ONLINE MATRIX FACTORIZATION FOR MARKOVIAN DATA AND APPLICATIONS TO NETWORK DICTIONARY LEARNING

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ABSTRACT. Online Matrix Factorization (OMF) is a fundamental tool for dictionary learning problems, giving an approximate representation of complex data sets in terms of a reduced number of extracted features. Convergence guarantees for most of the OMF algorithms in the literature assume independence between data matrices, and the case of a dependent data stream remains largely unexplored. In this paper, we show that the well-known OMF algorithm for i.i.d. stream of data proposed in [MBPS10], in fact converges almost surely to the set of critical points of the expected loss function, even when the data matrices form a Markov chain satisfying a mild mixing condition. Furthermore, we extend the convergence result to the case when we can only approximately solve each step of the optimization problems in the algorithm. For applications, we demonstrate dictionary learning from a sequence of images generated by a Markov Chain Monte Carlo (MCMC) sampler. Lastly, by combining online non-negative matrix factorization and a recent MCMC algorithm for sampling motifs from networks, we propose a novel framework of Network Dictionary Learning, which extracts 'network dictionary patches' from a given network in an online manner that encodes main features of the network. We demonstrate this technique on real-world text data.

1. INTRODUCTION

In modern data analysis, a central step is to find a low-dimensional representation to better understand, compress, or convey the key phenomena captured in the data. Matrix factorization provides a powerful setting for one to describe data in terms of a linear combination of factors or atoms. In this setting, we have a data matrix $X \in \mathbb{R}^{d \times n}$, and we seek a factorization of $X$ into the product $WH$ for $W \in \mathbb{R}^{d \times r}$ and $H \in \mathbb{R}^{r \times n}$. This problem has gone by many names over the decades, each with different constraints: dictionary learning, factor analysis, topic modeling, component analysis. It has applications in text analysis, image reconstruction, medical imaging, bioinformatics, and many other scientific fields more generally [SGH02, BB05, BBL+07, CWS+11, TN12, BMB+15, RPZ+18].

![Figure 1. Illustration of matrix factorization. Each column of the data matrix is approximated by a linear combination of the columns of the dictionary matrix.](image)

Online matrix factorization is a problem setting where data are accessed in a streaming manner and the matrix factors should be updated each time. That is, we get draws of $X$ from some distribution $\pi$ and seek the best factorization such that the expected loss $E_{X \sim \pi} \left[ \| X - WH \|_F^2 \right]$ is small. This is a relevant setting in today’s data world, where large companies, scientific instruments, and healthcare systems are collecting massive amounts of data every day. One cannot compute with the entire
dataset, and so we must develop online algorithms to perform the computation of interest while accessing them sequentially. There are several algorithms for computing factorizations of various kinds in an online context. Many of them have algorithmic convergence guarantees, however, all these guarantees require that data are sampled at each iteration i.i.d. with respect to previous iterations. In all of the application examples mentioned above, one may make an argument for (nearly) identical distributions, but never for independence. This assumption is critical to the analysis of previous works (see, e.g., [MBPS10, GTLY12, ZTX16]).

A natural way to relax the assumption of independence in this online context is through the Markovian assumption. In many cases one may assume that the data are not independent, but independent conditioned on the previous iteration. The central contribution of our work is to extend the analysis of online matrix factorization in [MBPS10] to the setting where the sequential data form a Markov chain. This is naturally motivated by the fact that the Markov chain Monte Carlo (MCMC) method is one of the most versatile sampling techniques across many disciplines, where one designs a Markov chain exploring the sample space that converges to the target distribution.

In the main result in the present paper, Theorem 4.1, we rigorously establish convergence of the online matrix factorization scheme from [MBPS10] when the data sequence \((X_t)_{t \geq 0}\) is a Markov chain with a mild mixing condition. One of the key ideas in our proof of Theorem 4.1 is to use conditioning on distant past in order to allow the Markov chain to mix close enough to the stationary distribution \(\pi\). This allows us to control the difference between the new and the average losses by concentration of Markov chains (see Proposition 7.5 and Lemma 7.6). Furthermore, in Theorem 4.3, we extend our convergence guarantee for a relaxed version of the same algorithm when one can only approximately find solutions to the optimization problems for the matrix factors at each iteration.

We demonstrate our results in two application contexts. First, we apply dictionary learning and reconstruction for images using Non-negative Matrix Factorization (NMF) for a sequence of Ising spin configurations generated by the Gibbs sampler (see Section 5). This illustrates that we can learn dictionary image patches from an MCMC trajectory of images. Second, we propose a novel framework for network data analysis that we call Network Dictionary Learning (see Section 6). This allows one to extract ‘network dictionary patches’ from a given network to see its fundamental features and to reconstruct the network using them. Two fundamental building blocks are online NMF on Markovian data, which is the main subject in this paper, and a recent MCMC algorithm for sampling motifs from networks, developed by Lyu together with Memoli and Sivakoff [LMS19].

2. Background and related work

2.1. Topic modeling and matrix factorization. Topic modeling (or dictionary learning) aims at extracting important features of a complex dataset so that one can approximately represent the dataset in terms of a reduced number of extracted features (topics) [BNJ03]. Topic models have been shown to efficiently capture latent intrinsic structures of text data in natural language processing tasks [SG07, BCD10]. One of the advantages of topic modeling based approaches is that the extracted topics are often directly interpretable, as opposed to the arbitrary abstraction of deep neural network based approach.

Matrix factorization is one of the fundamental tools in dictionary learning problems. Given a large data matrix \(X\), can we find some small number of ‘dictionary vectors’ so that we can represent each column of the data matrix has linear combination of dictionary vectors? More precisely, given a data matrix \(X \in \mathbb{R}^{d \times n}\) and sets of admissible factors \(\mathcal{C} \subseteq \mathbb{R}^{d \times r}\) and \(\mathcal{C}' \subseteq \mathbb{R}^{r \times n}\), we wish to factorize \(X\) into the product of \(W \in \mathcal{C}\) and \(H \in \mathcal{C}'\) by solving the following optimization problem

\[
\inf_{W \in \mathcal{C}, H \in \mathcal{C}'} \| X - WH \|_F^2,
\]
where $\|A\|_F^2 = \sum_{i,j} A_{ij}^2$ denotes the matrix Frobenius norm. Here $W$ is called the dictionary and $H$ is the code of data $X$ using dictionary $W$. A solution of such matrix factorization problem is illustrated in Figure 1.

When there are no constraints for the dictionary and code matrices, i.e., $C = \mathbb{R}^{d \times r}$ and $C' = \mathbb{R}^{r \times n}$, then the optimization problem (1) is equivalent to principal component analysis, which is one of the primary techniques in data compression and dictionary learning. In this case, the optimal dictionary $W$ for $X$ is given by the top $r$ eigenvectors of its covariance matrix, and the corresponding code $H$ is obtained by projecting $X$ onto the subspace generated by these eigenvectors. However, the dictionary vectors found in this way are often hard to interpret. This is in part due to the possible cancellation between them when we take their linear combination, with both positive and negative coefficients.

When the admissible factors are required to be non-negative, the optimization problem (1) is an instance of Nonnegative matrix factorization (NMF), which is one of the fundamental tools in dictionary learning problems that provides a parts-based representation of high dimensional data [LS99, LYC09]. Due to the non-negativity constraint, each column of the data matrix is then represented as a non-negative linear combination of dictionary elements (See Figure 1). Hence the dictionaries must be "positive parts" of the columns of the data matrix. When each column consists of a human face image, NMF learns the parts of human face (e.g., eyes, nose, and mouth). This is in contrast to principal component analysis and vector quantization: Due to cancellation between eigenvectors, each 'eigenface' does not have to be parts of face [LS99].

2.2. Online matrix factorization. Many iterative algorithms to find approximate solutions $WH$ to the optimization problem (1), including the well-known Multiplicative Update by Lee and Seung [LS01], are based on a block optimization scheme (see [Gil14] for a survey). Namely, we first compute its representation $H_t$ using the previously learned dictionary $W_{t-1}$, and then find an improved dictionary $W_t$ (see Figure 2 with setting $X_t = X$).

Despite their popularity in dictionary learning and image processing, one of the drawbacks of these standard iterative algorithms for NMF is that we need to store the data matrix (which is of size $O(dn)$) during the iteration, so they become less practical when there is a memory constraint and yet the size of data matrix is large. Furthermore, in practice only a random sample of the entire dataset is often available, in which case we are not able to apply iterative algorithms that require the entire dataset for each iteration.

The Online Matrix Factorization (OMF) problem concerns a similar matrix factorization problem for a sequence of input matrices. Namely, let $(X_t)_{t \geq 1}$ be a discrete-time stochastic process of data matrices taking values in a fixed sample space $\Omega \subseteq \mathbb{R}^{d \times n}$ with a unique stationary distribution $\pi$. Fix sets of admissible factors $C \subseteq \mathbb{R}^{d \times r}$ and $C' \subseteq \mathbb{R}^{r \times n}$ for the dictionaries and codes, respectively.
The goal of the OMF problem is to construct a sequence \((W_{t-1}, H_t)_{t \geq 1}\) of dictionaries \(W_t \in \mathcal{C} \subseteq \mathbb{R}^{r \times d}\) and codes \(H_t \in \mathcal{C}' \subseteq \mathbb{R}^{r \times n}\) such that, almost surely as \(t \to \infty\),

\[
\|X_t - W_{t-1} H_t\|_F^2 \to \inf_{W \in \mathcal{C}, H \in \mathcal{C}'} \mathbb{E}_{X \sim \pi} [\|X - WH\|_F^2].
\] (2)

Here and throughout, we write \(\mathbb{E}_{X \sim \pi}\) to denote the expected value with respect to the random variable \(X\) that has the distribution described by \(\pi\). Thus, we ask that the sequence of dictionary and code pairs provides a factorization error that converges to the best case average error. Since (2) is a non-convex optimization problem, it is reasonable to expect that \(W_t\) converges only to a locally optimal solution in general. Convergence guarantees to global optimum is a subject of future work.

2.3. Applications of online NMF in dictionary learning from images. One of the well-known applications of online NMF is for learning dictionary patches from images and image reconstruction. After we choose an appropriate patch size \(k \geq 1\), we first need to extract all \(k \times k\) image patches from the image. In terms of matrices, this is to consider the set of all \((k \times k)\) submatrices of the image with consecutive rows and columns. If there are \(N\) such image patches, we are forming \((k^2 \times N)\) patch matrix to which we apply NMF to extract dictionary patches. It is reasonable to believe that there are some fundamental features in the space of all image patches since nearby pixels in the image are likely to be spatially correlated. Since the number \(N\) of patches is typically large, one can use online NMF to learn dictionaries from independent batches of sample patches. A toy example for this application of online NMF is shown in Figure 3. See Section 5 for more details about applications on dictionary learning from MCMC trajectories.

![Figure 3: Reconstructing M.C. Escher’s Cycle (1938) by online NMF. 400316 patches of size 10 \times 10 are extracted from the original image, and then a random sample of size 10 is fed into online NMF algorithm for 500 iterations. Learned dictionaries (image patches) are shown in the left. Original and reconstructed image using the learned dictionary to the left are shown in the middle. The last shows the reconstructed image of Pierre-Auguste Renoir’s Two Sisters (1882) (original image omitted) using the dictionary patches learned from Escher’s Cycle in the left. Since the dictionary patches learned from Escher’s painting consists of basic local geometry, they are able to approximately reconstruct Renoir’s painting as well.](image-url)

2.4. Algorithm for online matrix factorization. In the literature of OMF, one of the crucial assumptions is that the sequence of data matrices \((X_t)_{t \geq 0}\) are drawn independently from the common distribution \(\pi\) (see., e.g., [MBPS10, GTLY12, ZTX16]). A cornerstone in the theory of OMF is the seminal
work of Mairal et al. [MBPS10]. They proposed the following scheme of OMF:

\[
\begin{align*}
H_t &= \arg\min_{H \in \mathbb{C}^{n \times k}} \|X_t - W_{t-1}H\|_F^2 + \lambda \|H\|_1 \\
A_t &= \frac{1}{t}((t-1)A_{t-1} + H_tH_t^T) \\
B_t &= \frac{1}{t}((t-1)B_{t-1} + H_tX_t^T) \\
W_t &= \arg\min_{W \in \mathbb{C}^{m \times n}} (\text{tr}(WA_tW^T) - 2\text{tr}(WB_t)),
\end{align*}
\]

where \(A_0\) and \(B_0\) are zero matrices of size \(r \times r\) and \(r \times d\), respectively. Note that the \(L_2\)-loss function is augmented with the \(L_1\)-regularization term \(\lambda \|H\|_1\) with regularization parameter \(\lambda > 0\), which forces the code \(H_t\) to be sparse. See Appendix A for more detailed algorithm implementing (3).

In the above scheme, the auxiliary matrices \(A_t \in \mathbb{R}^{r \times r}\) and \(B_t \in \mathbb{R}^{r \times d}\) effectively aggregate the history of data matrices \(X_1, \cdots, X_t\) and their best codes \(H_1, \cdots, H_t\). The previous dictionary \(W_{t-1}\) is updated to \(W_t\), which minimizes a surrogate loss function \(\text{tr}(WA_tW^T) - 2\text{tr}(WB_t)\). Under a mild assumption but with assuming that \(X_t\)'s are independently drawn from the stationary distribution \(\pi\), the authors of [MBPS10] proved that the sequence \((W_{t-1}, H_t)_{t \geq 0}\) converges to a critical point of the expected loss function in (2) augmented with the \(L_1\)-regularization term \(\lambda \|H\|_1\).

