Efficiently Factorizing Boolean Matrices using Proximal Gradient Descent

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Abstract

Addressing the interpretability problem of NMF on Boolean data, Boolean Matrix Factorization (BMF) uses Boolean algebra to decompose the input into low-rank Boolean factor matrices. These matrices are highly interpretable and very useful in practice, but they come at the high computational cost of solving an NP-hard combinatorial optimization problem. To reduce the computational burden, we relax BMF using a novel elastic BMF regularizer, from which we derive an efficient proximal point algorithm. Through an extensive set of experiments, we demonstrate that our method works well in practice: On synthetic data, we show that our algorithm converges quickly, recovers the ground truth precisely, and estimates the true matrix rank robustly. On real-world data, we improve upon the state of the art in recall, loss, and runtime, and a case study from the medical domain confirms that our results are easily interpretable and semantically meaningful.

1 Introduction

Discovering groups in data and expressing them in terms of common concepts is a central problem in many scientific domains and business applications, including cancer genomics [22], neuroscience [13], and recommender systems [17, 8]. This problem is often addressed using variants of *matrix factorization*, a family of methods that decompose the target matrix into a set of typically low-rank factor matrices whose product approximates the input well. Prominent examples of matrix factorization are Singular Value Decomposition (SVD) [10], Principal Component Analysis (PCA) [10], and Nonnegative Matrix Factorization (NMF) [30, 20, 21]. These methods differ in how they constrain the matrices involved: SVD and PCA require orthogonal factors, while NMF constrains the target matrix and the factors to be nonnegative.

SVD, PCA, and NMF achieve interpretable results—unless the data is Boolean. In this case, which is ubiquitous in the real world, their results are hard to interpret, because the input domain differs from the output domain. *Boolean Matrix Factorization* (BMF) addresses this problem by seeking two low-rank *Boolean* factor matrices whose Boolean product is close to the Boolean target matrix [23]. The output matrices, now lying in the same domain as the input, are interpretable and useful, but they come at the computational cost of solving an NP-hard combinatorial optimization problem [29, 23, 24]. To make BMF applicable in practice, we need efficient approximation algorithms.

There are many ways to approximate BMF—for example, by exploiting its underlying combinatorial or spatial structure [23, 5, 4], using probabilistic inference [36, 35, 34], or solving the related Bi-Clustering problem [27, 28]. Although these approaches achieve impressive results, they fall short when the input data is large and noisy. Hence, we take a different approach to overcome BMF's computational barrier. Starting from an NMF-like optimization problem, we derive a relaxation of the original BMF problem that allows intermediate solutions to be real-valued. Inspired by the elastic-net regularizer [42], we introduce the novel *elastic-BMF regularizer* to regularize towards Boolean factor

Submitted to 36th Conference on Neural Information Processing Systems (NeurIPS 2022). Do not distribute.

matrices. We obtain an efficient-to-compute *proximal operator* from our elastic-BMF regularizer that projects relaxed real-valued factors towards being Boolean, which allows us to leverage efficient gradient-based optimization procedures. In stark contrast to the state of the art [15, 16], which requires heavy post-hoc post-processing to actually achieve Boolean factors, we ensure a Boolean outcome upon convergence, by gradually increasing the projection strength using a *regularization rate*. We combine our relaxation, efficient proximal operator, and regularization rate into an *Elastic Boolean Matrix Factorization* algorithm (ELBMF) that is elegant, accurate, and efficient.

In summary, our main contributions are as follows:

1. We introduce the elastic BMF regularizer.
2. We overcome the computational hardness of BMF leveraging a novel relaxed BMF problem.
3. We efficiently solve the relaxed BMF problem using an optimization algorithm based on proximal gradient descent.

The remainder of the paper proceeds as follows. In Sec. 2, we formally introduce the BMF problem and its relaxation, define our elastic BMF regularizer and its proximal point operator, and show how to ensure a Boolean outcome upon convergence. We discuss related work in Sec. 3, validate our method through an extensive set of experiments in Sec. 4, and conclude with a discussion in Sec. 5.

2 Theory

Our goal is to factorize a given Boolean target matrix into at least two smaller, low-rank Boolean factor matrices, whose product comes close to the target matrix. Since the factor matrices are Boolean, this product follows the algebra of a Boolean semi-ring, i.e., it is identical to the standard outer product on a field where addition obeys $1 + 1 = 1$. We define the product between two Boolean matrices $\mathrm{U} \in \{0,1\}^{n\times k}$ and $\mathrm{V} \in \{0,1\}^{k\times m}$ on a Boolean semi-ring $(\{0,1\}, \vee, \wedge)$ as

$$[\mathrm{U} \circ \mathrm{V}]_{ij} = \bigvee_{l\in[k]} \mathrm{U}_{il}\mathrm{V}_{lk} \,, \tag{1}$$

where $[\mathrm{U} \circ \mathrm{V}] \in \{0,1\}^{n\times m}$. This gives rise to the BMF problem.

