),$$

where the random variable $\psi_{ij}(u)$ takes value a with probability proportional to

$$\exp(-L_{ij}(u, a)).$$

We observe each entry $(i, j) \in \Omega$. Then to find the maximum a posteriori (MAP) estimator (X, Y) of (\bar{X}, \bar{Y}) , we solve

$$\text{maximize } \exp\left(-\sum_{(i,j) \in \Omega} L_{ij}(x_i y_j, A_{ij})\right) \exp(-r(X)) \exp(-\tilde{r}(Y)),$$

which is equivalent, by taking logs, to the abstract generalized low rank model (17).

This interpretation gives us a simple way to interpret our procedure for denoising our data or imputing missing observations $(i, j) \notin \Omega$. We are simply computing the MAP estimator \hat{A}_{ij} .

Auto-encoder. The matrix X encodes the data; the matrix Y decodes it back into the full space. We can view (17) as providing the best linear auto-encoder for the data; among all linear encodings (X) and decodings (Y) of the data, the abstract generalized low rank model (17) minimizes the reconstruction error measured according to the loss functions L_{ij} .

Compression. We impose an information bottleneck by using a low rank auto-encoder to fit the data. The bottleneck is imposed by both the dimensionality reduction and the regularization, giving both soft and hard constraints on the information content allowed. The solution (X, Y) to problem (17) maximizes the information transmitted through this k -dimensional bottleneck, measured according to the loss functions L_{ij} . This X and Y give a compressed and real-valued representation that may be used to more efficiently store or transmit the information present in the data.

5.5 Offsets and scaling

Just as in the previous section, better practical performance can often be achieved by allowing an offset in the model as described in §3.3, and automatic scaling of loss functions as described in §4.3.

5.6 Numerical examples

Here, we give some small experiments illustrating the using of loss functions adapted to abstract data types, and comparing their performance with quadratically regularized PCA. To fit these models, we use alternating minimization and solve the subproblems with subgradient descent. This approach is explained more fully in §7.

Boolean PCA. For this experiment, we generate Boolean data $A \in \{-1, +1\}^{n \times m}$ as

$$A = \mathbf{sign}(X^{\text{true}}Y^{\text{true}}),$$

where $X^{\text{true}} \in \mathbf{R}^{n \times k_{\text{true}}}$ and $Y^{\text{true}} \in \mathbf{R}^{k_{\text{true}} \times m}$ have independent, standard normal entries. We consider a problem instance with $m = 50$, $n = 50$, and $k_{\text{true}} = k = 10$.

We fit two GLRMs to this data to compare their performance. Boolean PCA uses hinge loss $L(u, a) = \max(1 - au, 0)$ and quadratic regularization $r(u) = \tilde{r}(u) = .1\|u\|_2^2$, and produces the model $(X^{\text{bool}}, Y^{\text{bool}})$. Quadratically regularized PCA uses squared loss $L(u, a) = (u - a)^2$ and the same quadratic regularization, and produces the model $(X^{\text{real}}, Y^{\text{real}})$.

Figure 1 shows the results of fitting Boolean PCA to this data. The first column shows the original ground-truth data A ; the second shows the imputed data given the model, \hat{A}^{bool} , generated by rounding the entries of $X^{\text{bool}}Y^{\text{bool}}$ to the closest number in $0, 1$ (as explained in §5.3); the third shows the error $A - \hat{A}^{\text{bool}}$. Figure 1 shows the results of running quadratically regularized PCA on the same data, and shows A , \hat{A}^{real} , and $A - \hat{A}^{\text{real}}$.

As expected, Boolean PCA performs substantially better than quadratically regularized PCA on this data set. On average over 100 draws from the ground truth data distribution, the misclassification error (percentage of misclassified entries)

$$\epsilon(X, Y; A) = \frac{\#\{(i, j) \mid A_{ij} \neq \mathbf{sign}(XY)_{ij}\}}{mn}$$

is much lower using hinge loss ($\epsilon(X^{\text{bool}}, Y^{\text{bool}}; A) = 0.0016$) than squared loss ($\epsilon(X^{\text{real}}, Y^{\text{real}}; A) = 0.0051$). The average RMS errors

$$\text{RMS}(X, Y; A) = \left(\frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n (A_{ij} - (XY)_{ij})^2 \right)^{1/2}$$

using hinge loss ($\text{RMS}(X^{\text{bool}}, Y^{\text{bool}}; A) = 0.0816$) and squared loss ($\text{RMS}(X^{\text{real}}, Y^{\text{real}}; A) = 0.159$) also indicate an advantage for Boolean PCA.

Running the alternating subgradient method multiple times from different initial conditions yields different GLRMs, all with very similar (but not identical) fitting errors.

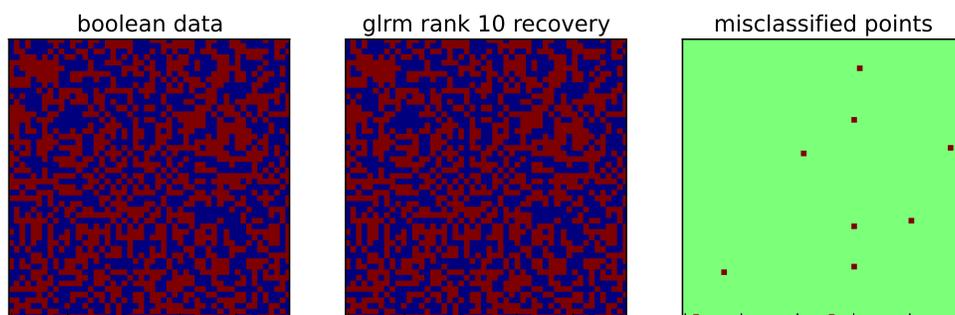


Figure 1: Boolean PCA on Boolean data.

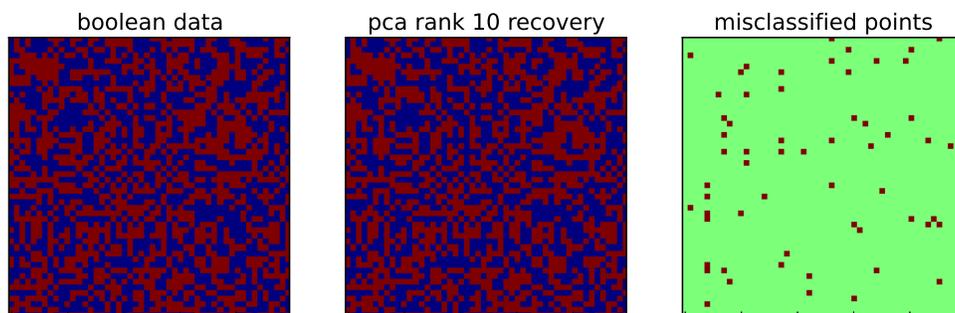


Figure 2: Quadratically regularized PCA on Boolean data.

Mixed data types. In this experiment, we fit a GLRM to a data table with numerical, Boolean, and ordinal columns generated as follows. Let $\mathcal{N}_1, \mathcal{N}_2$, and \mathcal{N}_3 partition the column indices $1, \dots, n$. Choose $X^{\text{true}} \in \mathbf{R}^{m \times k_{\text{true}}}$, $Y^{\text{true}} \in \mathbf{R}^{k_{\text{true}} \times n}$ to have independent, standard normal entries. Assign entries of A as follows:

$$A_{ij} = \begin{cases} x_i y_j & j \in \mathcal{N}_1 \\ \text{sign}(x_i y_j) & j \in \mathcal{N}_2 \\ \text{round}(3x_i y_j + 1) & j \in \mathcal{N}_3, \end{cases}$$

where the function **round** maps a to the nearest integer in the set $\{1, \dots, 7\}$. Thus, \mathcal{N}_1 corresponds to real-valued data; \mathcal{N}_2 corresponds to Boolean data; and \mathcal{N}_3 corresponds to ordinal data. We consider a problem instance in which $m = 100$, $n_1 = 40$, $n_2 = 30$, $n_3 = 30$, and $k_{\text{true}} = k = 10$.

