Learning Markov models via low-rank optimization

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Modeling unknown systems from data is a precursor of system optimization and sequential decision making. In this paper, we focus on learning a Markov model from a single trajectory of states. Suppose that the transition model has a small rank despite of a large state space, meaning that the system admits a low-dimensional latent structure. We show that one can estimate the full transition model accurately using a trajectory of length that is proportional to the total number of states. We propose two maximum likelihood estimation methods: a convex approach with nuclear-norm regularization and a nonconvex approach with rank constraint. We show that both estimators enjoy optimal statistical rates in terms of the Kullback-Leibler divergence and the $\ell_2$ error. For computing the nonconvex estimator, we develop a novel DC (difference of convex function) programming algorithm that starts with the convex M-estimator and then successively refines the solution till convergence. Empirical experiments demonstrate consistent superiority of the non-convex estimator over the convex one.

Key words: Markov Model, DC-programming, Non-convex Optimization, Rank Constrained Likelihood

1. Introduction

In engineering and management applications, one often has to collect data from unknown systems, learn their transition functions, and learn to make predictions and decisions. A critical precursor of decision making is to model the system from data. We study how to learn an unknown Markov
model of the system from its state-transition trajectories. When the system admits a large number of states, recovering the full model becomes sample expensive.

In this paper, we focus on Markov processes where the transition matrix has a small rank. The small rank implies that the observed process is governed by a low-dimensional latent process which we cannot see in a straightforward manner. It is a property that is (approximately) satisfied in a wide range of practical systems. Despite the large state space, the low-rank property makes it possible to accurate learning of a full set of transition density functions based on short empirical trajectories.

1.1. Motivating Examples

Practical state-transition processes with a large number of states often exhibit low-rank structures. For example, the sequence of stops made by a taxi turns out to follow a Markov model with approximately low rank structure \cite{Liu2012, Benson2017}. For another example, random walk on a lumpable network has a low-rank transition matrix \cite{Buchholz1994, E2008}. The transition kernel with fast decaying eigenvalues has been also observed in molecular dynamics \cite{Rohrdanz2011}, which can be used to find metastable states, coresets and manifold structures of complicated dynamics \cite{Chodera2007, Coifman2008}.

Low-rank Markov model is also related to dimension reduction for control systems and reinforcement learning. For example, the state aggregation approach for modeling a high-dimensional system can be viewed as a low-rank approximation approach \cite{Bertsekas1995, Bertsekas1995, Singh1995}. In state aggregation, one assumes that there exists a latent stochastic process \(\{z_t\} \subset [r]\) such that \(P(s_{t+1} \mid s_t) = \sum_z P(z_t = z \mid s_t)P(s_{t+1} \mid z_t = z)\), which is equivalent to a factorization model of the transition kernel \(P\). In the context of reinforcement learning, the nonnegative factorization model was referred to as the generalized to the rich observations model \cite{Azizzadenesheli2016}. The low-rank structure allows us to model and optimize the system using significantly fewer observations and less computation. Effective methods for estimating the low-rank Markov model would pave the way to better understanding of process data and more efficient decision making.
1.2. Our approach

We propose to estimate the low-rank Markov model based on an empirical trajectory of states, whose length is only proportional to the total number of states. We propose two approaches based on the maximum likelihood principle and low-rank optimization. The first approach uses a convex nuclear-norm regularizer to enforce the low-rank structure and a polyhedral constraint to ensure that optimization is over all probabilistic matrix. The second approach is to solve a rank-constrained optimization problem using difference-of-convex (DC) programming. For both approaches, we provide statistical upper bounds for the Kullback-Leibler (KL) divergence between the estimator and the true transition matrix as well as the $\ell_2$ risk. We also provide a information-theoretic lower bound to show that the proposed estimators are nearly rate-optimal. Note that low-rank estimation of Markov model was considered in Zhang and Wang (2017) where a spectral method with total variation bound is given. In comparison, the novelty of our methods lies in the use of maximum likelihood principle and low-rank optimization, which allows us to obtain the first and sharpest KL divergence bound for learning low-rank Markov models.