Problem 1 (Boolean Matrix Factorization) *For a given target matrix* $\mathrm{A} \in \{0,1\}^{n\times m}$ *and a given matrix rank* $\mathbb{N} \ni k \leq \min\{n, m\}$*, discover the factor matrices* $\mathrm{U} \in \{0,1\}^{n\times k}$ *and* $\mathrm{V} \in \{0,1\}^{k\times m}$ *that minimize*

$$\|\mathrm{A} - \mathrm{U} \circ \mathrm{V}\|_F^2 = \sum_{ij} \mathrm{A}_{ij} \oplus [\mathrm{U} \circ \mathrm{V}]_{ij} \,. \tag{2}$$

While beautiful in theory, we cannot solve this problem exactly for all but the smallest matrices, as it is NP-complete [24]. In practice, we have to rely on approximations. To do this, we relax the Boolean constraints of Eq. (2) to allow non-negative, *non-Boolean* 'intermediate' factor matrices during the optimization. In other words, we solve the non-negative matrix factorization (NMF) [30]

$$\|\mathrm{A} - \mathrm{U}\mathrm{V}\|_F^2 \,, \tag{3}$$

subject to $\mathrm{U} \in \mathbb{R}_+^{n\times k}$ and $\mathrm{V} \in \mathbb{R}_+^{k\times m}$. We can solve this problem efficiently, e.g., via a Gauss-Seidel scheme. Although efficient, using plain NMF, however, disregards the Boolean structure of our matrices and produces factor matrices from a different domain, which are consequently hard to interpret and potentially very dense. To benefit from efficient optimization and still arrive at Boolean outputs, we allow real-valued intermediate solutions and regularize them towards becoming Boolean.

To steer our optimization towards Boolean solutions, we penalize non-Boolean solutions using a regularizer. This idea has been explored in prior work. There exists the l_1-inspired PRIMP regularizer [15], which is $-\kappa[-|1-2x|+1]$ for values inside $[0,1]$ and ∞ otherwise, and the l_2-inspired bowl-shaped regularizer [41], which is $\lambda(x^2-x)^2/2$ everywhere on the real line. Although both have been successfully applied to BMF, both also have undesirable properties: The PRIMP regularizer penalizes well *inside* the interval $[0,1]$ but is non-differentiable on the outside, while the bowl-shaped regularizer is differentiable and penalizes well *outside* the interval $[0,1]$ but is almost flat on the inside. Hence, both regularizers are problematic if used individually. Combining them,

however, yields a regularizer that penalizes non-Boolean values well across the full real line. To combine l_1- and l_2-regularization, we use the *elastic-net regularizer*,

$$r(x) = \kappa\|x\|_1 + \lambda\|x\|_2^2 \ , \tag{4}$$

which, however, only penalizes *non-zero* solutions [42]. To penalize *non-Boolean* solutions, we combine two elastic-net regularizers into our (almost W-shaped) *elastic-BMF regularizer*,

$$R(X) = \sum_{x \in X} \min\{r(x), r(x-1)\} \ , \tag{5}$$

where $X \in \{\mathrm{U}, \mathrm{V}\}$. In Fig. 1, we show all three regularizers in the range of $[-1, 2]$, for $\lambda = \kappa = 0.5$. We see that only the elastic BMF regularizer penalizes non-Boolean solutions across the full spectrum, and summarize our regularized relaxed BMF as follows.

Problem 2 (Elastic Boolean Matrix Factorization) *For a given target matrix* $\mathrm{A} \in \{0,1\}^{n \times m}$ *and a given matrix rank* $\mathbb{N} \ni k \leq \min\{n, m\}$*, discover the factor matrices* $\mathrm{U} \in \mathbb{R}_+^{n \times k}$ *and* $\mathrm{V} \in \mathbb{R}_+^{k \times m}$ *that minimize*

$$\|\mathrm{A} - \mathrm{UV}\|_F^2 + R(\mathrm{U}) + R(\mathrm{V}) \ . \tag{6}$$

Although this is a relaxed problem, it is still non-convex. Therefore, we cannot straightforwardly solve it. However, the problem is suitable for the Gauss-Seidel optimization scheme. That is, we alternatingly fix one factor matrix to optimize the other. By doing so, we generate a sequence

$$\mathrm{U}_{t+1} \leftarrow \arg\min_{\mathrm{U}} \|\mathrm{A} - \mathrm{UV}_t\|_F^2 + R(\mathrm{U}) \ , \tag{7}$$

$$\mathrm{V}_{t+1} \leftarrow \arg\min_{\mathrm{V}} \|\mathrm{A} - \mathrm{U}_{t+1}\mathrm{V}\|_F^2 + R(\mathrm{V}) \ , \tag{8}$$