We fit a heterogeneous loss GLRM to this data with loss function

$$L_{ij}(u, a) = \begin{cases} L_{\text{real}}(u, a) & j \in \mathcal{N}_1 \\ L_{\text{bool}}(u, a) & j \in \mathcal{N}_2 \\ L_{\text{ord}}(u, a) & j \in \mathcal{N}_3, \end{cases}$$

where $L_{\text{real}}(u, a) = (u - a)^2$, $L_{\text{bool}}(u, a) = \max(0, 1 - au)$, and $L_{\text{ord}}(u, a)$ is defined in equation (19), and with quadratic regularization $r(u) = \tilde{r}(u) = .1\|u\|_2^2$. We fit the GLRM to produce the model $(X^{\text{mix}}, Y^{\text{mix}})$. For comparison, we also fit quadratically regularized PCA to the same data, using $L_{ij}(u, a) = (u - a)^2$ for all j and quadratic regularization $r(u) = \tilde{r}(u) = .1\|u\|_2^2$, to produce the model $(X^{\text{real}}, Y^{\text{real}})$.

Figure 3 shows the results of fitting the heterogeneous loss GLRM to the data. The first column shows the original ground-truth data A ; the second shows the imputed data given the model, \hat{A}^{mix} , generated by rounding the entries of $X^{\text{mix}}Y^{\text{mix}}$ to the closest number in $0, 1$ (as explained in §5.3); the third shows the error $A - \hat{A}^{\text{mix}}$. Figure 4 corresponds to quadratically regularized PCA, and shows A , \hat{A}^{real} , and $A - \hat{A}^{\text{real}}$.

To evaluate error for Boolean and ordinal data, we use the misclassification error ϵ defined above. For notational convenience, we let $Y_{\mathcal{N}_l}$ ($A_{\mathcal{N}_l}$) denote Y (A) restricted to the columns \mathcal{N}_l in order to pick out real valued columns ($l = 1$), Boolean columns ($l = 2$), and ordinal columns ($l = 3$).

Table 1 compare the average error (difference between imputed entries and ground truth) over 100 draws from the ground truth distribution for models using heterogeneous loss $(X^{\text{mix}}, Y^{\text{mix}})$ and quadratically regularized loss $(X^{\text{real}}, Y^{\text{real}})$. Columns are labeled by error metric. We use misclassification error ϵ for Boolean and ordinal data and MSE for numerical data.

	MSE($X, Y_{\mathcal{N}_1}; A_{\mathcal{N}_1}$)	$\epsilon(X, Y_{\mathcal{N}_2}; A_{\mathcal{N}_2})$	$\epsilon(X, Y_{\mathcal{N}_3}; A_{\mathcal{N}_3})$
$X^{\text{mix}}, Y^{\text{mix}}$	0.0224	0.0074	0.0531
$X^{\text{real}}, Y^{\text{real}}$	0.0076	0.0213	0.0618

Table 1: Average error for numerical, Boolean, and ordinal features using GLRM with heterogenous loss and quadratically regularized loss.

Missing data. Here, we explore the effect of missing entries on the accuracy of the recovered model. We generate data A as detailed above, but then censor one large block of entries in the table (constituting 3.75% of numerical, 50% of Boolean, and 50% of ordinal data), removing them from the observed set Ω .

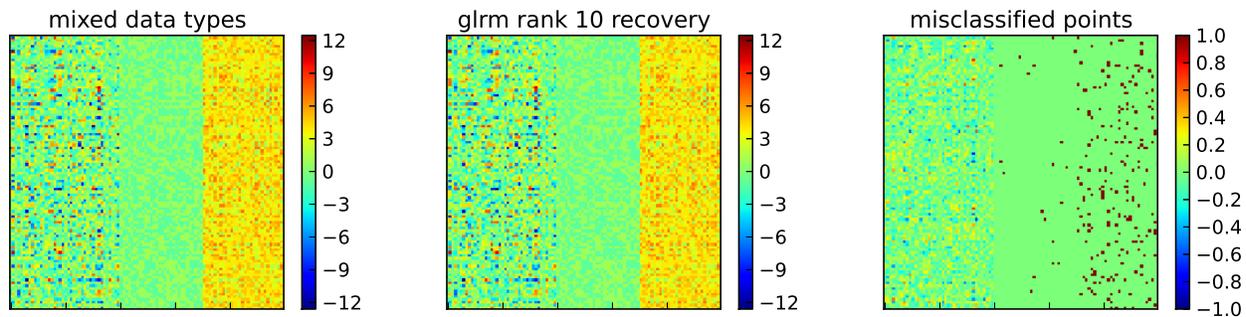


Figure 3: Heterogeneous loss GLRM on mixed data.

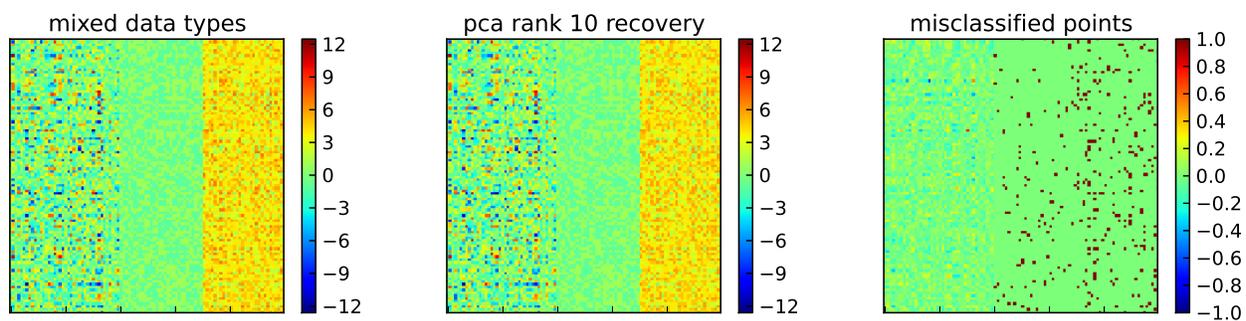


Figure 4: Quadratically regularized PCA on mixed data.

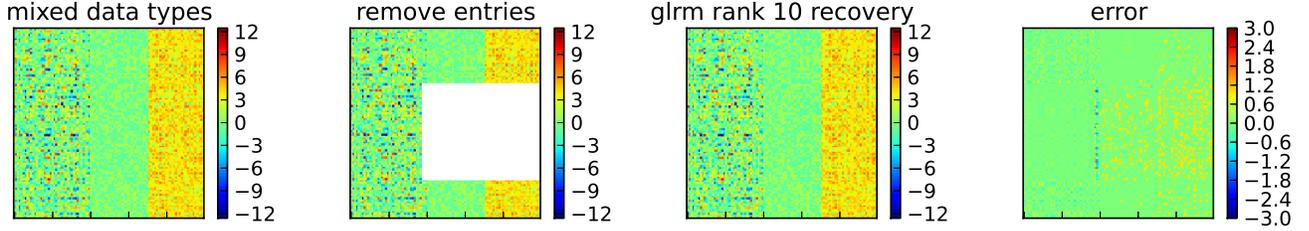


Figure 5: Heterogeneous loss GLRM on missing data.

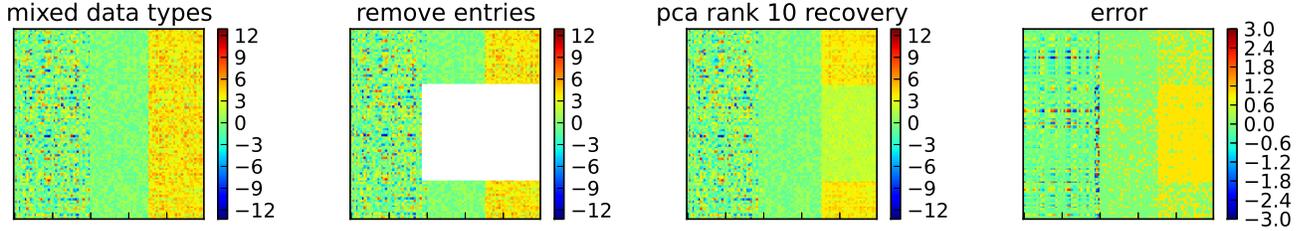


Figure 6: Quadratically regularized PCA on missing data.