Our second approach involves solving a rank constraint optimization problem over probabilistic matrices, which is a refinement of the convex nuclear-norm approach. Due to the non-convex rank constraint, the optimization problem is difficult - to the best of our knowledge, there is no efficient approach that directly solves the rank-constraint problem. In this paper, we develop a penalty approach to relax the rank constraint and transform the original problem into a DC (difference of convex functions) programming one. Furthermore, we develop a particular DC algorithm to solve the problem by initiating at the solution to the convex problem and successively refining the solution through solving a sequence of inner subproblems. Each subroutine is based on the multi-block alternating direction method of multipliers (ADMM). Empirical experiments show that the successive refinements through DC programming does improve the learning quality. As a byproduct of this research, we develop a new class of DC algorithms and a unified convergence analysis for solving non-convex non-smooth problems, which were not available in the literature to our best knowledge.
1.3. Contributions and paper outline

The paper provides a full set of solutions for learning low-rank Markov models. The main contributions are: (1) We develop statistical methods for learning low-rank Markov model with rate-optimal Kullback-Leibler divergence guarantee for the first time; (2) We develop low-rank optimization methods that are tailored to the computation problems for nuclear-norm regularized and rank-constrained M-estimation; (3) A byproduct is a generalized DC algorithm that applies to nonsmooth nonconvex optimization with convergence guarantee.

The rest of the paper is organized as follows. Section 2 surveys related literature. Section 3 proposes two maximum likelihood estimators based on low-rank optimization and establishes their statistical properties. Section 4 develops computation methods and establishes convergence of the methods. Section 5 presents the results of our numerical experiments.

2. Related literature

Model reduction for complicated systems has a long history. It traces back to variable-resolution dynamic programming (Moore 1991) and state aggregation for decision process (Sutton and Barto 1998). In the case of Markov process, (Deng et al. 2011, Deng and Huang 2012) considered low-rank reduction of Markov models with explicitly known transition probability matrix, but not the estimation of the reduced models.

Low-rank matrix approximation has been proved powerful in analysis of large-scale panel data, with numerous applications including network analysis (E et al. 2008), community detection (Newman 2013), ranking (Negahban et al. 2016), product recommendation (Keshavan et al. 2010) and many more. The main goal is to impute corrupted or missing entries of a large data matrix. Statistical theory and computation methods are well understood in the settings where a low-rank signal matrix is corrupted with independent Gaussian noise or its entries are missed independently.

In contrast, our problem is to estimate the transition density functions from dependent state trajectories, where statistical theory and efficient methods are under-developed. When the Markov model has rank 1, it becomes an independent process. In this case, our problem reduces to estimation of a discrete distribution from independent samples (Steinhaus 1957, Lehmann and Casella 1954).
For a rank-2 transition matrix, Huang et al. (2016) proposed an estimation method using a small number of independent samples. For estimation of general low-rank Markov models, the closest work to ours is Zhang and Wang (2017), in which a spectral method via truncated singular value decomposition was introduced and the upper and lower error bounds in terms of total variation were established. Yang et al. (2017) developed an online stochastic gradient method for computing the leading singular space of a transition matrix from random walk data. To our best knowledge, none of the existing works has analyzed efficient recovery of the Markov model with Kullback-Leiber divergence guarantee.

On the optimization side, we adopt DC programming to handle the rank constraint and replace it with the difference of two convex functions. DC programming was first introduced by Pham Dinh and Le Thi (1997) and has become a prominent tool for handling a class of nonconvex optimization problems (see also Pham Dinh and Le Thi (2005), Le Thi et al. (2012, 2017), Le Thi and Pham Dinh (2018)). In particular, Van Dinh et al. (2015) and Wen et al. (2017) considered the majorized DC algorithm, which motivated the particular optimization method developed in this paper. However, both Van Dinh et al. (2015) and Wen et al. (2017) used the majorization technique with restricted choices of majorants, and neither considered the introduction of the indefinite proximal terms. In addition, Wen et al. (2017) further assumes the smooth part in the objective to be convex. In comparison with the existing methods, our DC programming method applies to nonsmooth problems and is compatible with a more flexible and possibly indefinite proximal term.