of simpler-to-solve sub-problems, until convergence. Now, each sub-problem is again a sum of two $f(X) + R(X)$ functions, where f is the loss $\|\cdot\|_F^2$, and $R(X)$ is the regularizer. This allows us to follow a proximal gradient approach, i.e., we use *Proximal Alternating Linear Minimization* (PALM) [6, 32]. In a nutshell, we minimize a sub-problem by following the gradient ∇f of f, to then use the proximal operator for R to nudge its outcome towards a Boolean solution. That is, for the gradients $\nabla_{\mathrm{U}} f = \mathrm{UVV}^\top - \mathrm{AV}^\top$ and $\nabla_{\mathrm{V}} f = \mathrm{VU}^\top\mathrm{U} - \mathrm{A}^\top\mathrm{V}$, we compute the step

$$\mathrm{prox}_R(X - \eta\nabla f) \ , \tag{9}$$

where η represents the step size, which we compute in terms of Lipschitz constant, rather than relying on a costly line-search [6]. To further improve the convergence properties, we make use of an *inertial* term that linearly combines X_t with X_{t-1} before applying Eq. (9) (see [32] for a detailed description). We now derive the proximal operator for the elastic BMF regularizer, before discussing how we ensure that the factor matrices are Boolean, and summarizing our approach as an algorithm.

2.1 Proximal Mapping

To solve the sub-problem

$$\arg\min_X f(X) + R(X)$$

from Eq. (8), where $X \in \{\mathrm{U}, \mathrm{V}\}$, we need a proximal operator [31] that projects values towards a regularized point. This operator is the solution to

$$\mathrm{prox}(X) = \arg\min_Y \frac{1}{2}\|X - Y\|_2^2 + R(X) \ .$$

As Eq. (2.1) is coordinate-wise solvable, we can reduce this equation to a scalar proximal operator

$$\mathrm{prox}_{\kappa\lambda}(x) = \arg\min_{y \in \mathbb{R}} \frac{1}{2}(x-y)^2 + R(y) \ .$$

Although this scalar function may seem simple, due to R, it is non-convex, which—in general—rules out the existence of unique minima. We can, however, exploit the W-shape of R. That is, from the perspective of a fixed U_{ij}, the regularizer is locally convex after a case distinction. Starting with the case of $X_{ij} = x$, $x \leq 1/2$, we can simplify Eq. (2.1) to $\frac{1}{2}(x-y)^2 + \lambda'/2y^2 + \kappa|y|$, letting $\lambda' = 2\lambda$. Setting its derivative to 0, we get to $y = x - \kappa\,\mathrm{sign}(y)$. Asserting that a least-squares solution will always be of the same sign, we substitute the sign of x with $\mathrm{sign}(y)$. Repeating these steps analogously for $x > 1/2$, we obtain our proximal operator:

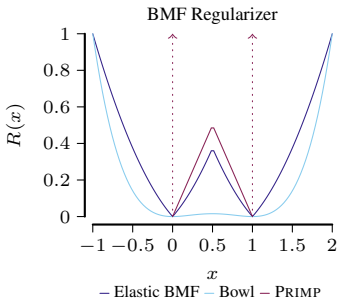


Figure 1: We show three BMF regularizer for $\lambda = \kappa = 0.5$.

Algorithm 1: ELBMF

Input: Matrix $\mathrm{A} \in \{0,1\}^{n \times m}$, rank $k \in \mathbb{N}$
Output: Factors $\mathrm{U} \in \{0,1\}^{n \times k}$, $\mathrm{V} \in \{0,1\}^{k \times m}$
initialize U, V uniformly at random
for $t = 1, 2, \ldots$ **until convergence do**
  $\mathrm{U} \leftarrow \arg\,\mathrm{reduce}_{\mathrm{U}}\, \ell_{\lambda_t}(\mathrm{A}, \mathrm{U}, \mathrm{V})$
  $\mathrm{V} \leftarrow \arg\,\mathrm{reduce}_{\mathrm{V}}\, \ell_{\lambda_t}(\mathrm{A}, \mathrm{U}, \mathrm{V})$
end

Definition 1 (Proximal Operator) *Given regularization coefficients κ and λ, our proximal operator for matrix X is $\mathrm{prox}_R(X) = [\mathrm{prox}_{\kappa\lambda}(X_{ij})]_{ij}$, where $\mathrm{prox}_{\kappa\lambda}$ is the scalar proximal operator*

$$\mathrm{prox}_{\kappa\lambda}(x) \equiv (1+\lambda)^{-1} \begin{cases} x - \kappa\,\mathrm{sign}(x) & \text{if } x \leq \frac{1}{2} \\ x - \kappa\,\mathrm{sign}(x-1) + \lambda & \text{otherwise .} \end{cases} \tag{10}$$

Although not strictly necessary, to improve the empirical convergence rate, we would like to constrain our factor matrices to be non-negative. As our proximal operator does not account for this, we impose non-negativity by using the *alternating projection* procedure to combine the non-negativity proximal operator [31] with Eq. (10) into $\max\{0, \mathrm{prox}_{\kappa\lambda}(x)\}$.