Figure 5 shows the results of fitting the heterogeneous loss GLRM described above on the censored data. The first column shows the original ground-truth data A ; the second shows the block of data that has been removed from the observation set Ω ; the third shows the imputed data given the model, \hat{A}^{mix} , generated by rounding the entries of $X^{\text{mix}}Y^{\text{mix}}$ to the closest number in $\{0, 1\}$ (as explained in §5.3); the fourth shows the error $A - \hat{A}^{\text{mix}}$. Figure 6 corresponds to running quadratically regularized PCA on the same data, and shows A , \hat{A}^{real} , and $A - \hat{A}^{\text{real}}$. While quadratically regularized PCA and the heterogeneous loss GLRM performed similarly when no data was missing, the heterogeneous loss GLRM performs much better than quadratically regularized PCA when a large block of data is censored.

We compare the average error (difference between imputed entries and ground truth) over 100 draws from the ground truth distribution in Table 2. As above, we use misclassification error ϵ for Boolean and ordinal data and MSE for numerical data.

	$\text{MSE}(X, Y_{\mathcal{N}_1}; A_{\mathcal{N}_1})$	$\epsilon(X, Y_{\mathcal{N}_2}; A_{\mathcal{N}_2})$	$\epsilon(X, Y_{\mathcal{N}_3}; A_{\mathcal{N}_3})$
$X^{\text{mix}}, Y^{\text{mix}}$	0.392	0.2968	0.3396
$X^{\text{real}}, Y^{\text{real}}$	0.561	0.4029	0.9418

Table 2: Average error over imputed data using a GLRM with heterogeneous loss and regularized quadratic loss.

6 Multi-dimensional loss functions

In this section, we generalize the procedure to allow the loss functions to depend on *blocks* of the matrix XY , which allows us to represent abstract data types more naturally. For example, we can now represent categorical values, permutations, distributions, and rankings.

We are given a loss function $L_{ij} : \mathbf{R}^{1 \times d_j} \times \mathcal{F}_j \rightarrow \mathbf{R}$, where d_j is the *embedding dimension* of feature j , and $d = \sum_j d_j$ is the total dimension of the embedded features. The loss $L_{ij}(u, a)$ describes the approximation error incurred when we represent a feature value $a \in \mathcal{F}_j$ by the vector $u \in \mathbf{R}^{d_j}$.

Let $x_i \in \mathbf{R}^{1 \times k}$ be the i th row of X (as before), and let $Y_j \in \mathbf{R}^{k \times d_j}$ be the j th block matrix of Y so the columns of Y_j correspond to the columns of embedded feature j . We now formulate a multi-dimensional generalized low rank model on the database A ,

$$\text{minimize } \sum_{(i,j) \in \Omega} L_{ij}(x_i Y_j, A_{ij}) + \sum_{i=1}^m r_i(x_i) + \sum_{j=1}^n \tilde{r}_j(Y_j), \quad (18)$$

with variables $X \in \mathbf{R}^{n \times k}$ and $Y \in \mathbf{R}^{k \times d}$, and with loss L_{ij} as above and regularizers $r_i(x_i) : \mathbf{R}^{1 \times k} \rightarrow \mathbf{R}$ (as before) and $\tilde{r}_j(Y_j) : \mathbf{R}^{k \times d_j} \rightarrow \mathbf{R}$. Note that the first argument of L_{ij} is a *row* vector with d_j entries, and the first argument of r_j is a matrix with d_j columns. When every entry A_{ij} is real-valued (*i.e.*, $d_j = 1$), then we recover the generalized low rank model (13) seen in the previous section.

6.1 Examples

Categorical PCA. Suppose that $a \in \mathcal{F}$ is a categorical variable, taking on one of d values or labels. Identify the labels with the integers $\{1, \dots, d\}$. In (18), set

$$L(u, a) = (1 - u_a)_+ + \sum_{a' \in \mathcal{F}, a' \neq a} (1 + u_{a'})_+,$$

and use the quadratic regularizer $r_i = \gamma \| \cdot \|_2^2$, $\tilde{r} = \gamma \| \cdot \|_2^2$.

Fixing X and optimizing over Y is equivalent to training one SVM per label to separate that label from all the others: the j th column of Y gives the weight vector corresponding the j th SVM. Optimizing over X identifies the low-dimensional feature vectors for each example that allow these SVMs to most accurately predict the labels.

The difference between categorical PCA and Boolean PCA is in how missing labels are imputed. To impute a label for entry (i, j) with feature vector x_i according to the procedure described above in 5.3, we project the representation Y_j onto the line spanned by x_i to form $u = x_i Y_j$. Given u , the imputed label is simply $\text{argmax}_l u_l$. This model has the interesting property that if column l' of Y_j lies in the interior of the convex hull of the columns of Y_j , then $u_{l'}$ will lie in the interior of the interval $[\min_l u_l, \max_l u_l]$ [BV04]. Hence the model will never impute label l' for any example.

We need not restrict ourselves to the loss function given above. In fact, any loss function that can be used to train a classifier for categorical variables (also called a multi-class classifier) can be used to fit a categorical PCA model, so long as the loss function depends

only on the inner products between the parameters of the model and the features corresponding to each example. The loss function becomes the loss function L used in (18); the optimal parameters of the model give the optimal matrix Y , while the implied features will populate the optimal matrix X . For example, it is possible to use loss functions derived from error-correcting output codes [DB95]; the Directed Acyclic Graph SVM [PCST99]; the Crammer-Singer multi-class loss [CS02]; or the multi-category SVM [LLW04].

Ordinal PCA. We saw in §5 one way to fit a GLRM to ordinal data. Here, we use a larger embedding dimension for ordinal features. The multi-dimensional embedding will be particularly useful when the best mapping of the ordinal variable onto a linear scale is not uniform; *e.g.*, if level 1 of the ordinal variable is much more similar to level 2 than level 2 is to level 3. Using a larger embedding dimension allows us to infer the relations between the levels from the data itself. Here we again identify the labels $a \in \mathcal{F}$ with the integers $\{1, \dots, d\}$.

One approach we can use for (multi-dimensional) ordinal PCA is to solve (18) with the loss function

$$L(u, a) = \sum_{a'=1}^{d-1} (1 - I_{a>a'} u_{a'})_+, \quad (19)$$

and with quadratic regularization. Fixing X and optimizing over Y is equivalent to training an SVM to separate labels $a \leq l$ from $a > l$ for each $l \in \mathcal{F}$. This approach produces a set of hyperplanes (given by the columns of Y) separating each level l from the next. The hyperplanes need not be parallel to each other.

Permutation PCA. Suppose that a is a permutation of the numbers $1, \dots, d$. Define the permutation loss

$$L(u, a) = \sum_{i=1}^{d-1} (1 - u_{a_i} + u_{a_{i+1}})_+.$$

This loss is zero if $u_{a_i} > u_{a_{i+1}} + 1$ for $i = 1, \dots, d-1$, and increases linearly when these inequalities are violated. Define $\mathbf{sort}(u)$ to return a permutation \hat{a} of the indices $1, \dots, d$ so that $u_{\hat{a}_i} \geq u_{\hat{a}_{i+1}}$ for $i = 1, \dots, d-1$. It is easy to check that $\operatorname{argmin}_a L(u, a) = \mathbf{sort}(u)$. Hence using the permutation loss function in generalized PCA (18) finds a low rank approximation of a given table of permutations.

Many variants on the permutation PCA problem are possible. For example, in *ranking PCA*, we interpret the permutation as a ranking of the choices $1, \dots, d$, and penalize deviations of many levels more strongly than deviations of only one level by choosing the loss

$$L(u, a) = \sum_{i=1}^{d-1} \sum_{j=i+1}^d (1 - u_{a_i} + u_{a_j})_+.$$

From here, it is easy to generalize to a setting in which the rankings are only partially observed. Suppose that we observe pairwise comparisons $a \subseteq \{1, \dots, d\} \times \{1, \dots, d\}$, where

$(i, j) \in a$ means that choice i was ranked above choice j . Then a loss function penalizing deviations from these observed rankings is

$$L(u, a) = \sum_{(i,j) \in a} (1 - u_{a_i} + u_{a_j})_+.$$

Many other modifications to ranking loss functions have been proposed in the literature that interpolate between the the two first loss functions proposed above, or which prioritize correctly predicting the top ranked choices. These losses include the area under the curve loss [Ste07], ordered weighted average of pairwise classification losses [UBG09], the weighted approximate-rank pairwise loss [WBU10], the k -order statistic loss [WYW13], and the accuracy at the top loss [BCMR12].