3. Minimax rate-optimal estimation of low-rank Markov chains

Consider an ergodic Markov chain $\mathcal{X} = \{X_0, X_1, \ldots, X_n\}$ on $p$ states $\mathcal{S} = \{s_j\}_{j=1}^p$ with the transition probability matrix $P \in \mathbb{R}^{p \times p}$ and stationary distribution $\pi$. We quantify the distance between two transition matrices $P$ and $\hat{P}$ in Frobenius norm $\|\hat{P} - P\|_F = \left\{\sum_{i,j=1}^p (\hat{P}_{ij} - P_{ij})^2\right\}^{1/2}$ and Kullback-Leibler divergence $D_{KL}(P, \hat{P}) = \sum_{i,j=1}^p \pi_i P_{ij} \log(P_{ij}/\hat{P}_{ij})$. Suppose that the unknown transition matrix $P$ has a small constant rank $r \ll p$. Our goal is to estimate the transition matrix $P$ via a state trajectory of length $n$. 
3.1. Spectral gap of nonreversible Markov chains

We first introduce the right $L_2$-spectral gap of $P$ [Fill 1991, Jiang et al. 2018], a quantity that measures the convergence speed of the Markov chain $\{X_n\}$ to its invariant distribution $\pi$. This quantity determines the ‘effective’ sample size in statistical rate of our proposed M-estimators. Let $L_2(\pi) := \{h \in \mathbb{R}^p : \sum_{j \in [p]} h_j^2 \pi_j < \infty\}$ be a Hilbert space endowed with the following inner product:

$$\langle h_1, h_2 \rangle_\pi := \sum_{j \in [p]} h_{1j} h_{2j} \pi_j.$$

The matrix $P$ induces a linear operator on $L_2(\pi)$: $h \mapsto Ph$, which we abuse $P$ to denote. Let $P^*$ be the adjoint operator of $P$ with respect to $L_2(\pi)$:

$$P^* = \text{Diag}(\pi)^{-1} P^\top \text{Diag}(\pi).$$

Note that the following four statements are equivalent: (a) $P$ is self-adjoint; (b) $P^* = P$; (c) the detailed balance condition holds: $\pi_i P_{ij} = \pi_j P_{ji}$; (d) the Markov chain is reversible. In our analysis, we do not require the Markov chain to be reversible. We therefore introduce the additive reversibilization of $P$ that is defined to be $(P + P^*)/2$, which is a self-adjoint operator on $L_2(\pi)$ and has the largest eigenvalue as 1. The right spectral gap of $P$ is defined as follows:

**Definition 1 (Right $L_2$-spectral gap).** We say that the right $L_2$-spectral gap of $P$ is $1 - \rho_+$ if

$$\rho_+ := \sup_{\langle h, 1 \rangle_\pi = 0, \langle h, h \rangle_\pi = 1} \frac{1}{2} \langle (P + P^*)h, h \rangle_\pi < 1,$$

where 1 in $\langle h, 1 \rangle$ refers to the all-one $p$-dimensional vector.

3.2. Estimation methods and statistical results

Now we are in position to present our methods and statistical results. Given the trajectory $\{X_1, \ldots, X_n\}$, we count the number of times that the state $s_i$ transitions to $s_j$:

$$n_{ij} := |\{1 \leq k \leq n \mid X_{k-1} = s_i, X_k = s_j\}|.$$
Let $n_i := \sum_{j=1}^p n_{ij}$ for $i = 1, \ldots, p$ and $n := \sum_{i=1}^p n_i$. The averaged negative log-likelihood function of $P$ based on the state-transition trajectory $\{x_0, \ldots, x_n\}$ is

$$\ell_n(P) := -\frac{1}{n} \sum_{k=1}^n \log((P, X_k)) = -\frac{1}{n} \sum_{i=1}^p \sum_{j=1}^p n_{ij} \log(P_{ij}), \quad (1)$$

where $X_k := e_i e_j^\top \in \mathbb{R}^{p \times p}$ if $x_k = s_i$ and $x_{k+1} = s_j$. We first impose the following assumptions on $P$ and $\pi$.

**Assumption 1.** (i) $\text{rank}(P) = r$; (ii) There exist some positive constants $\alpha, \beta > 0$ such that $\alpha/p \leq P_{jk} \leq \beta/p$ for all $1 \leq j,k \leq p$; (iii) $\pi_j \leq \beta/p$ for all $1 \leq j \leq p$.