A possible way to handle Markovian dependence in the input sequence of matrices is ‘downsampling’ the input into a sparse subsequence of nearly independent samples. Namely, if we keep only one Markov chain sample in every \(\tau\) iterations, then the remaining samples are asymptotically independent provided the epoch \(\tau\) is long enough compared to the mixing time of the Markov chain. A similar line of approach was used in [YBZW17] for a relevant but different problem of factorizing the unknown transition matrix of a Markov chain by observing its trajectory. On the other hand, our approach to handle the Markovian dependence is based on conditioning the future state of the Markov chain on a distant past so that the conditional expectation of the future state is very close to its stationary expectation. This allows us to control the difference between the new and the average losses by concentration of Markov chains (see Proposition 7.5 and Lemma 7.6).

2.5. **Notation.** Fix integers \(m, n \geq 1\). We denote by \(\mathbb{R}^{m \times n}\) the set of all \(m \times n\) matrices of real entries. For any matrix \(A\), we denote its \((i, j)\) entry, \(i\)th row, and \(j\)th column by \(A_{ij}\), \([A]_{i*}\), and \([A]_{*j}\). For each \(A = (A_{ij}) \in \mathbb{R}^{m \times n}\), denote its Frobenius and operator norms, denoted by \(\|A\|_F\), \(\|A\|_2\), and \(\|A\|_{op}\), by

\[
\|A\|_F = \sqrt{\sum_{ij} a_{ij}^2}, \quad \|A\|_2 = \sqrt{\sum_{ij} a_{ij}^2}, \quad \|A\|_{op} = \inf\{c > 0 : \|Ax\|_F \leq c \|x\|_F \text{ for all } x \in \mathbb{R}^n\}. \tag{4}
\]

For any subset \(\mathcal{A} \subset \mathbb{R}^{m \times n}\) and \(X \in \mathbb{R}^{n \times m}\), denote

\[
R(\mathcal{A}) = \sup_{X \in \mathcal{A}} \|X\|_F, \quad d_F(X, \mathcal{A}) = \inf_{Y \in \mathcal{A}} \|X - Y\|_F. \tag{5}
\]

For any continuous functional \(f : \mathbb{R}^{m \times n} \to \mathbb{R}\) and a subset \(A \subseteq \mathbb{R}^n\), we denote

\[
\arg\min_{x \in A} f(y) = \left\{ x \in A \mid f(x) = \min_{y \in A} f(y) \right\}. \tag{6}
\]

When \(\arg\min_{x \in A} f\) is a singleton \(\{x^*\}\), we identify \(\arg\min_{x \in A} f\) as \(x^*\).

For any event \(A\), we let \(1_A\) denote the indicator function of \(A\), where \(1_A(\omega) = 1\) if \(\omega \in A\) and \(0\) otherwise. We also denote \(1_A = 1(\omega)\) when convenient. For each \(x \in \mathbb{R}\), denote \(x^+ = \max(0, x)\) and \(x^- = \max(0, -x)\). Note that \(x = x^+ - x^-\) for all \(x \in \mathbb{R}\) and the functions \(x \to x^\pm\) are convex.

For each integer \(n \geq 1\), denote \([n] = \{1, 2, \cdots, n\}\). A simple graph \(G = ([n], A_G)\) is a pair of its node set \([n]\) and its adjacency matrix \(A_G\), where \(A_G\) is a symmetric 0-1 matrix with zero diagonal entries. We say nodes \(i\) and \(j\) are adjacent in \(G\) if \(A_G(i, j) = 1\).
3. Preliminary discussions

3.1. Markov chains on countable state space. We first give a brief account on Markov chains on countable state space (see, e.g., [LP17]). Fix a countable set \( \Omega \). A function \( P : \Omega^2 \to [0, \infty) \) is called a Markov transition matrix if every row of \( P \) sums to 1. A sequence of \( \Omega \)-valued random variables \((X_t)_{t \geq 0}\) is called a Markov chain with transition matrix \( P \) if for all \( x_0, x_1, \cdots, x_n \in \Omega \),
\[
\mathbb{P}(X_n = x_n \mid X_{n-1} = x_{n-1}, \cdots, X_0 = x_0) = \mathbb{P}(X_n = x_n \mid X_{n-1} = x_{n-1}) = P(x_{n-1}, x_n).
\]
(7)

We say a probability distribution \( \pi \) on \( \Omega \) a stationary distribution for the chain \((X_t)_{t \geq 0}\) if \( \pi = \pi P \), that is,
\[
\pi(x) = \sum_{y \in \Omega} \pi(y) P(y, x).
\]
(8)

We say the chain \((X_t)_{t \geq 0}\) is irreducible if for any two states \( x, y \in \Omega \) there exists an integer \( t \geq 0 \) such that \( P^t(x, y) > 0 \). For each state \( x \in \Omega \), let \( \mathcal{F}(x) = \{ t \geq 1 \mid P^t(x, x) > 0 \} \) be the set of times when it is possible for the chain to return to starting state \( x \). We define the period of \( x \) by the greatest common divisor of \( \mathcal{F}(x) \). We say the chain \( X_t \) is aperiodic if all states have period 1. Furthermore, the chain is said to be positive recurrent if there exists a state \( x \in \Omega \) such that the expected return time of the chain to \( x \) started from \( x \) is finite. Then an irreducible and aperiodic Markov chain has a unique stationary distribution if and only if it is positive recurrent [LP17, Thm 21.21].

Given two probability distributions \( \mu \) and \( \nu \) on \( \Omega \), we define their total variation distance:
\[
\| \mu - \nu \|_{TV} = \sup_{A \subseteq \Omega} |\mu(A) - \nu(A)|.
\]
(9)

If a Markov chain \((X_t)_{t \geq 0}\) with transition matrix \( P \) starts at \( x_0 \in \Omega \), then by (7), the distribution of \( X_t \) is given by \( P^t(x_0, \cdot) \). If the chain is irreducible and aperiodic with stationary distribution \( \pi \), then the convergence theorem (see, e.g., [LP17, Thm 21.14]) asserts that the distribution of \( X_t \) converges to \( \pi \) in total variation distance: As \( t \to \infty \),
\[
\sup_{x_0 \in \Omega} \| P^t(x_0, \cdot) - \pi \|_{TV} \to 0.
\]
(10)

See [MT12, Thm 13.3.3] for a similar convergence result for the general state space chains. When \( \Omega \) is finite, then the above convergence is exponential in \( t \) (see, e.g., [LP17, Thm 4.9]). Namely, there exists constants \( \lambda \in (0, 1) \) and \( C > 0 \) such that for all \( t \geq 0 \),
\[
\max_{x_0 \in \Omega} \| P^t(x_0, \cdot) - \pi \|_{TV} \leq CA^t.
\]
(11)

Markov chain mixing refers to the fact that, when the above convergence theorems hold, then one can approximate the distribution of \( X_t \) by the stationary distribution \( \pi \).

3.2. Naive solution minimizing empirical loss function. Define the following quadratic loss function of the dictionary \( W \in \mathbb{R}^{d \times r} \) with respect to data \( X \in \mathbb{R}^{d \times n} \)
\[
\ell(X, W) = \inf_{H \in \mathcal{C} \subset \mathbb{R}^{r \times n}} \| X - WH \|_F^2 + \lambda \| H \|_1,
\]
(12)

where \( \mathcal{C} \) denotes the set of admissible codes and \( \lambda > 0 \) is a fixed \( L_1 \)-regularization parameter. For each \( W \in \mathcal{C} \) define its expected loss by
\[
f(W) = \mathbb{E}_{X \sim \pi} [\ell(X, W)].
\]
(13)

Suppose arbitrary sequences of data matrices \((X_t)_{t \geq 0}\) and codes \((H_t)_{t \geq 0}\) are given. For each \( W \in \mathcal{C} \) and \( t \geq 0 \) define the empirical loss \( f_t(W) \)
\[
f_t(W) = \frac{1}{t} \sum_{s=1}^{t} \ell(X_s, W).
\]
(14)
Suppose \((X_t)_{t \geq 1}\) is an irreducible Markov chain on \(\Omega\) with unique stationary distribution \(\pi\). Note that by the Markov chain ergodic theorem (see, e.g., [Dur10, Thm 6.2.1, Ex. 6.2.4] or [MT12, Thm. 17.1.7]), for each dictionary \(W\), the empirical loss \(f_t(W)\) converges almost surely to the expected loss \(f(W)\):

\[
\lim_{t \to \infty} f_t(W) = f(W) \quad \text{a.s.} \tag{15}
\]

This observation suggests the following naive solution to OMF based on a block optimization scheme:

Upon arrival of \(X_t\):

\[
\begin{aligned}
H_t &= \arg\min_{H \in \mathcal{C}} \|X_t - W_{t-1} H\|_F^2 + \lambda \|H\|_1 \\
W_t &= \arg\min_{W \in \mathcal{C}} f_t(W).
\end{aligned} \tag{16}
\]

Finding \(H_t\) in (16) can be done using a number of known algorithms (e.g., LARS [EHJ+04], LASSO [Tib96], and feature-sign search [LBRN07]) in this formulation. However, there are some important issues in solving the optimization problem for \(W_t\) in (16). Namely, in order to compute the empirical loss \(f_t(W)\), we may have to store the entire history of data \(X_1, \cdots, X_t\), and we need to solve \(t\) instances of optimization problem (12) for each summand of \(f_t(W)\). Both of these are a significant requirement for memory and computation. These issues are addressed in the OMF scheme (3), as we discuss in the following subsection.

### 3.3. Asymptotic solution minimizing surrogate loss function

The idea behind the online NMF scheme (3) is to solve the following approximate problem

Upon arrival of \(X_t\):

\[
\begin{aligned}
H_t &= \arg\min_{H \in \mathcal{C}} \|X_t - W_{t-1} H\|_F^2 + \lambda \|H\|_1 \\
W_t &= \arg\min_{W \in \mathcal{C}} \hat{f}_t(W).
\end{aligned} \tag{17}
\]

with a given initial dictionary \(W_0 \in \mathcal{C}\), where \(\hat{f}_t(W)\) is a convex upper bounding surrogate for \(f_t(W)\) defined by

\[
\hat{f}_t(W) = \frac{1}{t} \sum_{s=1}^{t} (\|X_s - W H_s\|_F^2 + \lambda \|H_s\|_1). \tag{18}
\]

Namely, we recycle the previously found codes \(H_1, \cdots, H_t\) and use them as approximate solutions of the sub-problem (12). Hence, there is only a single optimization for \(W_t\) in the relaxed problem (17).

It seems that this might still require storing the entire history \(X_1, X_2, \cdots, X_t\) up to time \(t\). But in fact we only need to store two summary matrices \(A_t \in \mathbb{R}^{r \times t}\) and \(B_t \in \mathbb{R}^{r \times d}\). Indeed, (17) is equivalent to the optimization problem (3) stated in the introduction. To see this, define \(A_t = t^{-1} \sum_{s=1}^{t} H_s H_s^T\) and \(B_t = t^{-1} \sum_{s=1}^{t} H_s X_s^T\). Then \(A_t\) and \(B_t\) are defined by the recursive relations given in (3). Furthermore, note that

\[
\|X - WH\|_F^2 = \sum_{i=1}^{d} \|X_i^* - W_i^* H_i\|_F^2 \tag{19}
\]

\[
= \sum_{i=1}^{d} W_i^* H_i H_i^T W_i^T - W_i^* H_i X_i^T - X_i^* H_i^T W_i^T + X_i^* X_i^T \tag{20}
\]

\[
= \text{tr}(W HH^T W^T) - 2\text{tr}(WHX^T) + \text{tr}(XX^T). \tag{21}
\]

Hence we can write

\[
\hat{f}_t(W) = \text{tr}(WA_t W^T) - 2\text{tr}(WB_t) + \frac{1}{t} \sum_{s=1}^{t} (\text{tr}(X_s X_s^T) + \lambda \|H_s\|_1). \tag{22}
\]

This shows the equivalence of equations defining \(W_t\) in (17) and (3).
4. Statement of main results

4.1. Setup and assumptions. Fix integers $d, n, r \geq 1$ and a constant $\lambda > 0$. Here we list all technical assumptions required for our convergence theorems to hold.

(A1). Data matrices $X_t$ are drawn from a compact and countable subset $\Omega \subseteq Q^{d \times n}$.

(A2). Dictionaries $W_t$ are constrained to a compact subset $\mathcal{C} \subseteq \mathbb{R}^{d \times r}$.

(M1). $(X_t)_{t \geq 0}$ is an irreducible, aperiodic, and positive recurrent Markov chain on the countable state space $\Omega \subseteq Q^{d \times n}$. We let $P$ and $\pi$ denote its transition matrix and unique stationary distribution, respectively.

(M2). There exists a sequence $(a_t)_{t \geq 0}$ of non-decreasing non-negative integers such that
\[
\begin{align*}
a_t &= O(t (\log t)^{-2}), \\
\sup_{x \in \Omega} \| P^a_t(x, \cdot) - \pi \|_{TV} &= O((\log t)^{-2}).
\end{align*}
\]

(C1). The loss and expected loss functions $\ell$ and $f$ defined in (12) and (14) are continuously differentiable.

(C2). The eigenvalues of the positive semidefinite matrix $A_t$ defined in (3) are at least some constant $\kappa_1 > 0$ for all $t \geq 0$.

It is standard to assume compact support for data matrices as well as dictionaries. In order to make the state space $\Omega$ of the Markov chain countable, we further assume that both $\Omega$ and $\mathcal{C}$ are restricted to field of rational numbers as in (A1)-(A2). For all numerical and application purposes, this is with no loss of generality. We remark that our analysis and main results still hold in the general state space case, but this requires a more technical notion of positive Harris chains irreducibility assumption in order to use functional central limit theorem for general state space Markov chains [MT12, Thm. 17.4.4]. We restrict our attention to the countable state space Markov chains in this paper.