6.2 Offsets and scaling

Just as in the previous section, better practical performance can often be achieved by allowing an offset in the model as described in §3.3, and scaling loss functions as described in §4.3.

7 Algorithms

In this section, we discuss a number of algorithms that may be used to fit generalized low rank models.

Related work. The matrix factorization literature presents a wide variety of algorithms to solve special cases of our problem. For example, there are variants on alternating Newton methods [Gor02, SG08], (stochastic or incremental) gradient descent [NRRW11, RR11, LRS⁺10, BRRT12], conjugate gradients [RS05, SJ03], expectation minimization (EM) [SJ03], multiplicative updates [LS99] and semidefinite programming [SRJ04]. Generally, expectation minimization has been found to underperform relative to other methods [SG08], while semidefinite programming becomes computationally intractable for very large (or even just large) scale problems [RS05].

We have not previously seen a treatment of algorithms for this entire class of problems that can handle large scale data or take advantage of parallel computing resources. Below, we give a number of algorithms appropriate for this setting, including many that have not been previously proposed in the literature. Our algorithms are all based around alternating minimization and variations on that basic algorithm that are more suitable for large scale data and parallel computing environments.

7.1 Alternating minimization

We showed earlier how to use alternating minimization to find an (approximate) solution to a generalized low rank model. Algorithm (1) shows how to explicitly extend alternating minimization to a generalized low rank model (13) with observations Ω .

Algorithm 1

```
given  $X^0, Y^0$ 
for  $k = 1, 2, \dots$  do
  for  $i = 1, \dots, M$  do
     $x_i^k = \operatorname{argmin}_x \left( \sum_{j:(i,j) \in \Omega} L_{ij}(xy_j^{k-1}, A_{ij}) + r(x) \right)$ 
  end for
  for  $j = 1, \dots, N$  do
     $y_j^k = \operatorname{argmin}_y \left( \sum_{i:(i,j) \in \Omega} L_{ij}(x_i^k y, A_{ij}) + \tilde{r}(y) \right)$ 
  end for
end for
```

Parallelization. Alternating minimization parallelizes naturally over examples and features. In Algorithm 1, the loops over $i = 1, \dots, N$ and over $j = 1, \dots, M$ may both be executed in parallel.

7.2 Early stopping

It is not very useful to spend a lot of effort optimizing over X before we have a good estimate for Y . If an iterative algorithm is used to compute the minimum over X , it may make sense to stop the optimization over X early before going on to update Y . In general, we may consider replacing the minimization over x and y above by any update rule that moves towards the minimum. This templated algorithm is presented as Algorithm 2. Empirically, we find that this approach often finds a better local minimum than performing a full optimization over each factor in every iteration, in addition to saving computational effort on each iteration.

Algorithm 2

```
given  $X^0, Y^0$ 
for  $k = 1, 2, \dots$  do
  for  $i = 1, \dots, M$  do
     $x_i^k = \operatorname{update}_{L,r}(x_i^{k-1}, Y^{k-1}, A)$ 
  end for
  for  $j = 1, \dots, N$  do
     $y_j^k = \operatorname{update}_{L,\tilde{r}}(y_j^{(k-1)T}, X^{(k)T}, A^T)$ 
  end for
end for
```

We describe below a number of different update rules $\operatorname{update}_{L,r}$ by writing the X update. The Y update can be implemented similarly. (In fact, it can be implemented by substituting \tilde{r} for r , switching the roles of X and Y , and transposing all matrix arguments.) All of the approaches outlined below can still be executed in parallel over examples (for the X update) and features (for the Y update).

Gradient method. For example, we might take just one gradient step on the objective. This method can be used as long as L , r , and \tilde{r} do not take infinite values. (If any of these functions f is not differentiable, replace ∇f below by any subgradient of f [BXM03].)

We implement $\mathbf{update}_{L,r}$ as follows. Let

$$g = \sum_{j:(i,j) \in \Omega} \nabla L_{ij}(x_i y_j, A_{ij}) y_j + \nabla r(x_i).$$

Then set

$$x_i^k = x_i^{k-1} - \alpha_k g,$$

for some step size α_k . For example, a common step size rule is $\alpha_k = 1/k$, which guarantees convergence to the globally optimal X if Y is fixed [BXM03].

Proximal gradient method. If a function takes on the value ∞ , it need not have a subgradient at that point, which limits the stochastic gradient update to cases where the regularizer and loss are (finite) real valued. When either the loss or regularizer take on infinite values, we can use a proximal gradient method.

The proximal operator of a function f [PB13] is

$$\mathbf{prox}_f(z) = \operatorname{argmin}_x (f(x) + \frac{1}{2} \|x - z\|_2^2).$$

If f is the indicator function of a set \mathcal{C} , the proximal operator of f is just (Euclidean) projection onto \mathcal{C} .

A proximal gradient update $\mathbf{update}_{L,r}$ is implemented as follows. Let

$$g = \sum_{j:(i,j) \in \Omega} \nabla L_{ij}(x_i y_j, A_{ij}) y_j.$$

Then set

$$x_i^k = \mathbf{prox}_{\alpha_k r}(x_i^{k-1} - \alpha_k g),$$

for some step size α_k . The step size rule $\alpha_k = 1/k$ guarantees convergence to the globally optimal X if Y is fixed, while using a fixed, but sufficiently small, step size α guarantees convergence to a small $O(\alpha)$ neighborhood around the optimum [Ber11]. In numerical experiments, we find that using a fixed step size α on the order of $1/\|g\|_2$ gives fast convergence in practice.

Stochastic gradients. Instead of computing the full gradient of L with respect to x_i above, we can replace the gradient g in either the gradient or proximal gradient method by any *stochastic gradient* g , which is a vector that satisfies

$$\mathbf{E} g = \sum_{j:(i,j) \in \Omega} \nabla L_{ij}(x_i y_j, A_{ij}) y_j.$$

A stochastic gradient can be computed by sampling j uniformly at random from among observed features of i , and setting $g = \{\{j : (i, j) \in \Omega\} | \nabla L_{ij}(x_i y_j, A_{ij}) y_j\}$. More samples from $\{j : (i, j) \in \Omega\}$ can be used to compute a less noisy stochastic gradient.

7.3 Quadratic objectives

Here we describe an update rule for quadratic objectives and arbitrary regularizers that can be used along with the factorization caching technique described in §2.3. We assume here that the objective is given by

$$\|A - XY\|_F^2 + r(X) + \tilde{r}(Y).$$

We will concentrate here on the X update; as always, the Y update is exactly analogous.

As in the case of quadratic regularization, we first form the Gram matrix $G = Y^T Y$. Then the proximal gradient update is fast to evaluate:

$$\mathbf{prox}_{\alpha_k r}(X - \alpha_k(GX - AY^T)).$$

But we can take advantage of the ease of inverting the Gram matrix G to design a faster algorithm. Letting $f(X) = \|A - XY\|_F^2$, we can use the prox-prox update

$$X^{k+1} = \mathbf{prox}_{\alpha_k r}(\mathbf{prox}_{\alpha_k f}(X^k)).$$

This update is simply a proximal gradient step on the objective when f is replaced by the *Moreau envelope* of f ,

$$M_f(X) = \inf_{X'} (f(X') + \|X - X'\|_F^2).$$

(See [PB13] for details.) This objective has the same minimizers as the original objective. Thus, repeating this update t times produces an update

$$X^{k+1} = (\mathbf{prox}_{\alpha r}(\mathbf{prox}_{\alpha f}))^t(X)$$

that approaches the alternating minimization update $X^{k+1} = \operatorname{argmin}_X (f(X) + r(X))$ as $t \rightarrow \infty$, for any constant stepsize $\alpha \leq \|G\|_2^2$. (Here, $\|G\|_2 = \sup_{\|x\|_2 \leq 1} \|Gx\|_2$ is the operator norm of G .)