2.2 Ensuring Boolean Factors

Our proximal operator only nudges the factor matrices towards *becoming* Boolean. We, however, want to ensure that our results *are* Boolean. To this end, the state-of-the-art method PRIMP relies heavily on post-processing, performing a very expensive joint two-dimensional grid search to guess the 'best' pair of rounding thresholds, which are then used to produce Boolean matrices. Although this tends to work in practice, it is an inefficient post-hoc procedure—and thus, it would be highly desirable to have Boolean factors already upon convergence. To achieve this without rounding or clamping, we revisit our regularizer, which binarizes more strongly if we regularize more aggressively. Consequently, if we regularize too aggressively, we converge to a suboptimal solution, and if we regularize too mildly, we do not binarize our solutions. To prevent subpar solutions and still binarize our output, we start with a weak regularization and gradually increase its strength.

Considering Eq. (10), we see that a higher regularization strength increases the distance over which our proximal operator projects. Thus, if we set the l_1-distance controlling κ too high, we will immediately leap to a Boolean factor matrix, which will terminate the algorithm and yield a suboptimal solution. Regulating the l_2-distance controlling λ is a less delicate matter. Hence, we gradually increase λ to prevent a subpar solution and achieve a Boolean outcome, using a *regularization rate* $\lambda_t = \lambda \cdot \nu_t$ that gradually increases the proximal distance at a user-defined rate $\nu_t \geq 0\, \forall t \geq 0$.

We summarize the considerations laid out above as ELBMF in Alg. 1. The computational complexity of ELBMF is bounded by the complexity of computing the gradient, which is identical to the complexity of matrix multiplication. Therefore, for all practical purposes, ELBMF is sub-cubic $\mathcal{O}\left(n^{2.807}\right)$ using Strassen's algorithm.

3 Related Work

Matrix factorization is a well-established family of methods, whose members, such as SVD, PCA, or NMF, are used everywhere in machine learning. Almost all matrix factorization methods operate on real-valued matrices, however, while BMF operates under Boolean algebra. *Boolean Matrix Factorization* originated in the combinatorics community [26] and was later introduced to the data mining community [23], where many cover-based BMF algorithms were developed [5, 4,

23, 25]. In recent years, BMF has gained traction in the machine learning community, which tends to tackle the problem differently. Here, *relaxation-based approaches* that optimize for a relaxed but regularized BMF [15, 14, 41] are related to our method, but they differ especially in their regularization. Hess et al. [15] introduce a regularizer that is only partially differentiable and rely heavily on post-processing to force a Boolean solution, and Zhang et al. [41] regularize only weakly between 0 and 1. In contrast, our regularizer penalizes well across the full spectrum and yields a Boolean outcome upon convergence. Other recent approaches build on *probabilistic inference*. Rukat et al. [36, 35, 34], for example, combine Bayesian Modeling and sampling into their logical factor machine. A similar direction is taken by Ravanbakhsh et al. [33], who use graphical models and message passing, and Liang et al [22], who combine MAP-inference and sampling. A different, *geometry-based approach* lies in locating dense submatrices by ordering the data to exploit the consecutive-ones property [39, 37]. Since BMF is essentially solving a bipartite graph partitioning problem, it is also closely related to Bi-Clustering and Co-Clustering [27]. Neumann and Miettinen [28] use this relationship to efficiently solve BMF by means of a streaming algorithm. Although there are many different approaches to BMF, its biggest challenge to date remains scalability [24].

4 Experiments

We implement ELBMF in the Julia language and run experiments on 16 Cores of an AMD EPYC 7702 and a single NVIDIA A100 GPU, reporting wall clock time. We provide the source code, datasets, synthetic dataset generator, and other information needed for reproducibility.[1] We compare ELBMF against six methods: three dedicated BMF methods (ASSO [23], GRECOND [5], and PRIMP [15]), one streaming Bi-Clustering algorithm SOFA [28], one elastic-net-regularized NMF method leveraging proximal gradient descent (NMF [30, 20, 21]), and one interpretable Boolean autoencoder (BINAPS [9]). Since NMF outputs non-negative factor matrices, rather Boolean matrices, we cannot compare against NMF directly, so we clamp and round its solutions to the nearest Boolean outcome. To fairly compare against BINAPS, we task it with autoencoding the target matrix as a reconstruction, given the matrix ranks from our experiments as the number of latent dimensions. We perform three sets of experiments. First, we ascertain that ELBMF works reliably on synthetic data. Second, we verify that it generally performs well on real-world data. And third, we illustrate that its outputs are semantically meaningful through an exploratory analysis of a biomedical dataset.