Assumption (M1) is a standard assumption in Markov chain Monte Carlo. Namely, when one designs a Markov chain Monte Carlo to sample from a target distribution $\pi$, a standard approach is to devise a Markov chain that has $\pi$ as a stationary distribution, and then show that the chain is irreducible, aperiodic, and positive recurrent. Then by the general Markov chain theory we have summarized in Subsection 3.1, $\pi$ is the unique stationary distribution of the chain.

On the other hand, (M2) is a very weak assumption on the rate of convergence of the Markov chain $(X_t)_{t \geq 0}$ to its stationary distribution $\pi$. Note that (M2) follows from

(M2)' There exists a constant $\alpha > 0$ such that
\[
\sup_{x \in \Omega} \| P^t(x, \cdot) - \pi \|_{TV} = O(t^{-\alpha}).
\]

since we may then choose $a_t = \lfloor t (\log t)^{-2} \rfloor$. Now, (M2)' is trivially satisfied in the special case when $\Omega$ is finite, which in fact covers many practical situations. Indeed, assuming (M1) and that $\Omega$ is finite, the convergence theorem (11) provides an exponential rate of convergence of the empirical distribution of the chain to $\pi$, in particular implying the polynomial rate of convergence in (M2)'.

Our main result, Theorem 4.1, guarantees that both the empirical and surrogate loss processes $(f_t(W_t))$ and $(\hat{f}_t(W_t))$ converge almost surely under the assumptions (A1)-(A2) and (M1)-(M2). The assumptions (C1)-(C2), which are also used in [MBPS10], are sufficient to ensure that the limit point is a critical point of the expected loss function $f$ defined in (13).

We remark that (C1) follows from the following alternative condition (see [MBPS10, Prop. 1]):

(C1)' For each $X \in \Omega$ and $W \in \mathcal{C}$, the sparse coding problem in (12) has a unique solution.
In order to enforce (C1)', we may use the elastic net penalization by Zou and Hastie [ZH05]. Namely, we may replace the first equation in (3) by
\begin{equation}
H_t = \arg\min_{H \in \mathcal{C} \subset \mathbb{R}^{r \times n}} \|X_t - W_{t-1} H\|^2_F + \lambda \|H\|_1 + \frac{\kappa_2}{2} \|H\|^2_F
\end{equation}
for some fixed constant \(\kappa_2 > 0\). See the discussion in [MBPS10, Subsection 4.1] for more details.

On the other hand, (C2) guarantees that the eigenvalues of \(A_t\) produced by (3) are lower bounded by the constant \(\kappa_1 > 0\). It follows that \(A_t\) is invertible and \(\hat{f}_t\) is strictly convex with Hessian \(2A_t\). This is crucial in deriving Proposition 7.4, which is later used in the proof of Theorems 4.1 and 4.3. Note that (C2) can be enforced by replacing the last equation in (3) with
\begin{equation}
W_t = \arg\min_{W \in \mathcal{C} \subset \mathbb{R}^{r \times 1}} \{\text{tr}(W(A_t + \kappa_1 I)W^T) - 2\text{tr}(WB_t)\}.
\end{equation}
The same analysis for the algorithm (3) that we will develop in the later sections will apply for the modified version with (25) and (26), for which (C1)-(C2) are trivially satisfied.

4.2. Convergence theorems. Our main result in this paper, which is stated below in Theorem 4.1, asserts that under the OMF scheme (3), the induced stochastic processes \((f_t(W_t))\) and \((\hat{f}_t(W_t))\) converge as \(t \to \infty\) in expectation. Furthermore, the sequence \((W_t)_{t \geq 0}\) of learned dictionaries converge the set of critical points of the expected loss function \(f\).

Theorem 4.1. Suppose (A1)-(A2) and (M1)-(M2). Let \((W_{t-1}, H_t)_{t \geq 1}\) be a solution to the optimization problem (3). Then the following hold.

(i) \(\lim_{t \to \infty} \mathbb{E}[f_t(W_t)] = \lim_{t \to \infty} \mathbb{E}[\hat{f}_t(W_t)] < \infty\). Furthermore, if \(\Omega\) is finite, then
\begin{equation}
\lim_{t \to \infty} \mathbb{E}[f_t(W_t)] - \mathbb{E}[\hat{f}_t(W_t)] = O(t^{-1/2}).
\end{equation}

(ii) \(f_t(W_t) - \hat{f}_t(W_t) \to 0\) as \(t \to \infty\) almost surely.

(iii) Further assume (C1)-(C2). Then almost surely, \(\limsup_{t \to \infty} \|\nabla f(W_t)\|_{op} = 0\).

We remark that the \(L_1\)-convergence and the rate of convergence in the above result has not before been established even when \(X_t\)'s are i.i.d. [MBPS10].

Recall that \(W_t\) is the unique minimizer of the surrogate loss function \(\hat{f}_t\) over the compact set \(\mathcal{C}\) of dictionaries. Hence it is natural to expect that the surrogate loss \(\hat{f}_t(W_t)\) converges to some local minimum of some 'limiting' surrogate loss function. In [MBPS10], the convergence of surrogate loss is established by showing that it forms a quasi-martingale. Namely,
\begin{equation}
\sum_{t=0}^{\infty} \mathbb{E} \left[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \bigg| \mathcal{F}_t \right]^+ < \infty,
\end{equation}
where \(\mathcal{F}_t\) denotes the filtration of the information up to time \(t\). It is known that quasi-martingales converge to some limiting random variable almost surely [Fis65, Rao69]. However, the fact that the surrogate loss process \((\hat{f}_t(W_t))_{t \geq 0}\) forms a quasi-martingale crucially relies on the independence assumption on the data matrices. In fact, it is easy to see that this is false if this independence assumption is violated (e.g., when the data matrices deterministically alternate between two different matrices).

Our key innovation to overcome this issue is to use conditioning on distant past in order to allow the Markov chain to mix close enough to the stationary distribution \(\pi\) (see Proposition 7.5). Namely, we show
\begin{equation}
\sum_{t=0}^{\infty} \mathbb{E} \left[ \mathbb{E} \left[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \bigg| \mathcal{F}_{t-a_t} \right] \right]^+ < \infty
\end{equation}
for some sequence $1 \leq a_t \leq t$ satisfying (M2). The idea is to condition early on at time $t - a_t \ll t$ so that the chain has enough time $a_t$ to mix to its stationary distribution by time $t$. This gives enough control on the expected increments to show the convergence in expectation as stated in Theorem 4.1.

**Remark 4.2.** The condition (29) is not sufficient to derive almost sure convergence of $\hat{f}_t(W_t)$. For instance, let $(X_t)_{t \geq 0}$ be a sequence of i.i.d. random variables. Then clearly $X_t$ does not converge almost surely, but since $E[X_{t+1}] = E[X_t],$

$$\sum_{t=0}^{\infty} E[X_{t+1} - X_t | \mathcal{F}_{t-1}]^+ = \sum_{t=0}^{\infty} (E[X_{t+1}] - E[X_t])^+ = 0. \quad (30)$$

However, fortunately, almost sure convergence of $\hat{f}_t(W_t)$ is not necessary to deduce almost sure convergence of the dictionaries $W_t$ to the set of the critical points of $f$, as stated in Theorem 4.1 (ii).

Our last main result is a further generalization of Theorem 4.1. Note that any iterative algorithm designed to solve the optimization problems for $H_t$ and $W_t$ in (3) will give approximate solutions. Hence convergence of an approximate solution to (3) is a natural question that has both theoretical and practical interest. This has never been addressed even when $X_t$’s are i.i.d.

For each $X \in \mathbb{R}^{d \times n}$, $W \in \mathbb{R}^{d \times r}$, and $H \in \mathbb{R}^{r \times n}$, denote $\ell(X, W, H) = \|X - WH\|_F^2 + \lambda \|H\|_1$ and define $H^{opt}(X, W) = \arg\min_{H \in \mathcal{C}^r \subset \mathbb{R}^{r \times n}} \ell(X, W, H)$ (31)

Note that under (C2), there exists a unique minimizer of the function in the right hand side, with which we identify as $H^{opt}(X, W)$. We propose the following OMF scheme, which we call the relaxation of (3): For an arbitrary fixed constant $K > 0$,

Upon arrival of $X_t$:

$$\begin{align*}
\text{Find any } H_t & \in \mathcal{C}^r \subseteq \mathbb{R}^{r \times n} \text{ s.t. } \|H_t - H^{opt}(X_t, W_{t-1})\|_1 \leq K(\log t)^{-2} \\
A_t &= (t-1)^{-1} (t-1) + H_t H_t^T \\
B_t &= (t-1)^{-1} (t-1) + H_t X_t^T \\
\text{Find any } W_t & \in \mathcal{C} \text{ s.t. } \hat{g}_t(W_t) \leq \hat{g}_t(W_{t-1}),
\end{align*} \quad (32)$$

where we denote $\hat{g}_t(W) = \text{tr}(WA_t W^T) - 2\text{tr}(WB_t)$. (33)

Note that computing $H^{opt}$ is a convex optimization problem so it is easy to satisfy the condition for $H_t$ in (32). For instance, we may choose $\|V_H \ell(X_t, W_{t-1} \cdot)\|_F \leq K' (\log t)^{-2}$ for some constant $K'_t > 0$ (see Proposition 7.10). Also, finding $W_t \in \mathcal{C}$ such that $\hat{g}_t(W_t) \leq \hat{g}_t(W_{t-1})$ is easy since we can start with $W_t = W_{t-1}$ and apply projected gradient descent until the monotonicity condition $\hat{g}_t(W_t) \leq \hat{g}_t(W_{t-1})$ is first violated. See Proposition 7.10 and Appendix A for details.

Note that, according to (22), $W_{t+1}$ is the minimizer of the surrogate loss function $\hat{f}_{t+1}(W_{t+1})$. Hence (32) entails (3). Our key observation for the relaxed problem is that the asymptotic optimality of $H_t$ and the monotonicity of $W_t$ are enough to guarantee a similar convergence result, as stated in the following theorem.

**Theorem 4.3.** Suppose (A1)-(A2) and (M1)-(M2). Let $(W_{t-1}, H_t)_{t \geq 1}$ be any solution to the relaxed online NMF scheme (32). Then the following hold.

(i) $\lim_{t \to \infty} E[f_t(W_t)] = \lim_{t \to \infty} E[\hat{f}_t(W_t)] < \infty$. Furthermore, if $\Omega$ is finite and $H_t$ satisfies

$$\|H_t - H^{opt}(X_t, W_{t-1})\|_1 \leq K t^{-1/2} \quad (34)$$

for some fixed constant $K > 0$ and for all $t \geq 0$, then

$$\left| \lim_{t \to \infty} E[f_s(W_t)] - E[\hat{f}_t(W_t)] \right| = O(t^{-1/2}). \quad (35)$$
(ii) $f_t(W_t) - f_t(W_{t-1}) \to 0$ as $t \to \infty$ almost surely.

(iii) Further assume (C1)-(C2) for (32). Then almost surely,

$$\limsup_{t \to \infty} \| \nabla f_t(W_t) \|_{op} \leq \limsup_{t \to \infty} \| \nabla \hat{g}_t(W_t) \|_{op}. \quad (36)$$

Note that Theorem 4.3 implies Theorem 4.1, as (32) entails (3) and $\| \nabla \hat{g}_t(W_t) \|_{op} \equiv 0$ when $W_t$ is the minimizer of $\hat{g}_t$. A particular solution to (32) is when we choose $W_t = W$ for some fixed $W \in C$, which may not result in a good factorization of the data matrices. Nevertheless, Theorem 4.3 guarantees convergence of the empirical and surrogate loss functions as $t \to \infty$. However, since this does not try to minimize the surrogate loss $\hat{g}_t(W_t)$, the upper bound on the gradient in Theorem 4.3 might be large. Hence the limit of the loss functions may be far from a critical point in this case.

5. Application I: Learning features from MCMC trajectories

Suppose we want to learn features from a random element $X$ in a sample space $\Omega$ with distribution $\pi$. When the sample space is complicated, it is often not easy to directly sample a random element from it according to the prescribed distribution $\pi$. Two examples include sampling an Ising spin configuration from a Gibbs measure, and sampling a random sentence from a large corpus against a prior distribution. **Markov chain Monte Carlo (MCMC)** provides a fundamental sampling technique that uses Markov chains to sample a random element.

The idea behind MCMC sampling is the following. Given a distribution $\pi$ on a sample space $\Omega$, suppose we can construct a Markov chain $(X_t)_{t \geq 0}$ on $\Omega$ such that $\pi$ is its stationary distribution. If in addition the chain is irreducible and aperiodic, then by the convergence theorem (see (11) or [LP17, Thm 4.9]), we know that the distribution $\pi_t$ of $X_t$ converges to $\pi$ in total variation distance. Hence if we run the chain for long enough, the state of the chain is asymptotically distributed as $\pi$. In other words, we can sample a random element of $\Omega$ according to the prescribed distribution $\pi$ by emulating it through a suitable Markov chain.

Now suppose that we can sample a random element $X$ on $\Omega$ through a Markov chain $(X_t)_{t \geq 0}$. While we could build many independent MCMC samples of $X$, it would be much more efficient if we could learn features directly from a single MCMC trajectory $(X_t)_{t \geq 0}$. Our main results (Theorems 4.1 and 4.3) guarantee that we can apply the OMF scheme to learn features from a given MCMC trajectory. In the rest of this section, we demonstrate this through applying online NMF and image reconstruction technique to the two-dimensional Ising model.