This update can also be seen as a single iteration of ADMM when the dual variable in ADMM is initialized to 0; see [BPC⁺11]. Thus one can also use ADMM to efficiently compute the alternating minimization update for quadratic programs.

For quadratic objectives with Gram matrix $G = Y^T Y$, this update takes the simple form

$$\mathbf{prox}_{\alpha_k r}((G + \frac{1}{\alpha_k} I)^{-1}(AY^T + \frac{1}{\alpha_k} X)).$$

As in §2.3, we can compute $(G + \frac{1}{\alpha_k} I)^{-1}(AY^T + \frac{1}{\alpha_k} X)$ in parallel by first caching the factorization of $(G + \frac{1}{\alpha_k} I)^{-1}$. Hence it is advantageous to repeat this update many times before updating Y , since most of the computational effort is in forming G and AY^T .

For example, in the case of nonnegative least squares, this update is just

$$\Pi_+((G + \frac{1}{\alpha_k} I)^{-1}(AY^T + \frac{1}{\alpha_k} X)),$$

where Π_+ projects its argument onto the nonnegative orthant.

7.4 Convergence

Alternating minimization need not converge to the same solution (or indeed, the same objective values) when initialized at different starting points. Through examples, we explore this idea here, fitting two GLRMs using the serial Julia implementation (presented in §8) of the alternating proximal gradient updates method.

Global convergence for quadratically regularized PCA. Figure 7 shows the convergence of the alternating proximal gradient update method on a quadratically regularized PCA problem with randomly generated, fully observed data $A = X^{\text{true}}Y^{\text{true}}$, where entries of X^{true} and Y^{true} are drawn from a standard normal distribution. We pick five different random initializations of X and Y with standard normal entries to generate five different convergence trajectories. Quadratically regularized PCA is a simple problem with an analytical solution (see §2), and with no local minima (see Appendix A). Hence it should come as no surprise that the trajectories all converge to the same, globally optimal value.

Local convergence for nonnegative matrix factorization. Figure 8 shows convergence of the same algorithm on a nonnegative matrix factorization model, with data generated in the same way as in Figure 7. (Note that A has some negative entries, so the minimal objective value is strictly greater than zero.) Here, we plot the convergence of the objective value, rather than the suboptimality, since we cannot provably compute the global minimum of the objective function. We see that the algorithm converges to a different optimal value (and point) depending on the initialization of X and Y . Three trajectories converge to the same optimal value (though one does so much faster than the others), one to a value that is somewhat better, and one to a value that is substantially worse.

7.5 Initialization

Here, we discuss two approaches to initialization that result in provably good solutions, for special cases of the generalized low rank problem.

SVD. The SVD provides a provably good initialization for the quadratic matrix completion problem (8). In separate lines of research, [KMO10] and [JNS13] guarantee convergence of alternating minimization to the global optimum if the algorithm is initialized with the SVD of the data matrix (or of a slightly modified, or *trimmed*, matrix), so long as the number of entries in the matrix is sufficiently large, and the entries have been chosen uniformly at random. Indeed, the method even converges quickly: [JNS13] show that this approach achieves a quadratic convergence rate.

k -means++. The k -means++ algorithm is an initialization scheme designed for quadratic clustering problems. It consists of choosing an initial cluster centroid at random from the points, and then choosing the remaining $k - 1$ centroids from the points x that have not yet

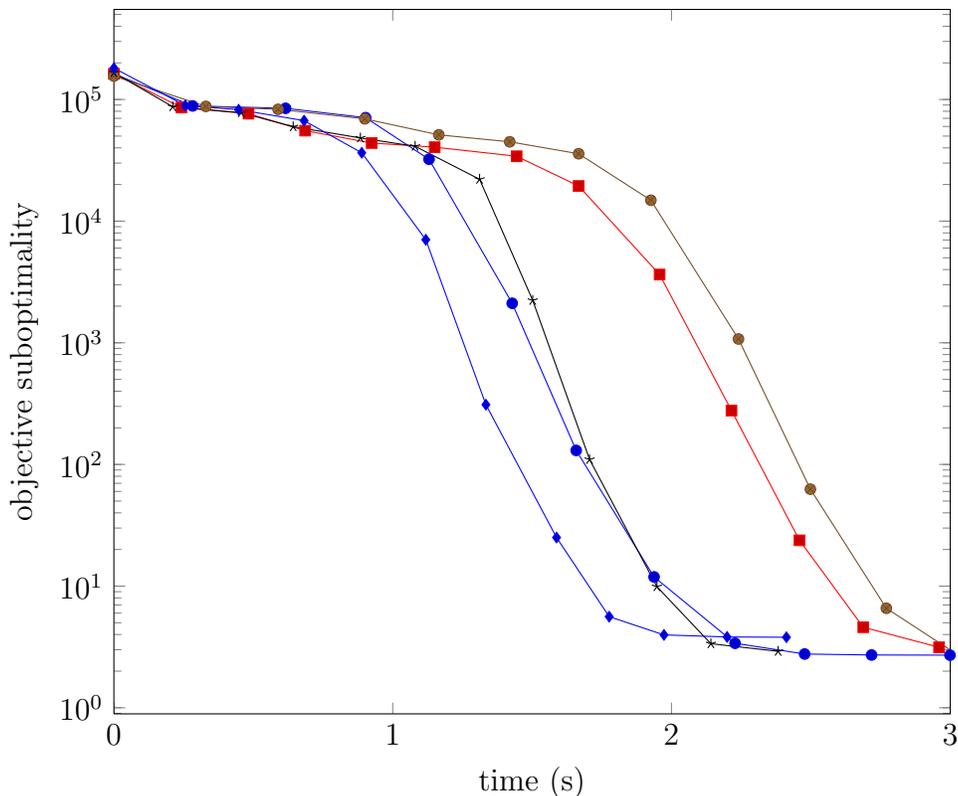


Figure 7: Convergence of alternating proximal gradient updates on quadratically regularized PCA for $n = m = 200$, $k = 2$.

been chosen with probability proportional to $D(x)^2$, where $D(x)$ is the minimum distance of x to any previously chosen centroid.

While quadratic clustering is known to be NP-hard, k -means++ followed by alternating minimization gives a solution with expected approximation ratio within $O(\log k)$ of the optimal value. (Here, the expectation is over the randomization in the initialization algorithm.) In contrast, an arbitrary initialization of the cluster centers for k -means can result in a solution whose value is arbitrarily worse than the true optimum.

Heuristic initializations for other models. These ideas provide good heuristic starting points for initializing more general low rank models.

If one desires a low rank model for the data, initializing with the SVD of the data (even if the data is incomplete, and the loss function is not quadratic) can sometimes help alternating minimization find a good local optimum.

Conversely, if the model rewards a solution that is spread out, as is the case in quadratic clustering or subspace clustering, it may be better to initialize the algorithm by choosing elements with probability proportional to a distance measure, as in k -means++. In the