4.1 Performance of ELBMF on Synthetic Data

In the following experiments, we ask three questions: (**1**) Does ELBMF converge?; (**2**) How well does ELBMF recover the information in the target matrix?; and (**3**) Does ELBMF estimate the true Boolean matrix rank correctly? To answer these questions, we generate synthetic data with known ground truth as follows. Starting with an all-zeros matrix, we randomly create rectangular, non-overlapping *tiles* full of ones, each spanning between 5 and 10 rows and columns. We then add noise by setting each cell to 1, uniformly at random, with varying noise probabilities.

How does ELBMF converge? To study how our method converges to a Boolean solution, we quantify relevant properties of the sequence of intermediate solutions (cf. Eq. (8)). First, to understand how quickly and stably ELBMF converges to a Boolean solution, we quantify the *Boolean gap*,

$$\sum_{X \in \{U_t, V_t\}} |X|^{-1} \sum_{x \in X} \min\{|x|, |x-1|\} \ .$$

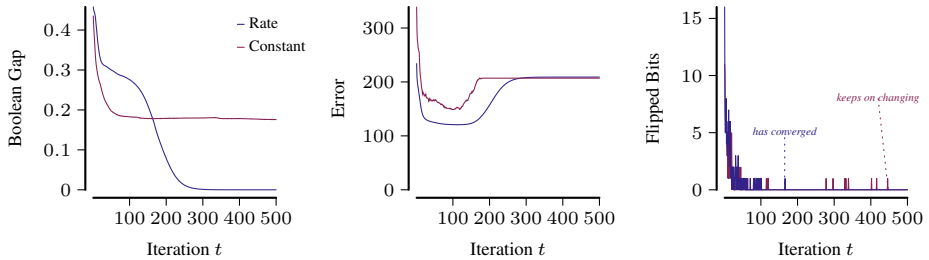
Second, to understand when we can safely round intermediate almost-Boolean solutions without losing information, we compute the fraction of bits that flip from iteration t to iteration $t+1$ as the *Hamming process*

$$|A|^{-1} \|\mathrm{B}_t - \mathrm{B}_{t+1}\|_1 \ ,$$

where B is a *rounded* intermediate reconstruction.

As shown in Fig. 2a, we achieve an almost-Boolean solution *without any rounding* after around 250 epochs, continuing until we reach an Boolean outcome. This is also the point at which the rounded

[1] dropbox.com/sh/gaoftnf0iyh27xq/AADRlhKxTV1S9LovwwnxVTCYa



(a) (b) (c)

Figure 2: Our method converges quickly under a regularization rate. We report the progression over time of the *Boolean gap* (a), *loss* and *loss of rounded factors* (b), as well as the *Hamming process* (c) of ELBMF on synthetic 40×30 matrices with 10% noise, under a constant regularization of $\lambda_t = 1$ or a regularization rate of $\lambda_t = 1.05^t$.

intermediate solution and its relaxation are almost identical, as illustrated in Fig. 2b. Considering the *rounded* solution sequence in Fig. 2c, we observe that ELBMF goes through an erratic bit-flipping-phase in the beginning, followed by only minor changes in each iteration until iteration $t = 100$. Afterwards, ELBMF has settled on a solution—under our regularization rate. When using constant regularization instead, we continue to observe bit flips until the end of the experiment (Fig. 2c). The constant regularization fits the data slightly better than the regularization rate (Fig. 2b), which is unsurprising, given that its factors are less constrained than the Boolean factors we use otherwise. However, under constant regularization, the Boolean gap hardly decreases over time (Fig. 2a). In other words, our regularization works well, and it allows us to safely binarize almost-converged factors that are ϵ-far from being Boolean by means of, e.g., our proximal operator.

How well does ELBMF recover the information in the target matrix? Having ensured that our method converges stably and quickly, we would like to assess whether it also converges to a high-quality factorization. To this end, we generate synthetic 40×30 matrices containing 5 random tiles, under additive noise levels between 0% (no noise) and 50%. We then compute the fraction of *ones* in the target matrix A that is covered by the reconstruction $\mathrm{B} = \mathrm{U} \circ \mathrm{V}$, i.e., the *recall* (higher is better)

$$\|\mathrm{A}\|_1^{-1} \|\mathrm{A} \odot \mathrm{B}\|_1 \ .$$

To ensure that we fit the *signal* in the data, we additionally report the recall regarding the generating, noise-free ground-truth tiles A^*, denoted as recall*. Finally, we compute the *Hamming similarity* (higher is better) between the target matrix and its reconstruction,

$$|\mathrm{A}|^{-1} \|\mathrm{A} - \mathrm{B}\|_1 \ ,$$

to rate the overall quality of the reconstruction including *zeros*.