5.1. The Ising model. Consider a general system of binary spins. Namely, let $G = (V, E)$ be a locally finite simple graph with vertex set $V$ and edge set $E$. Imagine each vertex (site) of $G$ can take either of the two states (spins) $+1$ or $-1$. A complete assignment of spins for each site in $G$ is given by a spin configuration, which we denote by a map $x : V \to \{-1, 1\}$. Let $\Omega = \{-1, 1\}^V$ denote the set of all spin configurations. In order to introduce a probability measure on $\Omega$, fix a function $H(\cdot; \theta) : \Omega \to \mathbb{R}$ parameterized by $\theta$, which is called a Hamiltonian of the system. For each choice of parameter $\theta$, we define a probability distribution $\pi_\theta$ on the set $\Omega$ of all spin configurations by

$$\pi_\theta(x) = \frac{1}{Z_\theta} \exp(-H(x; \theta)), \quad (37)$$

where the partition function $Z_\theta$ is defined by

$$Z_\theta = \sum_{x \in \Omega} \exp(-H(x; \theta)). \quad (38)$$

The induced probability measure $P_\theta$ on $\{-1, 1\}^{|V|}$ is called a Gibbs measure.
The Ising model, first introduced by Lenz in 1920 as a model of ferromagnetism [Len20], is one of the most well-known spin systems in the physics literature. The Ising model is defined by the following Hamiltonian

\[
H(x; T, h) = \frac{1}{T} \left( -\sum_{(u,v) \in E} x(u)x(v) - \sum_{v \in V} h(v)x(v) \right),
\]

where \(x\) is the spin configuration, the parameter \(T\) is called the temperature, and \(h : V \to \mathbb{R}\) the external field. In this paper we will only consider the case of zero external field. Note that, with respect to the corresponding Gibbs measure, a given spin configuration \(x\) has higher probability if the adjacent spins tend to agree, and this effect of adjacent spin agreement is emphasized (resp., diminished) for low (resp., high) temperature \(T\).

5.2. Gibbs sampler for the Ising model. One of the most extensively studied Ising models is when the underlying graph \(G\) is the two-dimensional square lattice (see [MW14] for a survey). It is well known that in this case the Ising model exhibits a sharp phase transition at the critical temperature \(T = T_c = 2/\log(1 + \sqrt{2}) \approx 2.2691\). Namely, if \(T < T_c\) (subcritical phase), then there tends to be large clusters of \(+1\)'s and \(-1\) spins; if \(T > T_c\) (supercritical phase), then the spin clusters are very small and fragmented; at \(T = T_c\) (criticality), the cluster sizes are distributed as a power law. (See Figure 4 for a simulation.)

In order to sample a random spin configuration \(x \in \Omega\), we use the following MCMC called the Gibbs sampler. Namely, let the underlying graph \(G = (V, E)\) to be a finite \(N \times N\) square lattice. We evolve a given spin configuration \(x_t : V \to \{-1, 1\}\) at iteration \(t\) as follows:

(i) Choose a site \(v \in V\) uniformly at random;
(ii) Let \(x^+\) and \(x^-\) be the spin configurations obtained from \(x_t\) by setting the spin of \(v\) to be 1 and \(-1\), respectively. Then

\[
P(x_{t+1}, x^+) = \frac{\pi(x^+)}{\pi(x^+) + \pi(x^-)}, \quad P(x_{t+1}, x^-) = \frac{\pi(x^-)}{\pi(x^+) + \pi(x^-)}.
\]

Note that \(P(x_{t+1}, x^+) = (1 + \exp(2T^{-1}\sum_{u \sim v} x_t(u)))^{-1}\), where the sum in the exponential is over all neighbors \(u\) of \(v\). Iterating the above transition rule generates a Markov chain trajectory \((x_t)_{t \geq 0}\) of Ising spin configurations, and it is well known that it is irreducible, aperiodic, and has the Boltzmann distribution \(\pi_T\) (defined in (37)) as its unique stationary distribution.

Figure 4. MCMC simulation of Ising model on 200 by 200 square lattice at temperature \(T = 0.5\) (left), \(T = 2.26\) (middle), and \(T = 5\) (right).
5.3. Learning features from Ising spin configurations. We now describe the setting of our simulation of online NMF algorithm on the Ising model. We consider a Gibbs sampler trajectory \( (x_t)_{t \geq 0} \) of the Ising spin configurations on the 200 \( \times \) 200 square lattice at three temperatures \( T = 0.5, 2.26, \) and 5. Initially \( x_0 \) is sampled so that each site takes +1 or -1 spins independently with equal probability. We then run the chain for \( 5 \times 10^6 \) iterations. By recording every 1000 iterations, we obtain a coarsened MCMC trajectory, which is represented as a 200 \( \times \) 200 \( \times \) 500 array \( A \) whose \( k \)th array \( A[\cdot;\cdot;k] \) corresponds to the spin configuration \( x_{1000k} \). If we denote \( X_k = x_{1000k} \), then \( (X_k)_{k \geq 0} \) also defines an irreducible and aperiodic Markov chain on \( \Omega \) with the same stationary distribution \( \pi_T \).
For each $X_t$, which is a $200 \times 200$ matrix of entries from $\{-1, 1\}$, we extract all possible $20 \times 20$ patches by choosing 20 consecutive rows and columns. There are $(200 - 20 + 1)^2 = 32761$ such patches, so after flattening each patch into a column vector, we obtain a $400 \times 32761$ matrix, which we denote by $\text{Patch}_{20}(X_k)$. We apply the online NMF scheme to the Markovian sequence $(\text{Patch}_{20}(X_k))_{k \geq 0}$ of data matrices to extract 100 dictionary patches. As the chain $(X_t)_{t \geq 0}$ is irreducible aperiodic and on finite state space, we can apply the main theorems (Theorems 4.1 and 4.3) to guarantee the almost sure convergence of the dictionary patches to the set of critical points of the expected loss function (13).

We apply the online NMF scheme and extract 100 dictionary patches of size $20 \times 20$ from the MCMC trajectory $(X_k)_{0 \leq k \leq 500}$ at a subcritical temperature $T = 0.5$ (Figure 5), near the critical temperature $T = 2.26$ (Figure 6), and a supercritical temperature $T = 5$ (Figure 7). We then use these dictionary patches to reconstruct an arbitrary Ising spin configuration at the corresponding temperatures. More precisely, we approximate the $200 \times 32761$ patch matrix $\text{Patch}_{20}(x)$ of a random Ising spin configuration $x$, and then paste all the patches back to a $200 \times 200$ spin configuration by averaging over the overlaps.

As shown in the corresponding figures, the learned dictionary patches are most effective in reconstructing the original image at the low temperature $T = 0.5$, and becomes less effective for higher temperatures, especially at $T = 5$. This is reasonable since the Ising spins become less correlated at higher temperatures, so we do not expect there are a few dictionary patches that could approximate the highly random configuration. The key takeaway here is that, while our convergence theorems (Theorems 4.1 and 4.3) guarantee that our dictionary patches will almost surely converge to local optimum, they do not tell us how effective they are in actually approximating the input sequence. This will depend on the model (e.g., temperature) as well as parameters of the algorithm (patch size, number of dictionaries, regularization, etc.). Moreover, as in the high temperature Ising model, effective dictionary learning may not be possible at all.
6. Application II: Network dictionary learning by online NMF and motif sampling

In this section, we propose a novel framework for network data analysis that we call Network Dictionary Learning, which enables one to extract ‘network dictionary patches’ from a given network to see its fundamental features and to reconstruct the network using the learned dictionaries. Network Dictionary Learning is based on two building blocks: 1) Online NMF on Markovian data, which is the main subject in this paper, and 2) a recent MCMC algorithm for sampling motifs from networks [LMS19].

6.1. Extracting patches from a network by motif sampling. For networks, we can think of a \((k \times k)\) patch as a sub-network induced onto a subset of \(k\) nodes. As we imposed to select \(k\) consecutive rows and columns to get patches from images, we need to impose a reasonable condition on the subset of nodes so that the selected nodes are strongly associated. For instance, if the given network is sparse, selecting three nodes uniformly at random would rarely induce any meaningful sub-network. Selecting such a subset of \(k\) nodes from networks can be addressed by the motif sampling technique introduced in [LMS19]. Namely, for a fixed ‘template graph’ (motif) \(F\) of \(k\) nodes, we would like to sample \(k\) nodes from a given network \(G\) so that the induced sub-network always contains a copy of \(F\). This guarantees that we are always sampling some meaningful portion of the network, where the prescribed graph \(F\) serves as a backbone.

Based on these ideas, we propose the following preliminary version of Network Dictionary Learning for simple graphs.

**Network Dictionary Learning: Static version for simple graphs:**

(i) Given two simple graphs \(G = ([n], A_G)\) and \(F = ([k], A_F)\), let \(\text{Hom}(F, G)\) denote the set of all homomorphisms \(F \rightarrow G\):

\[
\text{Hom}(F, G) = \left\{ \mathbf{x} : [k] \rightarrow [n] \mid \prod_{(i, j) \in E_F} A_G(\mathbf{x}(i), \mathbf{x}(j)) = 1 \right\}.
\] (41)

Compute \(\text{Hom}(F, G)\) and write \(\text{Hom}(F, G) = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}\).

(ii) For each homomorphism \(\mathbf{x}_i : F \rightarrow \mathcal{G}\), associate a \((k \times k)\) matrix \(A_{G\mathbf{x}_i}\), which we call the \(i\)th \(F\)-patch of \(G\), by

\[
A_{G\mathbf{x}_i}(a, b) = A_G(\mathbf{x}(a), \mathbf{x}(b)) \quad 1 \leq a, b \leq k.
\] (42)

Let \(X\) denote the \((k^2 \times N)\) matrix whose \(i\)th column is the \(k^2\)-dimensional vector corresponding to the \(i\)th \(F\)-patch of \(G\).

(iii) Factorize \(X \approx WH\) using NMF. Reshaping the columns of the dictionary matrix \(W\) into squares give the learned network dictionary patches.

**Example 7.1** (Network Dictionary Learning from torus). Let \(G\) be the \(n \times n\) torus graph and let \(F\) be the path of length 2. The adjacency matrix of \(G\) is shown in Figure 8 middle, and by labeling the center node as 1 (as in Figure 9), the adjacency matrix of \(F\) can be written as

\[
A_F = \begin{bmatrix}
0 & 1 & 1 \\
1 & 0 & 0 \\
1 & 0 & 0 \\
\end{bmatrix}.
\] (43)

Observe that there are \(N = 9n^2\) homomorphisms \(F \rightarrow G\), and if \(\mathbf{x} : F \rightarrow G\) is any homomorphism, the corresponding \(F\)-patch of \(G\) is always identical to \(A_F\) above. Hence the \(k^2 \times N\) matrix \(X\) of \(F\)-patches of \(G\) is of rank 1, generated by the 9-dimensional column vector corresponding to the \((3 \times 3)\) matrix \(A_F\) above. Hence in this case, we can bypass the problem of computing all homomorphisms \(F \rightarrow G\) in step (i)*.
Figure 8. (Left) Nine learned 3 by 3 network dictionary patches from Glauber chain sampling the ‘wedge motif’ $F = ([3], 1_{(1,2),(1,3)})$ from 10 by 10 torus. Black=1 and white = 0 with gray scale. The values below dictionaries indicate their ‘importance’, which is computed by the corresponding total row sums of the code matrices. (Middle) Heat map of the original adjacency matrix of the 10 by 10 torus where blue = 0 and yellow = 1. (Right) Heat map of the reconstructed adjacency matrix with the same colormap.

Figure 8 (left) shows nine learned $(3 \times 3)$ dictionary patches of $X$ learned by online NMF. Note that the three identical dictionary patches at matrix coordinates $(2,1)$, $(2,3)$, and $(3,3)$ correspond to the $(3 \times 3)$ matrix $A_F$ in (43). Since $X$ has rank 1, this should be the single dictionary patch that should be learned and used by online NMF to approximate all columns of $X$. Indeed, the figure also shows the ‘importance’ of each dictionary, which is computed by the corresponding row sum of the code matrix divided by the total sum. In the figure, the importance of the bottom right dictionary is 1, as expected.

Lastly, Figure 8 (right) shows the reconstructed adjacency matrix of $G$. This is done by approximating each $F$-patch of $G$ by a non-negative linear combination of the nine learned dictionaries, and then ‘patching up’ these approximations into a $(n \times n)$ matrix by averaging on overlaps. Since each $F$-patch of $G$ equals one of the dictionaries, we obtain a perfect reconstruction as shown in the figure.

6.2. Motif sampling from networks and MCMC sampler. There are two main issues in the preliminary Network Dictionary Learning scheme for simple graphs we described in the previous section. First, computing the full set $\text{Hom}(F,G)$ of homomorphisms $F \rightarrow G$ is computationally expensive with $O(n^k)$ complexity. Second, in the case of the general network with edge and node weights, some homomorphisms could be more important in capturing features of the network than others. In order to overcome the second difficulty, we introduce a probability distribution for the homomorphisms for the general case that takes into account the weight information of the network. To handle the first issue, we use a MCMC algorithm to sample from such a probability measure and apply online NMF to sequentially learn network dictionary patches.

We first give a precise definition of networks and motifs. A network as a mathematical object consists of a triple $G = ([n], A, \alpha)$ of information, where $[n]$ is the node set of individuals, $A : [n]^2 \rightarrow [0,\infty)$ is a (not necessarily symmetric) matrix describing interaction strength between individuals, and $\alpha : [n] \rightarrow (0,1]$ is a probability measure on $[n]$ giving significance of each individual. We are omitting the possibility of $\alpha(i) = 0$ for any $i \in [n]$ since in that case we can simply disregard the ‘invisible’ node $i$ from the network. Also note that any given $(n \times n)$ matrix $A$ taking values from $[0,1]$ can be regarded as a network $([n], A, \alpha)$ where $\alpha(i) \equiv 1/n$ is the uniform distribution on $[n]$. Fix an integer $k \geq 1$ and a

---

1When $G$ is a complete graph $K_q$ with $q$ nodes, computing homomorphisms $F \rightarrow K_q$ equals to computing all proper $q$-colorings of $F$. 
matrix $A_F : [k]^2 \rightarrow [0, \infty)$. Let $F = ([k], A_F)$ denote the corresponding edge-weighted graph, which we call a motif.