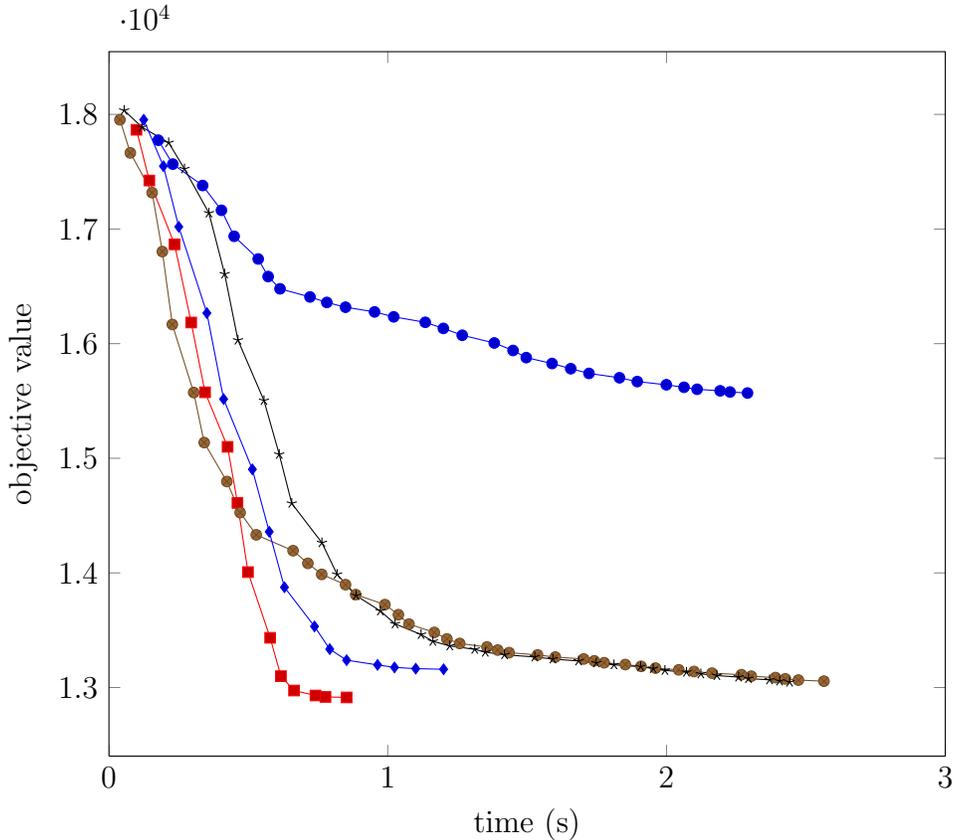


Figure 8: Convergence of alternating proximal gradient updates on NNMF for $n = m = 200$, $k = 2$.

k -means++ procedure, one can use the loss function $L(u)$ as the distance metric D .

7.6 Extensions

Homotopy methods. Suppose that we wish to understand the entire *regularization path* for a GLRM; that is, we would like to know the solution $(X(\gamma), Y(\gamma))$ to the problem

$$\text{minimize } \sum_{(i,j) \in \Omega} L_{ij}(x_i y_j, A_{ij}) + \gamma \sum_{i=1}^m r_i(x_i) + \gamma \sum_{j=1}^n \tilde{r}_j(y_j)$$

as a function of γ . Frequently, the regularization path may be computed almost as quickly as the solution for a single value of γ . We can achieve this by initially fitting the model with a very high value for γ , which is often a very easy problem. (For example, when r and \tilde{r} are norms, the solution is $(X, Y) = (0, 0)$ for sufficiently large γ .) Then we may solve problems corresponding to smaller and smaller values of γ by initializing the alternating minimization algorithm from our previous solution.

On-line optimization. Suppose that new examples or features are being added to our data set continuously, and we wish to perform *on-line optimization*, which means that we should have a good estimate at any time for the representations of those examples x_i or features y_j which we have seen. This model is equivalent to adding new rows or columns to the data table A as the algorithm continues. In this setting, alternating minimization performs quite well, and has a very natural interpretation. Given an estimate for Y , when a new example is observed in row i , we may solve

$$\text{minimize } \sum_{j:(i,j) \in \Omega} L_{ij}(A_{ij}, xy_j) + r(x)$$

with variable x to compute a representation for row i . This computation is exactly the same as one step of alternating minimization. Here, we are finding the best feature representation for the new example in terms of the (already well understood) archetypes Y . If the number of other examples previously seen is large, the addition of a single new example should not change the optimal Y by very much; hence if (X, Y) was previously the global minimum of (13), this estimate of the feature representation for the new example will be very close to its optimal representation (*i.e.*, the one that minimizes problem (13)). A similar interpretation holds when new columns are added to A .

8 Implementations

The authors have developed and released two codes for modelling and fitting generalized low rank models: a serial implementation written in Julia, and a distributed implementation written in Scala using the Spark framework. Both use the proximal gradient method described in §7 to fit GLRMs. In this section we briefly discuss these implementations, and report some timing results. For a full description and up-to-date information about available functionality, we encourage the reader to consult the on-line documentation.

8.1 Julia implementation

`LowRankModels` is a code written in Julia [BKSE12] for modelling and fitting GLRMs. The implementation is available on-line at

<https://github.com/madeleineudell/LowRankModels.jl>.

We discuss some aspects of the usage and features of the code here. For a full description and up-to-date information about available functionality, we encourage the reader to consult the on-line documentation.

Usage. To form a GLRM using `LowRankModels`, the user specifies

- the data A (A), which can be any array or array-like data structure (*e.g.*, a Julia `DataFrame`);

- the observed entries `obs` (Ω), a list of tuples of the indices of the observed entries in the matrix, which may be omitted if all the entries in the matrix have been observed;
- the list of loss functions `losses` ($L_j, j = 1, \dots, n$), one for each column of \mathbf{A} ;
- the regularizers `rx` (r) and `ry` (\tilde{r}); and
- the rank `k` (k).

For example, the following code forms and fits a k -means model with $k = 5$ on the matrix $A \in \mathbf{R}^{m \times n}$.

```
losses = fill(quadratic(),n) # quadratic loss
rx = onesparse()           # x is 1-sparse
ry = zeroreg()             # y is not regularized
glrm = GLRM(A,losses,rx,ry,k) # form GLRM
X,Y,ch = fit(glrm)         # fit GLRM
```

`LowRankModels` uses the proximal gradient method described in §7.2 to fit GLRMs. The optimal model is returned in the factors \mathbf{X} and \mathbf{Y} , while `ch` gives the convergence history.

Losses and regularizers must be of type `Loss` and `Regularizer`, respectively, and may be chosen from a list of supported losses and regularizers, which include

- quadratic loss `quadratic`,
- hinge loss `hinge`,
- ℓ_1 loss `l1`,
- huber loss `huber`,
- ordinal hinge loss `ordinal_hinge`,
- quadratic regularization `quadreg`,
- no regularization `zeroreg`,
- nonnegative constraint `nonnegative`, and
- 1-sparse constraint `onesparse`.

Users may also implement their own losses and regularizers.

Automatic modeling. `LowRankModels` is capable of adding offsets to a GLRM, and of automatically scaling the loss functions, as described in §4.3. It can also automatically detect the types of different columns of a data frame and select an appropriate loss. Using these features, `LowRankModels` implements a method

```
glrm(dataframe, k)
```

that forms a rank k model on a data frame, automatically selecting loss functions and regularization that suit the data well, and ignoring any missing (NA) element in the data frame. This GLRM can then be fit with the function `fit`.

Example. As an example, we fit a GLRM to the Motivational States Questionnaire (MSQ) data set [RA98]. This data set measures 3896 subjects on 92 aspects of mood and personality type, as well as recording the time of day the data were collected. The data include real-valued, Boolean, and ordinal measurements, and approximately 6% of the measurements are missing (NA).

The following code loads the MSQ data set and encodes it in two dimensions:

```
using RDatasets
using LowRankModels
# pick a data set
df = RDatasets.dataset("psych", "msq")
# encode it!
X,Y,labels,ch = fit(glrm(df,2))
```

Figure 9 uses the rows of Y as a coordinate system to plot some of the features of the data set. Here we see the automatic embedding separates positive from negative emotions along the y axis. This embedding is notable for being interpretable despite having been generated completely automatically; of course, better embeddings may be obtained by a more careful choice of loss functions, regularizers, scaling, and embedding dimension k .

8.2 Spark implementation

`SparkGLRM` is a code written in Scala, built on the Spark cluster programming framework [ZCF⁺10], for modelling and fitting GLRMs. The implementation is available on-line at

<http://git.io/glmspark>.

Design. In `SparkGLRM`, the data matrix A is split entry-wise across many machines, just as in [HMLZ14]. The model (factors X and Y) is replicated and stored in memory on every machine. Thus the total computation time required to fit the model is proportional to the number of nonzeros divided by the number of cores, with the restriction that the model should fit in memory. (The authors leave to future work an extension to models that do not fit in memory, *e.g.*, by using a parameter server [SSZ14].) Where possible, hardware acceleration (via breeze and BLAS) is used for local linear algebraic operations.