We run each method on our synthetic datasets, targeting a matrix rank of 5. To account for random fluctuations, we average over 10 samples per 10% increment in noise probability. In Fig. 3, we show similarity, recall, and recall*. We observe that in the noiseless case (0%), all methods except BINAPS recover the 5 ground-truth tiles with high accuracy, but only ASSO and ELBMF do so with perfect recalls. Starting with as little as 10% noise, both recalls of ASSO, GRECOND, SOFA, NMF, and BINAPS deteriorate quickly, while the similarity and both recalls of PRIMP and ELBMF remain high. In fact, ELBMF and PRIMP perform similarly across the board—which is highly encouraging, as unlike PRIMP, ELBMF does not require post-processing. For ASSO and GRECOND, recall and similarity drop considerably, but they exhibit a slightly higher recall*. This means that these methods are robust against noise, but they fail to recover the remaining information.

Does ELBMF estimate the true Boolean matrix rank correctly? When the true matrix rank is known, we can immediately apply ELBMF to factorize the data. In the real world, however, the true matrix rank might be unknown. In this case, we need to estimate an appropriate choice from the data, and we use synthetic data to ensure that ELBMF does so correctly.

Since a higher matrix rank usually also means a better fit, selecting the best rank according to recall, loss, or similarity leads to overfitting—unless we properly account for the growth in model complexity.

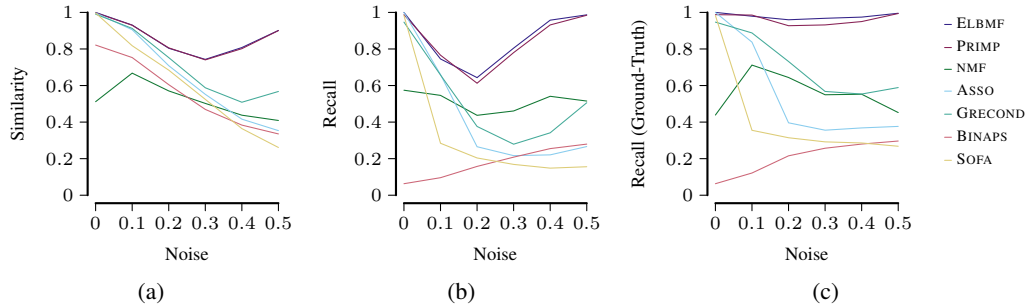


Figure 3: Overall, ELBMF reconstructs the noisy synthetic data well and recovers the ground-truth tiles. On synthetic data for additive noise levels increasing from 0% to 50%, we show *similarity* (a) and *recall* (b) w.r.t. the target matrix, and recall* w.r.t. the noise-free ground-truth tiles, for ASSO, GRECOND, SOFA, NMF, PRIMP, and ELBMF.

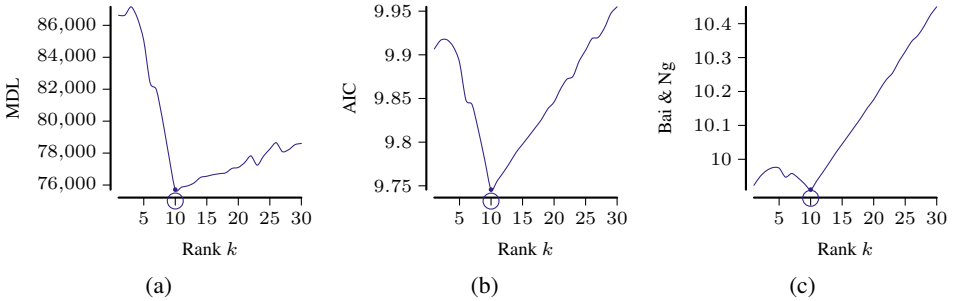


Figure 4: ELBMF robustly detects the correct rank and does not overfit the data under different model selection criteria, such as MDL, AIC, or Bai & Ng's first information criterion.

There are many *model selection criteria* that penalize complex models, such as AIC [1], Bai & Ng's criteria [3, 2], Nuclear-norm regularizing [19, 12], the information-theoretic Minimal Description Length principle (MDL) [11], or (Decomposed) Normalized Maximum Likelihood [18, 40]. We choose MDL, because it works very well in practice and is easily applied to our model. We use the log binomial $l(X) = \log \binom{|X|}{\|X\|_1}$ of any Boolean matrix X [25], to encode and sum the encoding lengths of the error matrix and the rows and columns of our factorization (assumed to be i.i.d.),

$$l(\mathrm{A} \oplus \mathrm{U} \circ \mathrm{V}) + \sum_{i \in [k]} l(\mathrm{U}_i^\top) + l(\mathrm{V}_i) + k \log(n \cdot m)\,,$$

as the *description length*, and select its *minimizer*.

To validate whether ELBMF recovers the right rank, we synthetically generate a ground-truth 400×300 matrix of rank 10 with 10% additive noise. In Fig. 4, we show MDL, AIC, and Bai & Ng's first criterion for each rank up to 30, finding that our method precisely discovers the true matrix rank.