For a given motif $F = ([k], A_F)$ and a $n$-node network $G = ([n], A, \alpha)$, we introduce the following probability distribution $\pi_{F \rightarrow G}$ on the set $[n]^{[k]}$ of all vertex maps $x : [k] \rightarrow [n]$ by

$$\pi_{F \rightarrow G}(x) = \frac{1}{Z} \prod_{1 \leq i, j \leq k} A(x(i), x(j))^{A_F(i,j)} \alpha(x(1)) \cdots \alpha(x(k)),$$

where $Z$ is the normalizing constant called the homomorphism density of $F$ in $G$. We call the random vertex map $x : [k] \rightarrow [n]$ distributed as $\pi_{F \rightarrow G}$ the random homomorphism of $F$ into $G$. Note that $\pi_{F \rightarrow G}$ becomes the uniform distribution on the set of all homomorphisms $F \rightarrow G$ when both $A$ and $A_F$ are matrices with 0/1 entries.

In order to sample a random homomorphism $F \rightarrow G$, we use the Glauber chain, which is an MCMC algorithm introduced in [LMS19]. This is the exact analogue of the Gibbs sampler for the Ising model we discussed in Subsection 5.2. Namely, we pick one node $i \in [k]$ of $F$ uniformly at random, and resample the current location $x_i(i) \in [n]$ of node $i$ in the network $G$ from the correct conditional distribution. This is illustrated in Figure 9 and see [LMS19, Sec. 5] for more details.

**Network Dictionary Learning: Online version for general networks**

(i) Given a network $G = ([n], A, \alpha)$ and a motif $F = ([k], A_F)$, generate a Glauber chain trajectory $(x_t)_{t \geq 0}$ of homomorphisms $F \rightarrow G$. Collect $N$ consecutive samples to form a sequence $(S_t)_{t \geq 0}$ of batches of $N$ homomorphisms:

$$S_t = (x_{N(t-1)+1}, x_{N(t-1)+2}, \cdots, x_{Nt}).$$

(ii) For each $t \geq 1$ and $1 \leq i \leq N$, denote by $A_{t,i}$ the $(k \times k)$ matrix

$$A_{t,i}(a, b) = A(x_{N(t-1)+i}(a), x_{N(t-1)+i}(b)) \quad 1 \leq a, b \leq k.$$

(iii) Apply online NMF to the Markovian sequence of matrices $(X_t)_{t \geq 0}$ to learn dictionary patches.

Note that, under the hypothesis of [LMS19, Thm 5.7], the Glauber chain $(x_t)_{t \geq 0}$ of homomorphisms $F \rightarrow G$ is a finite state Markov chain that is irreducible and aperiodic with unique stationary distribution $\pi_{F \rightarrow G}$. Moreover, the induced $N$-fold Markov chain $(X_t)_{t \geq 0}$ of $F$-patch matrices is also irreducible and aperiodic with a unique stationary distribution. Hence in this case Theorem 4.1 guarantees that the above Network Dictionary Learning scheme will converge to a locally optimal set of network dictionary patches.
Example 7.2 (Network Dictionary Learning from Word Adjacency Networks). In this example, we present a real-world application of Network Dictionary Learning that we have introduced in the previous section. Word Adjacency Networks (WANs) were recently introduced by Segarra, Eisen, and Ribeiro as a tool for authorship attribution [SER15]. Function words are the words that are used for grammatical purpose and do not carry lexical meaning on their own, such as “the”, “of”, and “which”. After fixing a list of $n$ function words, for a given article $A$, construct a $(n \times n)$ frequency matrix $M(A)$ whose $(i, j)$th entry $m_{ij}$ is the number of times that the $i$th function word is followed by the $j$th function word within a forward window of $D = 10$ consecutive words. One can think of a network associated to the article $A$, whose nodes are the function words and the edge weights are given by the frequency matrix with proper normalization.

In Figures 10 and 11 below, we apply Network Dictionary Learning on the Word Adjacency Network of Mark Twain’s novel *Adventures of Huckleberry Finn*. The article is encoded into a $(211 \times 211)$ frequency matrix, and we learn 36 $(3 \times 3)$ and $(7 \times 7)$ network dictionary patches using the general Network Dictionary Learning scheme. For motifs, we used the ‘wedge’ $F = ([3], 1_{[(1,2),(1,3)]})$, the ‘depth-2 wedge’ $F = ([5], 1_{[(1,2),(2,3),(1,4),(4,5)]})$, and the ‘depth-3 wedge’ $F = ([7], 1_{[(1,2),(2,3),(3,4),(1,5),(5,6),(6,7)]})$ to learn $(3 \times 3)$ and $(5 \times 5)$ dictionary patches, respectively. As before, importance of each learned dictionary patches are also shown in the figures. Unlike in the torus example, all the learned dictionaries have positive importance. These dictionary patches should encode some of the main patterns in chains of nearby function words in the article.

The reconstruction of the original network is done in an online manner, since storing $N$ homomorphisms $F \rightarrow \mathcal{G}$ requires large memory of order $O(Nn^6)$. Namely, we first learn the network dictionary patches using the Network Dictionary Learning algorithm. Next, for the reconstruction, we run the Glauber chain $(x_t)_{t \geq 0}$ of homomorphisms $F \rightarrow \mathcal{G}$ once more. For each $t \geq 0$, we reconstruct the $k \times k$ $F$-patch of $\mathcal{G}$ corresponding to the current homomorphism $x_t$ using the learned dictionaries. We keep track of the overlap count for each entry $A(a, b)$ that we have reconstructed up to time $t$, and...
Figure 11. (Left) 45 learned 5 by 5 network dictionary patches from Glauber chain sampling the ‘depth-2 wedge motif’ $F = ([5], [(1, 2), (2, 3), (1, 4), (4, 4)])$ from the Word Adjacency Matrix of “Mark Twain - Adventures of Huckleberry Finn”. Black=1 and white = 0 with gray scale. The values below dictionaries indicate their ‘importance’, which is computed by the corresponding total row sums of the code matrices. (Middle) Heat map of the original Word Adjacency Matrix of the 10 by 10 torus where blue = 0 and yellow = 1. (Right) Heat map of the reconstructed Word Adjacency Matrix with the same colormap. The Frobenius norms of the original, reconstructed, and their difference are 2.8317, 3.4296, and 1.7241, respectively.

Figure 12. (Left) 45 learned 7 by 7 network dictionary patches from Glauber chain sampling the ‘depth-3 wedge motif’ $F = ([7], [(1, 2, 3), (3, 4), (1, 5), (5, 6), (6, 7)])$ from the Word Adjacency Matrix of “Mark Twain - Adventures of Huckleberry Finn”. Black=1 and white = 0 with gray scale. The values below dictionaries indicate their ‘importance’, which is computed by the corresponding total row sums of the code matrices. (Middle) Heat map of the original Word Adjacency Matrix of the 10 by 10 torus where blue = 0 and yellow = 1. (Right) Heat map of the reconstructed Word Adjacency Matrix with the same colormap. The Frobenius norms of the original, reconstructed, and their difference are 2.8317, 4.0459, and 2.4928, respectively.

take the average of all the proposed values of each entry $A(a, b)$ up to time $t$. This only requires $O(n^2)$ memory. In our simulations, we used 50000 MCMC steps for reconstruction.

The reconstructed Word Adjacency Matrix in Figures 10, 11, and 12 seem to be very close to the original. Quantitatively, the Frobenius norm of the difference between the original and reconstructed matrices are 1.0275, 1.7241, and 2.4928, respectively. The Frobenius norms of the original and the
three reconstructed matrices are 2.8317, 3.0394, 3.4296, and 4.0459, respectively. We do observe that these reconstruction errors tend to drop as we increase the number of dictionaries and decrease the patch size. While the former trend is easy to understand, the latter seems to be coming from how the frequency matrix for the text data is constructed. Namely, recall that the frequency matrix records the frequency of seeing pairs of \(i\)th and \(j\)th function word within the range of \(D = 10\) consecutive words. Hence if we extract \(7 \times 7\) patches using the 3-wedge motif described in Figure 12, for example, this could span the range of 60 consecutive words in the document, which could even cover a short paragraph. It is reasonable that the patterns in collections of function words become weaker as the words are allowed to span a longer range in the document.

We also notice that the diagonal entries in the reconstruction are more pronounced, unlike the torus reconstruction in Example 7.1. A possible explanation is that, since it is much harder to embed a path into the Mark Twain network in a ‘proper way’ (like in the torus), often times the paths are just shrunk into a single node with positive self-loop. Since we are taking time average of the evolution of path embeddings into the network, this could emphasize the diagonal entries in the network.

7. Proof of Theorems 4.1 and 4.3

7.1. Preliminary bounds. In this subsection, we derive some key inequalities and preliminary bounds toward the proof of Theorem 4.1.

**Proposition 7.1.** Let \((W_{t-1}, H_t)_{t \geq 1}\) be a solution to the optimization problem (3). Then for each \(t \geq 0\),
the following hold almost surely:

(i) \[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right). \]

(ii) \[ 0 \leq \frac{1}{t+1} \left( \hat{f}_t(W_t) - f_t(W_t) \right) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right) + \hat{f}_t(W_t) - \hat{f}_{t+1}(W_{t+1}). \]

**Proof.** First recall that \(\hat{f}_t(W) \geq f_t(W)\) for all \(t \geq 0\) and \(W \in \mathbb{R}_{t \geq 0}^{d \times r}\). Also note that
\[ \hat{f}_{t+1}(W_t) = \frac{1}{t+1} \left( t \hat{f}_t(W_t) + \ell(X_{t+1}, W_t) \right) \]
for all \(t \geq 0\). It follows that
\[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) = \hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t+1}(W_t) + \hat{f}_{t+1}(W_t) - \hat{f}_t(W_t) \]
\[ = \hat{f}_{t+1}(W_{t+1}) - \hat{f}_{t+1}(W_t) + \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right) + \hat{f}_t(W_t) - \hat{f}_{t+1}(W_{t+1}) \]
\[ \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t) - f_t(W_t) \right). \]
This shows (i). Using the second equality above and the fact that \(\hat{f}_{t+1}(W_{t+1}) \leq \hat{f}_{t+1}(W_t)\), this also shows (ii). \(\square\)

Next, we show that if the data are drawn from compact sets, then the set of all possible codes also form a compact set. This also implies the boundedness of the matrices \(A_t \in \mathbb{R}^{r \times r}\) and \(B_t \in \mathbb{R}^{r \times n}\), which aggregate sufficient statistics up to time \(t^-\) (defined in 17). Also recall the optimal code \(H_{opt}(X, W) \in \mathcal{C}' \subseteq \mathbb{R}^{r \times n}\) defined in (31).

**Proposition 7.2.** Assume (A1) and let \(R(\Omega) < \infty\) be as defined in (5). Then the following hold:

(i) For all \(X \in \Omega\) and \(W \in \mathcal{C}'\),
\[ \|H_{opt}(X, W)\|_{F}^2 \leq \lambda^{-2} R(\Omega)^4 \]
(ii) For any sequence \((X_t)_{t \geq 1} \subseteq \Omega\) and \((W_t)_{t \geq 1} \subseteq \mathcal{C}\), define
\[
A_t = \frac{1}{t} \sum_{k=1}^{t} H_{\text{opt}}^{(1)}(X_k, W_k) H_{\text{opt}}^{(2)}(X_k, W_k)^T, \quad B_t = \frac{1}{t} \sum_{k=1}^{t} H_{\text{opt}}^{(1)}(X_k, W_k) X_k^T. \tag{52}
\]
Then for all \(t \geq 1\), we have
\[
\|A_t\|_F \leq \lambda^{-2} R(\Omega)^4, \quad \|B_t\|_F \leq \lambda^{-1} R(\Omega)^3 \tag{53}
\]

**Proof.** From (31), we have
\[
\lambda \|H_{\text{opt}}^{(1)}(X, W)\|_1 \leq \inf_{H \in \mathcal{C} \subset \mathbb{R}^{d \times n}} \left(\|X - WH\|_F^2 + \lambda \|H\|_1\right) \leq \|X\|_2^2 \leq R(\Omega)^2. \tag{54}
\]
Note that \(\|H\|_F^2 \leq \|H\|_F^2\) for any \(H\). This yields (i). To get (ii), we observe \(\|XY\|_F \leq \|X\|_F \|Y\|_F\) from the Cauchy-Schwarz inequality. Then (ii) follows immediately from (i) and triangle inequality. \(\Box\)

Lastly, in this subsection, we show the Lipschitz continuity of the loss function \(\ell(\cdot, \cdot)\). Since \(\Omega\) and \(\mathcal{C}\) are both compact, this also implies that \(f_t^*\) and \(f_t\) are Lipschitz for all \(t \geq 0\).