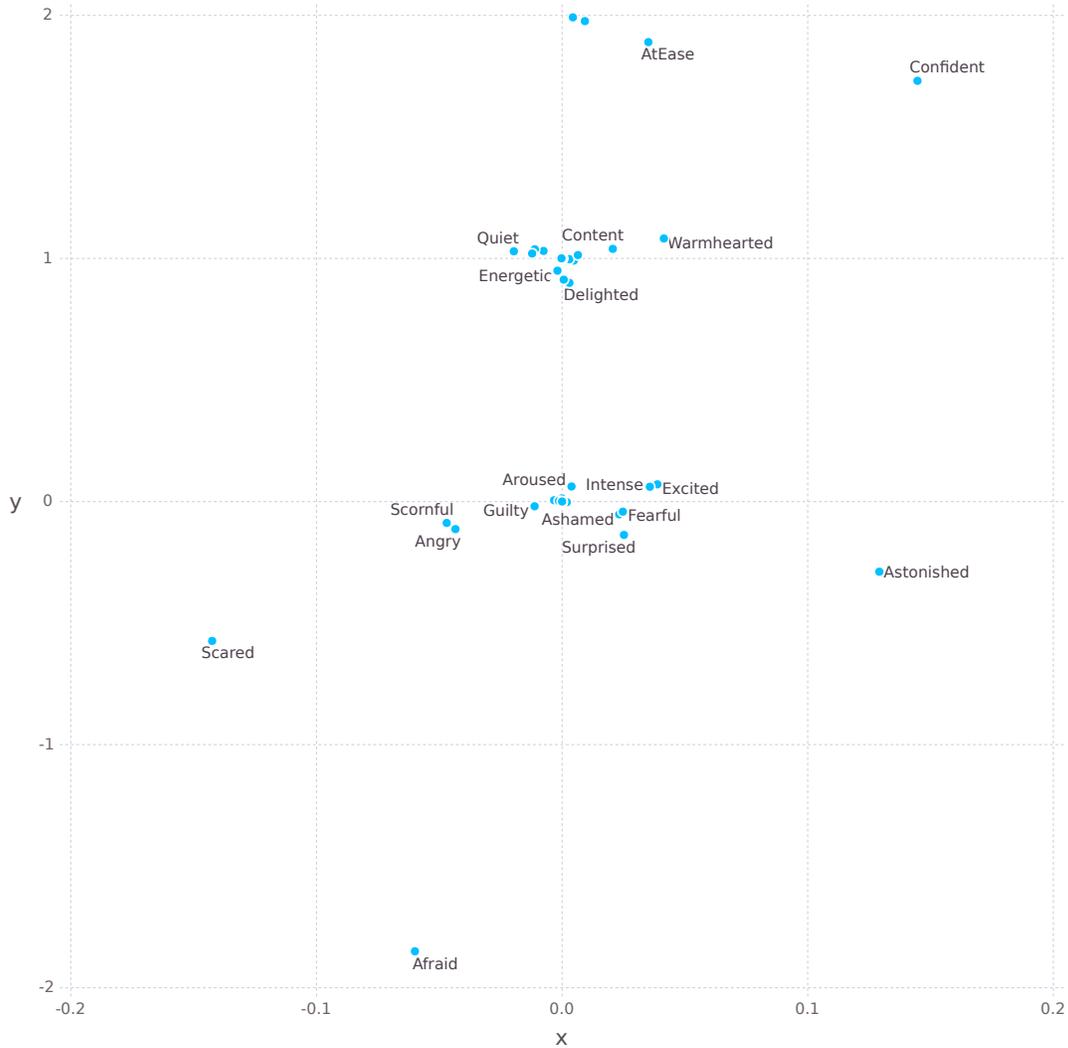


Figure 9: An automatic embedding of the MSQ [RA98] data set into two dimensions.

At every iteration, the current model is broadcast to all machines, so there is only one copy of the model on each machine. This is particularly important in machines with many cores, because it avoids duplicating the model on those machines. Each core on a machine will process a partition of the input matrix, using the local copy of the model.

Usage. The user provides loss functions indexed by $i = 0, \dots, m - 1$ and $j = 0, \dots, n - 1$, so a different loss function can be defined for each entry. Each loss function is defined by its

gradient (or a subgradient). The method signature is

```
loss_grad(i: Int, j: Int, prediction: Double, actual: Double)
```

whose implementation can be customized by particular i and j . As an example, the following line implements squared error loss for all entries:

```
prediction - actual
```

Similarly, the user provides functions implementing the prox operator of the regularizers r and \tilde{r} , which take a dense vector and perform the appropriate prox operation.

Experiments. We ran experiments on several large matrices. For size comparison, a very popular matrix in the recommender systems community is the Netflix Prize Matrix, which has 17770 rows, 480189 columns, and 100480507 nonzeros. Below we report results on several larger matrices, up to 10 times larger. The matrices are generated by fixing the dimensions and number of nonzeros per row, then uniformly sampling the locations for the nonzeros, and finally filling in those locations with a uniform random number in $[0, 1]$.

We report iteration times using an Amazon EC2 cluster with 10 slaves and one master, of instance type “c3.4xlarge”. Each machine has 16 CPU cores and 30 GB of RAM. We ran **SparkGLRM** to fit two GLRMs on matrices of varying sizes. Table 3 gives results for quadratically regularized PCA (*i.e.*, quadratic loss and quadratic regularization) with $k = 5$. To illustrate the capability to write and fit more specialized loss functions, we also fit a GLRM using a custom loss function

$$L_{ij}(u, a) = \begin{cases} |u - a| & i + j \text{ is even} \\ (u - a)^2 & i + j \text{ is odd,} \end{cases}$$

with $r(x) = \|x\|_1$ and $\tilde{r}(y) = \|y\|_2^2$, setting $k = 10$. We report results for this custom GLRM in Table 4.

Matrix size	# nonzeros	Time per iteration (s)
$10^6 \times 10^6$	10^6	7
$10^6 \times 10^6$	10^9	11
$10^7 \times 10^7$	10^9	227

Table 3: SparkGLRM for quadratically regularized PCA, $k = 5$.

The table gives the time per iteration. The number of iterations required for convergence depends on the size of the ambient dimension. On the matrices with the dimensions shown in Tables 3 and 4, convergence typically requires about 100 iterations, but we note that useful GLRMs often emerge after only a few tens of iterations.

Matrix size	# nonzeros	Time per iteration (s)
$10^6 \times 10^6$	10^6	9
$10^6 \times 10^6$	10^9	13
$10^7 \times 10^7$	10^9	294

Table 4: SparkGLRM for custom GLRM, $k = 10$.

Acknowledgements

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A Quadratically regularized PCA

In this appendix we describe some properties of the quadratically regularized PCA problem (2),

$$\text{minimize } \|A - XY\|_F^2 + \gamma\|X\|_F^2 + \gamma\|Y\|_F^2. \quad (20)$$

In the sequel, we let $U\Sigma V^T = A$ be the SVD of A and let r be the rank of A . We assume for convenience that all the nonzero singular values $\sigma_1 > \sigma_2 > \dots > \sigma_r > 0$ of A are distinct.

A.1 Solution

Problem (2) is the only problem we will encounter that has an analytical solution. A solution is given by

$$X = \tilde{U}\tilde{\Sigma}^{1/2}, \quad Y = \tilde{\Sigma}^{1/2}\tilde{V}^T, \quad (21)$$

where \tilde{U} and \tilde{V} are defined as in (4), and $\tilde{\Sigma} = \mathbf{diag}((\sigma_1 - \gamma)_+, \dots, (\sigma_k - \gamma)_+)$.

To prove this, let's consider the optimality conditions of (2). The optimality conditions are

$$-(A - XY)Y^T + \gamma X = 0, \quad -(A - XY)^T X + \gamma Y^T = 0.$$

Multiplying the first optimality condition on the left by X^T and the second on the left by Y and rearranging, we find

$$X^T(A - XY)Y^T = \gamma X^T X, \quad Y(A - XY)^T X = \gamma Y Y^T,$$

which shows, by taking a transpose, that $X^T X = Y Y^T$ at any stationary point.

We may rewrite the optimality conditions together as

$$\begin{aligned} \begin{bmatrix} -\gamma I & A \\ A^T & -\gamma I \end{bmatrix} \begin{bmatrix} X \\ Y^T \end{bmatrix} &= \begin{bmatrix} 0 & XY \\ (XY)^T & 0 \end{bmatrix} \begin{bmatrix} X \\ Y^T \end{bmatrix} \\ &= \begin{bmatrix} X(Y Y^T) \\ Y^T(X^T X) \end{bmatrix} \\ &= \begin{bmatrix} X \\ Y^T \end{bmatrix} (X^T X), \end{aligned}$$

where we have used the fact that $X^T X = Y Y^T$.