**Remark 1.** The entrywise bounds on $P$ and $\pi$ are for technical convenience and may not be necessary in practice. Specifically, the entry-wise upper and lower bounds $\alpha, \beta$ of $P$ ensure that (i) the gradient of the log-likelihood $\nabla \ell_n(P)$ is well controlled and exhibits exponential concentration around its population mean (see (EC.1) for the reason we need $\alpha$ there); (ii) $\ell_n(Q)$ enjoys restricted strong convexity around $P$ as characterized in Lemma 3 (see (EC.5) for the reason we need $\beta$ there); (iii) the converter between the $\ell_2$-risk $\|\hat{P} - P\|_F$ ($\|\hat{P}' - P\|_F$ resp.) and KL-divergence $D_{KL}(P, \hat{P})$ ($D_{KL}(P, \hat{P}')$ resp.) depends on $\alpha$ and $\beta$, as per (EC.14). The entry-wise upper and lower bounds are common in statistical analysis of count data, e.g., Poisson matrix completion (Cao and Xie 2016, Equation (10)), Poisson sparse regression (Jiang et al. 2015, Assumption 2.1), Point autoregressive model (Hall et al. 2016, Definition of $A_s$), etc.

Next we propose and analyze a nuclear-norm regularized maximum likelihood estimator (MLE) of $P$ that is defined as follows:

$$\hat{P} := \arg\min Q \in \mathbb{R}^{p \times p} \ell_n(Q) + \lambda \|Q\|_* \quad \text{s.t.} \quad Q1_p = 1_p, \quad \alpha/p \leq Q_{ij} \leq \beta/p, \quad \forall 1 \leq i,j \leq p, \quad (2)$$

where $\lambda > 0$ is a tuning parameter. Our first theorem shows that with an appropriate choice of $\lambda$, $\hat{P}$ exhibits sharp statistical accuracy.
Theorem 1 (Statistical guarantee for the nuclear-norm regularized estimator).

Suppose that the initial state $X_0$ is drawn from the stationary distribution $\pi$, that Assumption 7 holds, and that $n > p \log p/(1 - \rho_+).$ For any $\xi > 0$, choose

$$\lambda = \left\{\frac{C_1 \xi^2 p \log p}{(1 - \rho_+)n} \right\}^{1/2} + \frac{C_2 \xi p \log p}{n},$$

where $C_1$ and $C_2$ depend only on $\alpha$ and $\beta$. Then there exist universal constants $C_3, C_4 > 0$, depending only on $\alpha$ and $\beta$, such that with probability at least $1 - C_3 \exp(-\xi) - 3p^{-\xi-1}$, we have that

$$\|\hat{P} - P\|_F \leq C_4 \xi \left\{\frac{rp \log p}{(1 - \rho_+)n}\right\}^{1/2} \quad \text{and} \quad D_{KL}(P, \hat{P}) \leq \frac{C_4^2 \xi^2 \beta^2}{\alpha^2} \frac{rp \log p}{(1 - \rho_+)n}.$$

Remark 2. Theorem 1 suggests that the ‘effective’ sample size of learning the Markov model is $n(1 - \rho_+)$, where the discount factor is the spectral gap of the true Markov kernel. When $\rho_+ = 0$, the Markov model has rank 1 and our result reduces to the typical results under independent sampling scheme.

Remark 3. When $r = 1$, $P$ can be written as $1v^\top$ for some vector $v \in \mathbb{R}^p$, and then estimating $P$ essentially reduces to estimating a discrete distribution from multinomial count data. Our upper bound in Theorem 1 nearly matches (up to a log factor) the classical results of discrete distribution estimation $\ell_2$ risks (see, e.g., Lehmann and Casella (2006, Pg. 349)).

Then we move on to a second approach – using rank-constrained MLE to estimate $P$:

$$\hat{P}^r := \arg\min \ell_n(Q)$$

$$\text{s.t. } Q1_p = 1_p, \quad \alpha/p \leq Q_{ij} \leq \beta/p, \quad \forall 1 \leq i, j \leq p, \quad \text{rank}(Q) \leq r. \quad (3)$$

In contrast to $\hat{P}$, the rank-constrained MLE $\hat{P}^r$ enforces the prior knowledge “$P$ is low-rank” exactly without inducing any additional bias. It requires solving a non-convex and non-smooth optimization problem, to which we will provide a solution based on DC programming in Section 4.2. Here we first present its statistical guarantee.
Theorem 2 (Statistical guarantee for the rank-constrained estimator). Suppose that Assumption \( \mathbb{A} \) holds and that \( n > p \log p / (1 - \rho_+) \). There exist \( C_1, C_2 > 0 \), depending only on \( \alpha \) and \( \beta \), such that for any \( \xi > 0 \), we have with probability at least \( 1 - C_1 \exp(-\xi) - 3^{-\xi} \) that

\[
\| \hat{P} - P \|_F \leq C_2 \xi \left( \frac{rp \log p}{(1 - \rho_+) n} \right)^{1/2} \quad \text{and} \quad D_{KL}(P, \hat{P}) \leq \frac{C_2^2 \xi^2 \beta^2}{\alpha^2} \frac{rp \log p}{(1 - \rho_+) n}.
\]

Remark 4. The proof of the rank constrained method requires fewer inequality steps and is more straightforward than the that of the nuclear method. Although our upper bounds of the nuclear norm regularized method and the rank constrained one have the same rate (Theorems 1 and 2), the difference of their proofs may implicitly suggest the advantage of the rank constrained method in the constant, as further illustrated by our numerical studies.