**Proposition 7.3.** Suppose (A1) and (A2) hold, and let \(M = 2R(\Omega) + R(\mathcal{C})R(\Omega)^2/\lambda\). Then for each \(X_1, X_2 \in \Omega\) and \(W_1, W_2 \in \mathcal{C}\),
\[
|\ell(X_1, W_1) - \ell(X_2, W_2)| \leq M \left(\|X_1 - X_2\|_F + \lambda^{-1} R(\Omega) \|W_1 - W_2\|_F\right). \tag{55}
\]

**Proof.** Fix \(X \in \Omega \subseteq \mathbb{R}^{d \times n}\) and \(W_1, W_2 \in \mathcal{C}\). Denote \(H^* = H_{\text{opt}}^{(1)}(X_2, W_2)\) and \(H_+ = H_{\text{opt}}^{(1)}(X_1, W_1)\). According to Proposition 7.2, the norm of \(H^*\) and \(H_+\) are uniformly bounded by \(R(\Omega)^2/\lambda\). Note that for any \(A, B \in \Omega\), the triangle inequality implies
\[
\|a\|_F - \|b\|_F = (\|a\|_F + \|b\|_F) (\|a\|_F + \|b\|_F) \leq \|a - b\|_F (\|a\|_F + \|b\|_F). \tag{56}
\]
Also, the Cauchy-Schwarz inequality, (A1)-(A2), and Proposition 7.2 imply
\[
\|X_1 - W_1 H^*\|_F + \|X_2 - W_2 H^*\|_F \leq \|X_1\|_F + \|W_1\| + \|H^*\|_F + \|X_2\|_F \tag{58}
\]
\[
\leq 2R(\Omega) + R(\mathcal{C})R(\Omega)^2/\lambda. \tag{59}
\]
Denoting \(M = 2R(\Omega) + R(\mathcal{C})R(\Omega)^2/\lambda\), we have
\[
|\ell(X_1, W_1) - \ell(X_2, W_2)| \leq M \left(\|X_1 - W_1 H^*\|_F^2 + \lambda \|H^*\|_1\right) - \left(\|X_2 - W_2 H^*\|_F^2 + \lambda \|H^*\|_1\right) \tag{60}
\]
\[
\leq M \|X_1 - X_2\| + (W_2 - W_1) H^*\|_F \tag{61}
\]
\[
\leq M \left(\|X_1 - X_2\|_F + \|W_1 - W_2\|_F \|H^*\|_F\right) \tag{62}
\]
\[
\leq M \left(\|X_1 - X_2\|_F + \lambda^{-1} R(\Omega)^2 \|W_1 - W_2\|_F\right). \tag{63}
\]
This shows the assertion. \(\Box\)

**Proposition 7.4.** Let \((W_t, H_t)_{t \geq 1}\) be any solution to the relaxed online NMF scheme (32). Assume (A1)-(A2) and (C2) for (32). Then there exists some constant \(c > 0\) such that for all \(t \geq 1\),
\[
\|W_{t+1} - W_t\|_F \leq \frac{c}{\lambda^2 t}. \tag{64}
\]

**Proof.** The argument is inspired by the proof of [MBPS10, Lem.1]. Let \(A_t\) and \(B_t\) be as in (32). Denote \(\hat{g}_t(W) = \text{tr}(W A_t W^T) - 2\text{tr}(W B_t)\) and \(\hat{h}_t := \hat{g}_t - \hat{g}_{t+1}\). We first claim that there exists a constant \(c > 0\) such that
\[
|\hat{h}_t(W) - \hat{h}_t(W')| \leq c \|W - W'\|_F. \tag{65}
\]
for all $W, W' \in \mathcal{C}$ and $t \geq 0$. To see this, we first write
\[ \hat{h}_t(W) = \text{tr}(W(A_t - A_{t+1})W^T) - 2\text{tr}(W(B_t - B_{t+1})). \] (66)
The Cauchy-Schwartz inequality yields $\text{tr}(AB) = \|AB\|_F^2 \leq \|A\|_F \|B\|_F$, so we have
\[ \|\hat{h}_t(W) - \hat{h}_t(W')\|_F \leq |\text{tr}((W - W')(A_t - A_{t+1})W^T)| + |\text{tr}(W'(A_t - A_{t+1})(W - W')^T)| + 2|\text{tr}(W - W')(B_t - B_{t+1})| \] (67)
\[ \|\hat{h}_t(W) - \hat{h}_t(W')\|_F \leq 2(R(\mathcal{C})\|A_t - A_{t+1}\|_F + \|B_t - B_{t+1}\|_F) \cdot \|W - W'\|_F, \] (68)
where $R(\mathcal{C}) = \sup_{W \in \mathcal{C}} \|W\|_F < \infty$ by (A2). Note that for each fixed $t$ such that $H_t F \leq \|H_t\|_F \leq \|H^\text{new}(X_t, W_{t-1})\|_F + c_2$ for all $t \geq 0$. Hence by Proposition 7.2, it follows that $\|A_t\|_F$ and $\|B_t\|_F$ are uniformly bounded in $t$. Thus there exists a constant $C > 0$ such that for all $t \geq 0$,
\[ \|A_t - A_{t+1}\|_F = \frac{1}{t(t+1)} \|(A_1 + \cdots + A_t - tA_{t+1})\|_F \leq \frac{C}{t}, \] (70)
and similarly
\[ \|B_t - B_{t+1}\|_F \leq \frac{C'}{t} \] (71)
for some other constant $C' > 0$. Hence the claim (65) follows.

To finish the proof, note that (C2) implies that $\hat{g}_t$ satisfies the second order growth condition:
\[ |\hat{g}_t(W) - \hat{g}_t(W')| \geq \kappa_1 \|W - W'\|_F^2. \] (72)
Moreover, using (ii) and the monotonicity condition $\hat{g}_{t+1}(W_{t+1}) \leq \hat{g}_t(W_t)$, we have
\[ 0 \leq \hat{g}_t(W_{t+1}) - \hat{g}_t(W_t) = \hat{g}_t(W_t) - \hat{g}_{t+1}(W_{t+1}) + \hat{g}_{t+1}(W_{t+1}) - \hat{g}_{t+1}(W_t) + \hat{g}_{t+1}(W_t) - \hat{g}_t(W_t) \] (73)
\[ \leq \hat{g}_t(W_{t+1}) - \hat{g}_{t+1}(W_{t+1}) + \hat{g}_{t+1}(W_t) - \hat{g}_t(W_t) = \hat{h}(W_{t+1}) - \hat{h}(W_t). \] (74)
Hence by (72) and the claim (65), we get
\[ \kappa_1 \|W_t - W_{t+1}\|_F^2 \leq \hat{g}_t(W_{t+1}) - \hat{g}_t(W_t) \leq \frac{C}{t} \|W_t - W_{t+1}\|_F. \] (76)
This shows the assertion. \(\square\)

7.2. Convergence of the empirical and surrogate loss. We prove Theorem 4.1 in this subsection. According to Proposition 7.1, it is crucial to bound the quantity $\ell(X_{t+1}, W_t) - f_t(W_t)$. When $X_t$’s are i.i.d., we can condition on the information $\mathcal{F}_t$ up to time $t$ so that
\[ \mathbb{E} \left[ \ell(X_{t+1}, W_t) - f_t(W_t) \mid \mathcal{F}_t \right] = f_t(W_t) - f_t(W_t). \] (77)
Note that for each fixed $W \in \mathcal{C}$, $f_t(W) \rightarrow f(W)$ almost surely as $t \rightarrow \infty$ by the strong law of large numbers. To handle time dependence of $W_t$, one can instead look at the convergence of the supremum $\|f_t - f\|_\infty$ over the compact set $\mathcal{C}$, which is provided by the classical Glivenko-Cantelli theorem. This is the approach taken in [MBPS10] for i.i.d. input.

However, the same approach breaks down when $(X_t)_{t \geq 0}$ is a Markov chain. This is because, conditional on $\mathcal{F}_t$, the distribution of $X_{t+1}$ is not necessarily the stationary distribution $\pi$. Our key innovation to overcome this difficulty is to condition much early on – at time $t - N$ for some suitable $N = N(t)$. Then the Markov chain runs $N + 1$ steps up to time $t + 1$, so if $N$ is large enough for the chain to mix, then the distribution of $X_{t+1}$ conditional on $\mathcal{F}_{t-N}$ is close to the stationary distribution.
$\pi$. The error of approximating the stationary distribution by the $N + 1$ step distribution is controlled using total variation distance and mixing bound.

**Proposition 7.5.** Suppose (A1)-(A2) and (M1). Fix $W \in \mathcal{C}$. Then for each $t \geq 0$ and $0 \leq N < t$, conditional on the information $\mathcal{F}_{t-N}$ up to time $t-N$,

$$
\left| \mathbb{E}\left[ \mathcal{L}(X_{t+1}, W) - f_t(W) \right] \right| \leq \left| \mathcal{L}(W) - f_{t-N}(W) \right| + \frac{N}{t} \left( f_{t-N}(W) + \|\mathcal{L}(\cdot, W)\|_\infty \right)
$$

(78)

$$
+ 2\|\mathcal{L}(\cdot, W)\|_\infty \sup_{x \in \Omega} \|P^{N+1}(x, \cdot) - \pi\|_{TV}.
$$

(79)

**Proof.** Recall that for each $s \geq 0$, $\mathcal{F}_s$ denotes the $\sigma$-algebra generated by the history of data matrices $X_1, X_2, \ldots, X_s$. Fix $x \in \Omega$ and suppose $X_{t-N} = x$. Then by the Markov property, the distribution of $X_{t+1}$ conditional on $\mathcal{F}_{t-N}$ equals $P^{N+1}(x, \cdot)$, where $P$ denotes the transition kernel of the chain $(X_t)_{t \geq 0}$. Using the fact that $2\|\mu - \nu\|_{TV} = \sum |\mu(x) - \nu(x)|$ (see [LP17, Prop. 4.2]), it follows that

$$
\mathbb{E}\left[ \mathcal{L}(X_{t+1}, W) \right| \mathcal{F}_{t-N} ] = \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) P^{N+1}(x, x') \right| \mathcal{F}_{t-N} ]
$$

(80)

$$
= \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) \pi(x') \right| \mathcal{F}_{t-N} ] + \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) (P^{N+1}(x, x') - \pi(x')) \right| \mathcal{F}_{t-N} ]
$$

(81)

$$
\leq \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) \pi(x') \right| \mathcal{F}_{t-N} ] + 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV}
$$

(82)

$$
= f(W) + 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV}.
$$

(83)

Similarly, we have

$$
f(W) = \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) \pi(x') \right| \mathcal{F}_{t-N} ]
$$

(84)

$$
= \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) P^{N+1}(x, x') \right| \mathcal{F}_{t-N} ] + \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) (\pi(x') - P^{N+1}(x, x')) \right| \mathcal{F}_{t-N} ]
$$

(85)

$$
\leq \sum_{x' \in \Omega} \mathbb{E}\left[ \mathcal{L}(x', W) P^{N+1}(x, x') \right| \mathcal{F}_{t-N} ] + 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV}
$$

(86)

$$
= \mathbb{E}\left[ \mathcal{L}(x', W) \right| \mathcal{F}_{t-N} ] + 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV}.
$$

(87)

Also, observe that

$$
\mathbb{E}\left[ f_t(W) \right| \mathcal{F}_{t-N} ] = \frac{t-N}{t} f_{t-N}(W) + \frac{1}{t} \mathbb{E}\left[ \sum_{k=t-N+1}^{t} \mathcal{L}(X_k, W) \right| \mathcal{F}_{t-N} ]
$$

(88)

Since the last term in the last equation is bounded by 0 and $\frac{N}{t} \|\mathcal{L}(\cdot, W)\|_\infty$, we have

$$
\mathbb{E}\left[ \mathcal{L}(X_{t+1}, W) - f_t(W) \right| \mathcal{F}_{t-N} ] \leq \left( f(W) + 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV} \right)
$$

(89)

$$
- \left( \frac{t-N}{t} f_{t-N}(W) + \frac{1}{t} \mathbb{E}\left[ \sum_{k=t-N+1}^{t} \mathcal{L}(X_k, W) \right| \mathcal{F}_{t-N} ] \right)
$$

(90)

$$
\leq f(W) - f_{t-N}(W) + \frac{N}{t} f_{t-N}(W)
$$

(91)

$$
+ 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV}
$$

(92)

and

$$
\mathbb{E}\left[ f_t(W) - \mathcal{L}(X_{t+1}, W) \right| \mathcal{F}_{t-N} ] \leq \left( \frac{t-N}{t} f_{t-N}(W) + \frac{1}{t} \mathbb{E}\left[ \sum_{k=t-N+1}^{t} \mathcal{L}(X_k, W) \right| \mathcal{F}_{t-N} ] \right)
$$

(93)

$$
- \left( f(W) + 2\|\mathcal{L}(\cdot, W)\|_\infty \|P^{N+1}(x, \cdot) - \pi\|_{TV} \right)
$$

(94)
Then combining the two bounds by the triangle inequality gives the assertion.

Next, we use the Glivenko-Cantelli theorem and the functional central theorem for Markov chains together with the mixing condition (M2) to show that the surrogate loss process \((\hat{f}_t(W_t))_{t \geq 0}\) has the bounded positive expected variation.

**Lemma 7.6.** Let \((W_{t-1}, H_t)_{t \geq 1}\) be a solution to the optimization problem (3). Suppose \((A1)-(A2)\) and \((M1)\) hold.

(i) Let \((a_t)_{t \geq 0}\) be a sequence of non-decreasing non-negative integers such that \(a_t \in o(t)\). Then there exists absolute constants \(C_1, C_2, C_3 > 0\) such that for all sufficiently large \(t \geq 0\),

\[
E \left[ \left\| \sum_{i=0}^{t} \left( \frac{\ell(X_{t+1}, W_i) - f_t(W_i)}{t+1} \right) \mathcal{F}_{t-a_t} \right\| \right] \leq C_1 \frac{1}{t^{3/2}} + C_2 \left( \frac{1}{t^2} a_t + \frac{C_3}{t} \sup_{x \in \Omega} \| P^{a_t+1}(x, \cdot) - \pi \|_{TV} \right).
\]

(ii) Further assume that (M2) holds. Then we have

\[
\sum_{t=0}^{\infty} \left( E \left[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \right] \right)^+ \leq \sum_{t=0}^{\infty} E \left[ \left\| \frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t+1} \right\| \right] < \infty.
\]

**Proof.** Since \((X_t, W_t) \in \Omega \times \mathcal{C}\) for all \(t \geq 0\) and since both \(\Omega\) and \(\mathcal{C}\) are compact, we have

\[
L := \sup_{X \in \Omega, W \in \mathcal{C}} \ell(X, W) < \infty.
\]

Denote

\[
\Delta_t := \sup_{x \in \Omega} \| P^t(x, \cdot) - \pi \|_{TV}.
\]

Note that \(\| f_s \|_{\infty} \leq L\) for any \(s \geq 0\). Hence according to Propositions 7.5, we have

\[
E \left[ \left\| \frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t+1} \right\| \mathcal{F}_{t-a_t} \right] \leq \| f - f_{t-a_t} \|_{\infty} \frac{2L}{t} + 2a_t + \frac{L \Delta_t}{t}.
\]

Since \(a_t = o(t)\), we have \(a_t \leq t/2\) for all sufficiently large \(t \geq 0\). Then by the uniform functional CLT for Markov chains [Lev88, Thm 5.9], for all sufficiently large \(t \geq 0\), we have

\[
E \left[ \sqrt{t/2} \| f - f_{t-a_t} \|_{\infty} \right] \leq E \left[ \sqrt{t-a_t} \| f - f_{t-a_t} \|_{\infty} \right] = O(1).
\]

It follows that there exists a constant \(C_1 > 0\) such that

\[
E \left[ \frac{\| f - f_{t-a_t} \|_{\infty}}{t} \right] \leq E \left[ \frac{\sqrt{t/2} \| f - f_{t-a_t} \|_{\infty}}{t^{3/2}} \right] \leq \frac{C_1}{t^{3/2}}
\]

for all sufficiently large \(t \geq 1\). Hence taking expectation on both sides of (101) with respect to the information from time \(t - a_t\) to \(t\) yields the first assertion.