Now we see that (X, Y^T) lies in an *invariant subspace* of the matrix $\begin{bmatrix} -\gamma I & A \\ A^T & -\gamma I \end{bmatrix}$. Recall that V is an invariant subspace of a matrix A if $AV = VM$ for some matrix M . If $\text{Rank}(M) \leq \text{Rank}(A)$, we know that the eigenvalues of M are eigenvalues of A , and that the corresponding eigenvectors lie in the span of V .

Thus the eigenvalues of $X^T X$ must be eigenvalues of $\begin{bmatrix} -\gamma I & A \\ A^T & -\gamma I \end{bmatrix}$, and (X, Y^T) must span the corresponding eigenspace. More concretely, notice that $\begin{bmatrix} -\gamma I & A \\ A^T & -\gamma I \end{bmatrix}$ is (symmetric,

and therefore) diagonalizable, with eigenvalues $-\gamma \pm \sigma_i$. The larger eigenvalues $-\gamma + \sigma_i$ correspond to the eigenvectors (u_i, v_i) , and the smaller ones $-\gamma - \sigma_i$ to $(u_i, -v_i)$.

Now, $X^T X$ is positive semidefinite, so the eigenvalues shared by $X^T X$ and $\begin{bmatrix} -\gamma I & A \\ A^T & -\gamma I \end{bmatrix}$ must be positive. Hence there is some set $|\Omega| \leq k$ with $\sigma_i \geq \gamma$ for $i \in \Omega$ such that X has singular values $\sqrt{-\gamma + \sigma_i}$ for $i \in \Omega$. (Recall that $X^T X = Y Y^T$, so Y has the same singular values as X .) Then (X, Y^T) spans the subspace generated by the vectors (u_i, v_i) for $i \in \Omega$. We say the stationary point (X, Y) has active subspace Ω . It is easy to verify that $XY = \sum_{i \in \Omega} u_i(\sigma_i - \gamma)v_i^T$.

Each active subspace gives rise to an orbit of stationary points. If (X, Y) is a stationary point, then $(XT, T^{-1}Y)$ is also a stationary point so long as

$$-(A - XY)Y^T T^{-T} + \gamma XT = 0, \quad -(A - XY)^T XT + \gamma Y^T T^{-T} = 0,$$

which is always true if $T^{-T} = T$, *i.e.*, T is orthogonal. This shows that the set of stationary points is invariant under orthogonal transformations.

To simplify what follows, we choose a representative element for each orbit. Represent any stationary point with active subspace Ω by

$$X = U_\Omega(\Sigma_\Omega - \gamma I)^{1/2}, \quad Y = (\Sigma_\Omega - \gamma I)^{1/2}V_\Omega^T,$$

where by U_Ω we denote the submatrix of U with columns indexed by Ω , and similarly for Σ and V . At any value of γ , let $k'(\gamma) = \max\{i : \sigma_i \geq \gamma\}$. Then we have $\sum_{i=0}^{k'} \binom{k'}{i}$ (representative) stationary points, one for each choice of Ω . The number of (representative) stationary points is decreasing in γ ; when $\gamma > \sigma_1$, the only stationary point is $X = 0, Y = 0$.

These stationary points can have quite different values. If (X, Y) has active subspace Ω , then

$$\|A - XY\|_F^2 + \gamma(\|X\|_F^2 + \|Y\|_F^2) = \sum_{i \notin \Omega} \sigma_i^2 + \sum_{i \in \Omega} (\gamma^2 + 2\gamma|\sigma_i - \gamma|).$$

From this form, it is clear that we should choose Ω to include the top singular values $i = 1, \dots, k'(\gamma)$. Choosing any other subset Ω will result in a higher (worse) objective value: that is, the other stationary points are *not* global minima.

A.2 Fixed points of alternating minimization

Theorem 1. The quadratically regularized PCA problem (2) has only one local minimum, which is the global minimum.

Our proof is similar to that of [BH89], who proved a related theorem for the case of PCA (1).

Proof. We showed above that every stationary point of (2) has the form $XY = \sum_{i \in \Omega} u_i d_i v_i^T$, with $\Omega \subseteq \{1, \dots, k'\}$, $|\Omega| \leq k$, and $d_i = \sigma_i - \gamma$. We use the representative element from each stationary orbit described above, so each column of X is $u_i \sqrt{d_i}$ and each row of Y is $\sqrt{d_i} v_i^T$ for some $i \in \Omega$. The columns of X are orthogonal, as are the rows of Y .

If a stationary point is not the global minimum, then $\sigma_j > \sigma_i$ for some $i \in \Omega$, $j \notin \Omega$. Below, we show we can always find a descent direction if this condition holds, thus showing that the only local minimum is the global minimum.

Assume we are at a stationary point with $\sigma_j > \sigma_i$ for some $i \in \Omega$, $j \notin \Omega$. We will find a descent direction by perturbing XY in direction $u_j v_j^T$. Form \tilde{X} by replacing the column of X containing $u_i \sqrt{d_i}$ by $(u_i + \epsilon u_j) \sqrt{d_i}$, and \tilde{Y} by replacing the row of Y containing $\sqrt{d_i} v_i^T$ by $\sqrt{d_i} (v_i + \epsilon v_j)^T$. Now the regularization term increases slightly:

$$\begin{aligned} \gamma(\|\tilde{X}\|_F^2 + \|\tilde{Y}\|_F^2) - \gamma(\|X\|_F^2 + \|Y\|_F^2) &= \sum_{i' \in \Omega, i' \neq i} (2\gamma t_{i'}) + 2\gamma d_i (1 + \epsilon^2) - \sum_{i' \in \Omega} 2\gamma t_{i'} \\ &= 2\gamma d_i \epsilon^2. \end{aligned}$$

Meanwhile, the approximation error decreases:

$$\begin{aligned} \|A - \tilde{X}\tilde{Y}\|_F^2 - \|A - XY\|_F^2 &= \|u_i \sigma_i v_i^T + u_j \sigma_j v_j^T - (u_i + \epsilon u_j) d_i (v_i + \epsilon v_j)^T\|_F^2 - (\sigma_i - d_i)^2 - \sigma_j^2 \\ &= \|u_i (\sigma_i - d_i) v_i^T + u_j (\sigma_j - \epsilon^2 d_i) v_j^T - \epsilon u_i d_i v_j^T - \epsilon u_j d_i v_i^T\|_F^2 \\ &\quad - (\sigma_i - d_i)^2 - \sigma_j^2 \\ &= \left\| \begin{bmatrix} \sigma_i - d_i & -\epsilon d_i \\ -\epsilon d_i & \sigma_j - \epsilon^2 d_i \end{bmatrix} \right\|_F^2 - (\sigma_i - d_i)^2 - \sigma_j^2 \\ &= (\sigma_i - d_i)^2 + (\sigma_j - \epsilon^2 d_i)^2 + 2\epsilon^2 d_i^2 - (\sigma_i - d_i)^2 - \sigma_j^2 \\ &= -2\sigma_j \epsilon^2 d_i + \epsilon^4 d_i^2 + 2\epsilon^2 d_i^2 \\ &= 2\epsilon^2 d_i (d_i - \sigma_j) + \epsilon^4 d_i^2, \end{aligned}$$

where we have used the rotational invariance of the Frobenius norm to arrive at the third equality above. Hence the net change in the objective value in going from (X, Y) to (\tilde{X}, \tilde{Y}) is

$$\begin{aligned} 2\gamma d_i \epsilon^2 + 2\epsilon^2 d_i (d_i - \sigma_j) + \epsilon^4 d_i^2 &= 2\epsilon^2 d_i (\gamma + d_i - \sigma_j) + \epsilon^4 d_i^2 \\ &= 2\epsilon^2 d_i (\sigma_i - \sigma_j) + \epsilon^4 d_i^2, \end{aligned}$$

which is negative for small ϵ . Hence we have found a descent direction, showing that any stationary point with $\sigma_j > \sigma_i$ for some $i \in \Omega$, $j \notin \Omega$ is not a local minimum. \square

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