4.2 Performance of ELBMF on Real-World Data

Having ascertained that ELBMF works well on synthetic data, we turn to its performance in the real world. Here, we use nine publicly available datasets and anonymized[2] from different domains. To cover the *biomedical domain*, we extract the network containing empirical evidence of protein-protein interactions in *homo sapiens* from the STRING database. From the GRAND repository, we take the gene regulatory networks sampled from *Glioblastoma (GBM)* and *Lower Grade Glioma (LGG)* brain cancer tissues, as well as from non-cancerous *Cerebellum* tissue. The *TCGA* dataset

[2] GRAND.NETWORKMEDICINE.ORG STRING-DB.ORG CANCER.GOV/TCGA INTERNATIONALGENOME.ORG PATENTSVIEW.ORG GROUPLENS.ORG/DATASETS/MOVIELENS KAGGLE.COM/DATASETS/NETFLIX-INC/NETFLIX-PRIZE-DATA

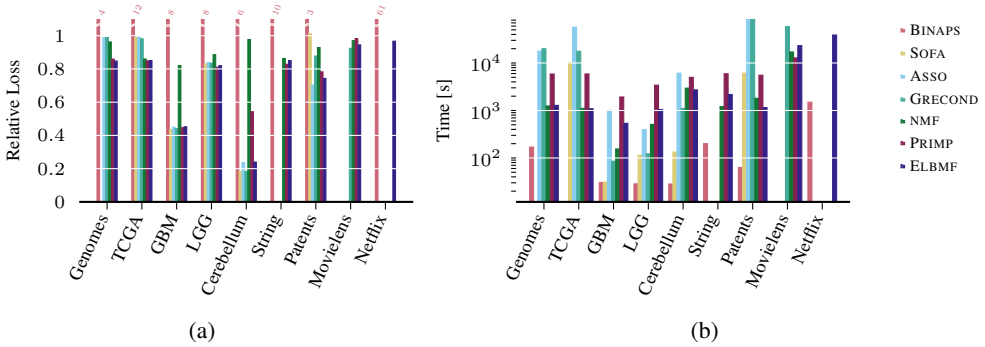


Figure 5: Our method factorizes real-world data with low relative loss and runtime. We report relative loss (a) and runtime (b) between real-world target matrices and their reconstructions from ASSO, GRECOND, SOFA, BINAPS, NMF, and ELBMF. Tilted numbers in (a) report relative loss of BINAPS.

contains binarized gene expressions from cancer patients, and we further obtain the single nucleotide polymorphism (SNP) mutation data from the 1*k Genomes* project, following processing steps from the authors of BINAPS [9]. In the *entertainment domain*, we use the user-movie datasets *Movielens* and *Netflix*, binarizing the original 5-star-scale ratings by setting only reviews with more than 3.5 stars to 1. Finally, as data from the *innovation domain*, we derive a directed citation network between patent groups from patent citation and classification data provided by *PatentsView*. For each dataset with a given number of groups, such as cancer types or movie genres, we set the matrix rank k to 33 (TCGA), 28 (Genomes), 136 (Patents), 20 (Movielens), and 20 (Netflix). When the number of subgroups is unknown, we estimate the rank using MDL and ELBMF, resulting in 100 (GBM), 32 (LGG), 100 (String), and 450 (Cerebellum).

As we can achieve a high similarity with an all-zeros reconstruction (in the case of sparse data), or a perfect recall with an all-ones reconstruction, we also report the *relative loss* (lower is better),

$$\|\mathrm{A}\|_1 \|\mathrm{A} - \mathrm{U} \circ \mathrm{V}\|_1 \,,$$

between the target matrices and their reconstructions. In Fig. 5, we show recall and runtime of ASSO, GRECOND, SOFA, BINAPS, NMF, and ELBMF, applied to all datasets. We see in Fig. 5a that ELBMF often has the lowest loss, outperforming ASSO, GRECOND, SOFA, BINAPS, and NMF. In many cases, ELBMF also has a loss lower than PRIMP. We observe the largest gap between the two on the Cerebellum dataset, where PRIMP's grid search procedure fails to find suitable thresholds. This is a highly impressive result, as ELBMF does not necessitate heavy post-processing, which is required by PRIMP. In Fig. 5b (log scale), we see how post-processing degrades runtime, observing that PRIMP is always much slower than ELBMF. For example, PRIMP does not finish on the Netflix data, where only ELBMF and BINAPS succeeded. Notably, without much extra care, NMF's performance is surprisingly good: It often outperforms the dedicated BMF methods ASSO, GRECOND, and SOFA.

4.3 Exploratory Analysis of Gene Expression Data with ELBMF

Knowing that ELBMF performs well quantitatively, we ask whether its outputs are also interpretable. To this end, we take a closer look at the *TCGA* data, which contains the expression levels of 20 530 genes from 10 459 patients, who are labeled with 33 cancer types. Since we are interested in retaining high gene expression levels only, we set expression levels to one if their Z-scores fall into the top 5% quantile, and to zero otherwise [22]. We run ELBMF on this dataset, targeting a rank of 33.