Now we show the second assertion. The first inequality in (98) follows from Proposition 7.1 (i). To show the second inequality, denote \(Y_t = (t+1)^{-1} \ell(X_{t+1}, W) - f_t(W)\). Note that by the first assertion and (M2), there exists a constant \(C > 0\) such that almost surely for all \(t \geq 0\),

\[
E \left[ \left\| Y_t \mid \mathcal{F}_{t-a_t} \right\| \right] \leq \frac{C}{t (\log t)^2}.
\]

Then by iterated expectation and Jensen's inequality, it follows that

\[
|E[Y_t]| = E \left[ E \left[ Y_t \mid \mathcal{F}_{t-a_t} \right] \right] \leq E \left[ \left\| Y_t \mid \mathcal{F}_{t-a_t} \right\| \right] \leq \frac{C}{t (\log t)^2}.
\]

Since the last expression is integrable, (ii) follows from Proposition 7.1. □
Proposition 7.7. Let \((a_n)_{n \geq 0}\) and \((b_n)_{n \geq 0}\) be non-negative real sequences such that
\[
\sum_{n=0}^{\infty} a_n = \infty, \quad \sum_{n=0}^{\infty} a_n b_n < \infty.
\] (106)
Further assume that there exists a constant \(K > 0\) such that \(|b_{n+1} - b_n| \leq Ka_n\) for all \(n \geq 0\). Then
\[
\lim_{n \to \infty} b_n = 0.
\]

Proof. See [MBPS10, Lem. 3] or [Ber99, Prop. 1.2.4].

Now we prove the main result in this paper, Theorem 4.1.

Proof of Theorem 4.1. Suppose (A1)-(A2) and (M1)-(M2) hold. We first show (i). In order to show that
\[
\mathbb{E}[\hat{f}_t(W_t)]
\]
converges as \(t \to \infty\), since \(f_t(W_t)\) is bounded uniformly in \(t\), it suffices to show that the sequence \((\mathbb{E}[\hat{f}_t(W_t)])_{t \geq 0}\) has a unique limit point. To this end, observe that for any \(x, y \in \mathbb{R}\), \((x + y)^+ \leq x^+ + y^+\). Note that, for each \(m, n \geq 1\) with \(m > n\),
\[
\left(\mathbb{E}[\hat{f}_m(W_m)] - \mathbb{E}[\hat{f}_n(W_n)]\right)^+ \leq \sum_{k=n}^{m-1} \left(\mathbb{E}[\hat{f}_{k+1}(W_{k+1})] - \mathbb{E}[f_k(W_k)]\right)^+
\] (107)
\[
\leq \sum_{k=n}^{\infty} \left(\mathbb{E}[\hat{f}_{k+1}(W_{k+1})] - \mathbb{E}[f_k(W_k)]\right)^+.
\] (108)
The last expression converges to zero as \(n \to \infty\) by Lemma 7.9 (ii). This implies that the sequence
\[(\mathbb{E}[\hat{f}_t(W_t)])_{t \geq 0}\]
has a unique limit point, as desired.

Furthermore, suppose that the state space \(\Omega\) for the Markov chain \((X_t)_{t \geq 0}\) is finite. Then by the convergence theorem (see., e.g., [LP17, Thm. 4.9] or (11)), by choosing \(a_t = \lceil \sqrt{t} \rceil\) in Lemma 7.9 (i), we get
\[
\mathbb{E}\left[\left|\left|\frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t + 1}\right|\right|_{\mathcal{F}_{t-a_t}}\right] \leq C_1 \frac{1}{t^{3/2}} + \frac{C_2 A^{3/2}}{t}
\] (109)
for some constants \(C_1, C_2 \geq 1\) and \(\lambda \in (0, 1)\). Then Proposition 7.1 gives
\[
\mathbb{E}[\hat{f}_m(W_m)] - \mathbb{E}[\hat{f}_n(W_n)] \leq \sum_{t=n}^{\infty} \left(\frac{C_1}{t^{3/2}} + \frac{C_2 A^{3/2}}{t}\right) \leq C' n^{-1/2}
\] (110)
for some constant \(C' > 0\). Since we have just shown that \(\mathbb{E}[\hat{f}_t(W_t)]\) converges as \(t \to \infty\), letting \(m \to \infty\) in the above inequality will show that
\[
\lim_{m \to \infty} \mathbb{E}[\hat{f}_m(W_m)] - \mathbb{E}[\hat{f}_n(W_n)] \leq \sum_{t=n}^{\infty} \left(\frac{C_1}{t^{3/2}} + \frac{C_2 A^{3/2}}{t}\right) \leq C' n^{-1/2}.
\] (111)
Below we will show that \(\lim_{t \to \infty} \mathbb{E}[f_t(W_t)]\) exists and equals to \(\lim_{t \to \infty} \mathbb{E}[\hat{f}_t(W_t)]\), so this will complete the proof of (i).

Next, we show the assertions for the empirical loss process \((f_t(W_t))_{t \geq 0}\). We claim that
\[
\mathbb{E}\left[\sum_{t=0}^{\infty} \frac{\hat{f}_t(W_t) - f_t(W_t)}{t + 1}\right] = \sum_{t=0}^{\infty} \mathbb{E}\left[\frac{\hat{f}_t(W_t) - f_t(W_t)}{t + 1}\right] < \infty.
\] (112)
The first equality follows from Fubini's theorem by noting that \(\hat{f}_t(W) - f_t(W) \geq 0\) for any \(W \in \mathcal{C}\). On the other hand, by using Proposition 7.1 (ii),
\[
\sum_{t=0}^{\infty} \mathbb{E}\left[\frac{\hat{f}_t(W_t) - f_t(W_t)}{t + 1}\right] \leq \sum_{t=0}^{\infty} \mathbb{E}\left[\frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t + 1}\right] - \sum_{t=0}^{\infty} \mathbb{E}[\hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t)]
\] (113)
The first sum on the right hand side is finite by Lemma 7.6 (ii), and the second sum is also finite since we have just shown that \( \mathbb{E}[\hat{f}_t(W_t)] \) converges as \( t \to \infty \). This shows the claim.

Now, note that the claim (112) also implies
\[
\sum_{t=0}^{\infty} \frac{\hat{f}_t(W_t) - f_t(W_t)}{t+1} < \infty \quad \text{a.s.} \tag{114}
\]
since the expectation in the left hand side of (112) is finite. Both \( \hat{f}_t \) and \( f_t \) are uniformly bounded and Lipschitz by Proposition 7.3. Also, note that Proposition 7.4 applies in the current situation since (3) we have just shown that

\[
\text{Thus, according to Proposition 7.7, it follows from (114) that}
\lim_{t \to \infty} (\hat{f}_t(W_t) - f_t(W_t)) = 0 \quad \text{a.s.} \tag{117}
\]
Similarly, Jensen's inequality and above estimates imply
\[
\left| \mathbb{E}[\hat{f}_{t+1}(W_{t+1})] - \mathbb{E}[f_{t+1}(W_{t+1})] \right| - \left| \hat{f}_{t+1}(W_t) - f_t(W_t) \right| = O(t^{-1}). \tag{118}
\]

Since \( \mathbb{E}[\hat{f}_t(W_t)] \geq \mathbb{E}[f_t(W_t)] \), the claim (112) and Proposition 7.7 give
\[
\lim_{t \to \infty} \mathbb{E}[f_t(W_t)] = \lim_{t \to \infty} \mathbb{E}[\hat{f}_t(W_t)] + \lim_{t \to \infty} \mathbb{E}[\hat{f}_t(W_t)] - \mathbb{E}[\hat{f}_t(W_t)] = \lim_{t \to \infty} \mathbb{E}[\hat{f}_t(W_t)] \in (1, \infty). \tag{119}
\]
This complete the proof of (i) and (ii).

Lastly, we show (iii). Let \( W_\infty \in \mathcal{C} \) be any accumulation point of the sequence \( W_t \in \mathcal{C} \). It suffices to show that
\[
\| \nabla_W f(W_\infty) \|_{\text{op}} = 0. \tag{120}
\]
To this end, we first choose a subsequence \((t_k)_{k \geq 1}\) such that \( W_{t_k} \to W_\infty \). Denote \( C_t = t^{-1} \sum_{s=1}^{t} X_s X_s^T \) and \( D_t = t^{-1} \sum_{s=1}^{t} \lambda \| H_s \|_1 \). Recall that the sequence \((A_t, B_t, C_t, D_t)_{t \geq 0}\) is bounded by Proposition 7.2 and (A1). Hence we may choose a further subsequence of \((t_k)_{k \geq 1}\), which we will still denote by \((t_k)_{k \geq 1}\), so that \((A_{t_k}, B_{t_k}, C_{t_k}, D_{t_k}) \to (A_\infty, B_\infty, C_\infty, D_\infty) \in \mathbb{R}^{r \times r} \times \mathbb{R}^{r \times n} \times \mathbb{R}^{d \times d} \times \mathbb{R}\) a.s. as \( k \to \infty \).

Define a function
\[
\hat{f}(W) = \text{tr}(WA_\infty W^T) - 2\text{tr}(WB_\infty) + C_\infty + D_\infty. \tag{121}
\]
According to (C1)-(C2) and the optimality, \( W_t \) is a minimizer of the strictly convex function \( \hat{f} \). Hence \( \nabla_W \hat{f}(W_t) = 0 \) for all \( t \geq 0 \). It follows that
\[
\nabla_W \hat{f}(W_\infty) = \nabla_W f(W_\infty) - \nabla_W \hat{f}_{t_k}(W_{t_k}) = 2W(A_\infty - A_{t_k}) - 2(B_{\infty}^T - B_{t_k}). \tag{122}
\]
Hence by letting \( k \to \infty \), we have \( \| \nabla_W \hat{f}(W_\infty) \|_{\text{op}} = 0 \).

Note that \( \hat{f}_t \geq f_t \) for all \( t \geq 0 \) and over all \( \mathcal{C} \). Hence, for each \( W \in \mathcal{C} \), almost surely,
\[
\hat{f}(W) = \lim_{k \to \infty} \hat{f}_{t_k}(W) \geq \lim_{k \to \infty} f_{t_k}(W) = f(W), \tag{123}
\]
where the last equality follows from Markov chain ergodic theorem (see, e.g., [Dur10, Thm. 6.2.1, Ex. 6.2.4] or [MT12, Thm. 17.1.7]). Moreover, by part (i), we know that
\[
\hat{f}(W_\infty) = \lim_{k \to \infty} \hat{f}_{t_k}(W_{t_k}) = f(W_\infty) \in (0, \infty) \tag{124}
\]
almost surely. Therefore, almost surely,
\[
\| \nabla_W \hat{f}(W_\infty) \|_{\text{op}} \leq \| \nabla_W \hat{f}(W_\infty) \|_{\text{op}} = 0. \tag{125}
\]

This completes the proof of the theorem.

\[ \square \]

7.3. **Proof of Theorem 4.3.** In this subsection, we prove Theorem 4.3. Most of the arguments are exactly same for the proof of Theorem 4.1. 

Recall that, in the proof of Proposition 7.1, we only used the fact that \( \hat{f}_{t+1}(W_{t+1}) \leq \hat{f}_t(W_t) \), not the full optimality of \( W_{t+1} \) in minimizing \( \hat{f}_{t+1} \). Hence exactly the same argument will show the following statement.

**Proposition 7.8.** Let \( (W_{t-1}, H_t)_{t \geq 1} \) be a solution to the relaxed optimization problem (32). Then for each \( t \geq 0 \), the following hold almost surely:

(i) \( \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t, H_{t+1}) - f_t(W_t) \right) \).

(ii) \( 0 \leq \frac{1}{t+1} \left( \hat{f}_t(W_t) - f_t(W_t) \right) \leq \frac{1}{t+1} \left( \ell(X_{t+1}, W_t, H_{t+1}) - f_t(W_t) \right) + \left( \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \right) \).

Moreover, recall that Lemma 7.6 follows from Proposition 7.5 and the uniform functional CLT. Hence a minor modification of the same argument using Proposition 7.8 instead will show the following lemma:

**Lemma 7.9.** Let \( (W_{t-1}, H_t)_{t \geq 1} \) be a solution to the optimization problem (32). Suppose (A1)-(A2) and (M1). Let \( \ell(\cdot, \cdot, \cdot) \) be the loss function defined above in (31).