To learn whether our method groups patients meaningfully, we visualize the target matrix and its reconstruction. As the target matrix is high-dimensional, we embed both the target matrix and the reconstruction into a two-dimensional space using t-SNE [38] as illustrated in Fig. 6, where each color corresponds to one cancer type. In Fig. 6a, we show that when embedding the target matrix directly, the cancer types are highly overlapping and hard to distinguish without the color coding. In contrast, when embedding our reconstruction, depicted in Fig. 6b, we see a clean segmentation into clusters that predominantly contain a single cancer type.

To better understand these results, we quantify the association between our 33 estimated groups and the ground-truth cancer types by computing the *mutual information* matrix. This matrix is noticeably

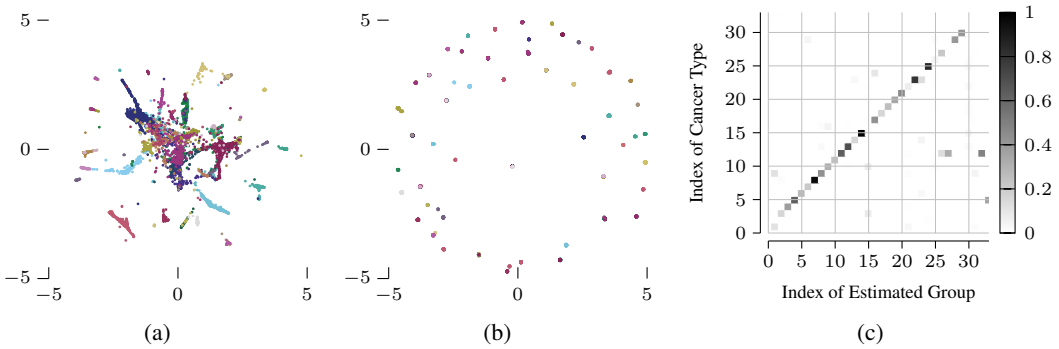


Figure 6: ELBMF discovers the hidden structure in gene expression data. We show the two-dimensional t-SNE embedding of the TCGA dataset (a) and the embedding of its reconstruction from ELBMF (b), where each point corresponds to one of the 10 459 patients, colored by cancer type. While the cancer types are hard to differentiate in the embedding of the original dataset (a), they are separated into easily distinguishable clusters in the embedding of our reconstruction (b). In (c), we show the renormalized mutual information between estimated groups and cancer types, and observe that there is an almost 1-to-1 correspondence between our estimated groups and the cancer types.

sparse (Fig. 6c), leading to a clean segmentation. Upon closer inspection with ENRICHR [7], the associations we discover turn out to be biologically meaningful. For example, we find that ELBMF associates a group of 356 genes to patients with *thyroid carcinoma*. This group is associated with *thyroid hormone generation* and *thyroid gland development*, and *statistically significantly* so—even under a strict False Discovery Control, with p-values as low as 2.574×10^{-8} and 6.530×10^{-6}.

5 Conclusion

We introduced ELBMF to efficiently factorize Boolean matrices using an elegant and simple algorithm that, unlike its closest competitors, does not rely on heavy post-processing. ELBMF considers a novel relaxed BMF problem, which allows intermediate solutions to be real-valued. It solves this problem by leveraging an efficiently computable proximal operator, derived from the innovative elastic BMF regularizer, and using a regularization rate to obtain Boolean factors upon convergence. Experimentally, we have shown that ELBMF works well in practice. It operates reliably on synthetic data, outperforms the state of the art on real-world data, and yields interpretable results even in difficult domains—without relying on rounding.

Although ELBMF works overall, it has two bottlenecks. First, by randomly initializing factors, we start with highly dense matrices, thus prohibiting efficient sparse matrix operations. This is not ideal for sparse datasets that are too large to fit into memory, and future research on sparse initialization of *Boolean* factors will benefit not only ELBMF but also many other methods. Second, the larger the datasets, the higher the cost of computing gradients, and future work might adapt stochastic gradient methods for ELBMF to mitigate this problem.

Broader Impact

ELBMF is a method for factorizing Boolean matrices, which permits interpretable, rather than black box data analysis. As such, it can help to make explicit any biases that may be present in the data. Just like any other method for interpretable data analysis, the insights they yield us can be used for good (e.g., insight into cancer-causing mutations) or for bad, and the ultimate quality of the outcome also depends on the behavior of the user. In our experiments we focus on *good* applications, and only consider anonymized open data.

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6 Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Sec. 5.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Sec. 5.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Sec. 2.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Sec. 2 and appendix.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Sec. 4, appendix, and under dropbox.com/sh/gaoftnf0iyh27xq/AADRlhKxTV1S9LovwwnxVTCYa.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Sec. 4 and appendix
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See appendix.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Sec. 4
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
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   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] See Sec. 4. All datasets are publicly available.
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5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]