(i) Let \( (a_t)_{t \geq 0} \) be a sequence of non-decreasing non-negative integers such that \( a_t \in o(t) \). Then there exists constants \( C_2, C_3, C_4 > 0 \) such that for all sufficiently large \( t \geq 0 \),

\[
E \left[ \left| E \left[ \frac{\ell(X_{t+1}, W_t, H_{t+1}) - f_t(W_t)}{t+1} \big| \mathcal{F}_{t-a_t} \right] \right| \right] \leq \frac{C_1}{t^{3/2}} + \frac{C_2}{t} a_t + \frac{C_3}{t} \sup_{x \in \Omega} \| P^{a_t+1}(x, \cdot) - \pi \|_{TV} \tag{126}
\]

\[
+ \frac{C_4}{t} \| H_{t+1} - H_{opt}(X_{t+1}, W_t) \|_1 \tag{127}
\]

(ii) Further assume that (M2) holds. Then we have

\[
\sum_{t=0}^{\infty} E \left[ \hat{f}_{t+1}(W_{t+1}) - \hat{f}_t(W_t) \right]^+ \leq \sum_{t=0}^{\infty} E \left[ \frac{\ell(X_{t+1}, W_t, H_{t+1}) - f_t(W_t)}{t+1} \right] < \infty \tag{128}
\]

**Proof.** Denote \( H_{opt} = H_{opt}(X_{t+1}, W_t) \), for which the loss \( \ell(X_{t+1}, W_t, H) \) is minimized. Fix \( H \in \mathcal{C} \subseteq \mathbb{R}^{r \times n} \) and denote \( M = 2R(\Omega) + R(\mathcal{C})R(\Omega)^2 / \lambda \). Then as in the proof of Proposition 7.2,

\[
\| \ell(X_{t+1}, W_t, H) - \ell(X_{t+1}, W_t) \| = \left( \| X_{t+1} - W_t H \|_F^2 + \lambda \| H \|_1 \right) - \left( \| X_{t+1} - W_t \hat{H}_{opt} \|_F^2 + \lambda \| H_{opt} \|_1 \right) \tag{129}
\]

\[
\leq M \left( \| W_t \|_F \| H - \hat{H}_{opt} \|_F + \lambda \| H - H_{opt} \|_1 \right) \tag{130}
\]

\[
\leq M \left( \| W_t \|_F \| H - \hat{H}_{opt} \|_F + \lambda \| H - H_{opt} \|_1 \right) \tag{131}
\]

\[
\leq M (R(\mathcal{C}) + \lambda) \| H - H_{opt} \|_1 \tag{132}
\]

Hence we can write

\[
E \left[ \frac{\ell(X_{t+1}, W_t, H_{t+1}) - f_t(W_t)}{t+1} \big| \mathcal{F}_{t-a_t} \right] \leq E \left[ \frac{\ell(X_{t+1}, W_t) - f_t(W_t)}{t+1} \big| \mathcal{F}_{t-a_t} \right] \tag{133}
\]

\[
+ \frac{M(R(\mathcal{C}) + \lambda)}{t+1} \| H_{t+1} - H_{opt}(X_{t+1}, W_t) \|_1 \tag{134}
\]

Now using the same argument as in the proof of Lemma 7.6 (i), one can show that for the first term on the right hand side, the same bound as in Lemma 7.6 (i) holds. This shows (i). Moreover, by the hypothesis on \( H_{t+1} \) in (32), the second term on the right hand side is of order \( O(t^{-1}(\log t)^{-2}) \). Then (ii) follows from (i) and integrating out the conditioning on \( \mathcal{F}_{t-a_t} \) as in the proof of Lemma 7.6 (ii). \( \square \)

Now we can show Theorem 4.3.
Proof of Theorem 4.3. Suppose (A1)-(A2) and (M1)-(M2). Using Lemma 7.9, the proof of (i) is exactly the same as before in Theorem 4.1. For (ii), using Proposition 7.8 and a similar argument, we can derive (114) for the current case. Furthermore, using Proposition 7.4, we still have (115). Hence by Proposition 7.7 we can deduce (117). This shows (ii).

To show (iii), suppose (C1)-(C2) and let $W_\infty \in \mathcal{C}$ be any accumulation point of the sequence $W_t \in \mathcal{C}$. As before, choose a subsequence $(t_k)_{k \geq 1}$ such that $W_{t_k} \to W_\infty$. Denote $C_t = t^{-1} \sum_{s=1}^t X_s X_s^T$ and $D_t = t^{-1} \sum_{s=1}^t \lambda \|H_s\|_1$. Recall that the sequence $(A_t, B_t, C_t, D_t)_{t \geq 0}$ is bounded by Proposition 7.2 and (A1). Hence we may choose a further subsequence of $(t_k)_{k \geq 1}$, which we will still denote by $(t_k)_{k \geq 1}$, so that $(A_{t_k}, B_{t_k}, C_{t_k}, D_{t_k}) \to (A_\infty, B_\infty, C_\infty, D_\infty) \in \mathbb{R}^{r \times r} \times \mathbb{R}^{r \times n} \times \mathbb{R}^{d \times d} \times \mathbb{R}$ a.s. as $k \to \infty$. Define a function

$$ \hat{f}(W) = \text{tr}(WA_\infty W^T) - 2\text{tr}(WB_\infty) + C_\infty + D_\infty. $$

(135)

Since $\hat{f}_t \equiv f_t$ for all $t \geq 0$ and over all $\mathcal{C}$, it holds that, for all $W \in \mathcal{C}$,

$$ \hat{f}(W) = \lim_{k \to \infty} \hat{f}_{t_k}(W) \geq \lim_{k \to \infty} f_{t_k}(W) = f(W). $$

(136)

Moreover, by part (i), we know that, almost surely,

$$ \hat{f}(W_\infty) = \lim_{k \to \infty} \hat{f}_{t_k}(W_{t_k}) = f(W_\infty). $$

(137)

This and (C2) yields, almost surely,

$$ \|\nabla_W f(W_\infty)\|_{op} \leq \|\nabla_W \hat{f}(W_\infty)\|_{op} \leq \limsup_{t \to \infty} \|\nabla_W \hat{f}_t(W_t)\|_{op}. $$

(138)

This completes the proof of the theorem.

Lastly, we give an easy sufficient condition to guarantee the condition $\|H_t - H_{opt}(X_t, W_{t-1})\|_1 = O((\log t)^{-2})$ in the relaxed online NMF scheme (32). For each matrix $A$, let $\sigma_{\min}(A)$ denote its minimum singular value.

Proposition 7.10 (Stopping criteria for $H_t$). For each $X \in \mathbb{R}^{d \times n}, W \in \mathbb{R}^{d \times r},$ and $H \in \mathbb{R}^{r \times n}$, we have

$$ \|H - H_{opt}(X, W)\|_1 \leq \frac{rn}{2\sigma_{\min}(W)^2} \|\nabla_H \ell(X, W, H)\|_F. $$

(139)

Proof. First, by a similar calculation in (21), we can write

$$ \ell(X, W, H) = \text{tr}(H^T W^T W H) - 2\text{tr}(H^T W X) + \text{tr}(X X^T) + \lambda \|H\|_1. $$

(140)

It follows that

$$ \nabla_H \ell(X, W, H) = 2W^T WH - 2W^T X + \lambda J, $$

(141)

where $J$ is the $r \times n$ matrix whose entries are all 1. Denote $H_{opt} = H_{opt}(X, W)$. Using the fact that $\nabla_H \ell(X, W, H_{opt}) = 0$,

$$ \nabla_H \ell(X, W, H) = \nabla_H \ell(X, W, H) - \nabla_H \ell(X, W, H_{opt}) = 2W^T W (H - H_{opt}). $$

(142)

Using the singular value decomposition, one can easily show that

$$ \|AB\|_F \geq \sigma_{\min}(A) \|B\|_F, $$

(143)

where $\sigma_{\min}(A)$ denotes the minimum singular value of $A$. It then follows that

$$ \|\nabla_H \ell(X, W, H)\|_F = \|2W^T W (H - H_{opt})\|_F $$

$$ \geq 2\sigma_{\min}(W^T W) \|H - H_{opt}\|_F $$

$$ = 2\sigma_{\min}(W)^2 \|H - H_{opt}\|_F $$

$$ \geq \frac{2\sigma_{\min}(W)^2}{nr} \|H - H_{opt}\|_1, $$

(144)

(145)

(146)

(147)
where the last inequality follows from Cauchy-Schwartz inequality. \qed

**Remark 7.11.** If we use \( \ell_F(X, W, H) := \|X - WH\|_F^2 + \lambda \|H\|_F \) to define the loss function \( \ell \) and optimal code \( H_{\text{opt}}(X, W) \) for (32), then we would need to have \( \|H_t - H_{\text{opt}}(X_t, W_{t-1})\|_F = O((\log t)^{-2}) \) instead of the 1-norm bound. According to (145), this could be ensured by the similar bound as in Proposition 7.10 without the factor \( r n \).

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Appendix A. Algorithm for the Relaxed Online NMF Scheme

In this appendix, we state an algorithm for the relaxed online NMF scheme (32). We denote by $\Pi_S : \mathbb{R}^{p \times q} \rightarrow S \subseteq \mathbb{R}^{p \times q}$ the projection onto $S$. The main algorithm, Algorithm 1 below, is a direct implementation of (32). The main algorithm has two sub algorithms, Algorithms 2 and 3, for computing $H_t$ and $W_t$, respectively. In the former, the small gradient condition (152) indeed implies

$$\|H_t - H_t^{opt}(X_t, W_{t-1})\|_F \leq \frac{K}{(\log t)^2} \quad \forall t \geq 0$$

(148)

according to Proposition 7.10. Hence the criteria in the first line of (32) is satisfied.

On the other hand, Algorithm 3 is the same dictionary update algorithm in [MBPS10] except that we have added the monotonicity condition (153) to guarantee convergence of the algorithm. In the ideal case when $W_t = \arg\min_{W \in \mathcal{G}} \hat{g}_t(W_t)$, (153) is automatically satisfied. However, this condition is not necessarily guaranteed if we iterate the column-wise gradient descent with projection (154) for a fixed finite number of times. Instead, we start by setting $W_t = W_{t-1}$ so that $\hat{g}_t(W_t) = \hat{g}_t(W_{t-1})$, and then incrementally update the entries of $W_t$ using gradient descent type rule until the first time that the condition $\hat{g}_t(W_t) \leq \hat{g}_t(W_{t-1})$ is violated. We also remark that the specific coordinate descent algorithms (151) and (154) can be replaced by any other algorithms, as long as the conditions (152) and (153) are satisfied.

Algorithm 1 online NMF for Markovian data

1: Variables:
2: $X_t \in \Omega \subseteq Q^{d \times n}$: data matrix at time $t \geq 0$
3: $W_{t-1} \in \mathcal{G} \subseteq \mathbb{R}^{d \times r}$: learned dictionary at time $t$
4: $(A_{t-1}, B_{t-1}) \in \mathbb{R}^{r \times r} \times \mathbb{R}^{r \times d}$: aggregate sufficient statistic up to time $t$
5: $\lambda, K > 0$: parameters
6: $\mathcal{G} \subseteq \mathbb{R}^{r \times n}$: constraint set of codes
7: Upon arrival of $X_t$:
8: Compute $H_t$ using Algorithm 2 so that

$$\left\|H_t - \left( \arg\min_{H \in \mathcal{G} \subseteq \mathbb{R}^{r \times n}} (\|X_t - W_{t-1}H\|_F^2 + \lambda \|H\|_1) \right) \right\|_F \leq \frac{K}{(\log t)^2}.$$  

(149)

9: $A_t \leftarrow t^{-1}((t-1)A_{t-1} + H_tH_t^T)$, $B_t \leftarrow t^{-1}((t-1)B_{t-1} + H_tX_t^T)$.
10: Compute $W_t$ using Algorithm 3, with $W_{t-1}$ as a warm restart, so that

$$\hat{g}_t(W_t) \leq \hat{g}_t(W_{t-1}),$$

(150)

where $\hat{g}_t(W) = \text{tr}(WA_tW^T) - 2\text{tr}(WB_t)$.

Algorithm 2 Sparse coding

1: Variables:
2: $X_t \in \Omega \subseteq Q^{d \times n}$: data matrix at time $t \geq 0$
3: $W_{t-1} \in \mathcal{G} \subseteq \mathbb{R}^{d \times r}$: learned dictionary at time $t$
4: $\lambda, K > 0$: parameters
5: $\mathcal{G} \subseteq \mathbb{R}^{r \times n}$: constraint set of codes
6: Repeat until convergence:
7: Do

$$H_t \leftarrow \Pi_{\mathcal{G}} \left( H_t - \frac{1}{\text{tr}(W_{t-1}^TW_{t-1})} (W_{t-1}^TW_{t-1}H_t - W_{t-1}^TX_t + \lambda J) \right)$$

(151)

8: Until

$$\|\nabla_H \ell(X_t, W_{t-1}, H)\|_F \leq \frac{K\sigma_{min}(W_{t-1})^2}{r(n\log t)^2}.$$  

(152)

9: Return $H_t$
Algorithm 3 Dictionary update

1: Variables:
2: $W_{t-1} \in \mathcal{S} \subseteq \mathbb{R}^{d \times r}$: learned dictionary at time $t$
3: $(A_t, B_t) \in \mathbb{R}^{r \times r} \times \mathbb{R}^{r \times d}$: aggregate sufficient statistic up to time $t$
4: $\lambda, \kappa_1 > 0$: parameters
5: Do $W_t \leftarrow W_{t-1}$
6: While:
7: \[ \hat{g}_t(W_t) \leq \hat{g}_t(W_{t-1}) \] (153)
8: Repeat until convergence:
9: For $i = 1$ to $d$:
10: \[ [W_t]_{*,i} \leftarrow \Pi_{\mathcal{S}} \left( [W_{t-1}]_{*,i} - \frac{1}{|A_t|_{jj}} (W_{t-1}[A_t]_{*,j} - [B_t^T]_{*,j}) \right) \] (154)
11: Return $W_t$