To assess the quality of the established statistical guarantee, we further provide a lower bound result below. It shows that when \( (1 - \rho_+), \alpha, \beta \) are constants, both estimators \( \hat{P} \) and \( \hat{P}_r \) are rate-optimal up to a logarithmic factor. Informally speaking, they are not improvable for estimating the class of rank-\( r \) Markov chains.

Theorem 3 (Minimax error lower bound for estimating low-rank Markov models).

Consider the following set of low-rank transition matrices

\[
\Theta := \{ P : P \geq 0, P 1_p = 1_p, \text{rank}(P) \leq r \}.
\]

There exist universal constants \( c, C > 0 \) such that when \( n \geq Cpr \), we have that

\[
\inf_{\hat{P}} \sup_{P \in \Theta} \mathbb{E}\{ D_{KL}(P, \hat{P}) \} \geq c \frac{rp}{n} \quad \text{and} \quad \inf_{\hat{P}} \sup_{P \in \Theta} \mathbb{E}\| \hat{P} - P \|_F^2 \geq c \frac{rp}{n}.
\]

In addition to the full transition matrix \( P \), the leading left and right singular subspaces of \( P \), say \( U, V \in \mathbb{R}^{p \times r} \), also play important roles in Markov chain analysis. For example, by performing \( k \)-means on the reliable estimators of \( U \) or \( V \) for a state aggregatable Markov chain, one can achieve good performance of state aggregation (Zhang and Wang 2017). Based on the previous results, one can further establish the error bounds on singular subspace estimation for Markov transition matrix.
Theorem 4. Under the setting of Theorem 1, suppose the left and right singular subspaces of \( \hat{P} \) are \( \hat{U} \in \mathbb{R}^{p \times r} \) and \( \hat{V} \in \mathbb{R}^{p \times r} \) respectively. Then there exists a constant \( C \), depending only on \( \alpha \) and \( \beta \), such that for any \( \xi > 0 \), one has

\[
\max(\| \sin \Theta(\hat{U}, U) \|^2_F, \| \sin \Theta(\hat{V}, V) \|^2_F) \leq \min \left\{ \frac{C \xi^2 pr \log p}{(1 - \rho_+) n \sigma_r^2(P), r} \right\}
\]

with probability at least \( 1 - K \exp(-\xi) - 3p^{-(\xi - 1)} \). Here, \( \sigma_r(P) \) is the \( r \)-th largest singular value of \( P \) and \( \| \sin \Theta(\hat{U}, U) \|_F := (r - \| \hat{U}^\top U \|_F^2)^{1/2} \) is the Frobenius norm \( \sin \Theta \) distance between \( \hat{U} \) and \( U \).

3.3. Proof outline of Theorems 1, 2

In this section, we elucidate the roadmap to Theorems 1 and 2. Complete proofs are deferred to the supplementary materials. We mainly focus on Theorem 1 for the nuclear-norm penalized MLE \( \hat{P} \), as Theorem 2 uses similar ideas.

We first show in the forthcoming Lemma 1 that when the regularization parameter \( \lambda \) is sufficiently large, the statistical error \( \hat{\Delta} := \hat{P} - P \) falls in a restricted nuclear-norm cone. This cone structure is crucial to establishing strong statistical guarantee for estimation of low-rank matrices with high-dimensional scaling (Negahban and Wainwright 2011). Define a linear subspace \( \mathcal{N} \) by

\[
\mathcal{N} := \left\{ Q : \sum_{k=1}^p Q_{jk} = 0, \forall j = 1, \ldots, p \right\}
\]

and denote the corresponding projection operator by \( \Pi_\mathcal{N} \). In other words, for any \( Q \in \mathcal{N} \) and any \( j = 1, \ldots, p \), the summation of all the entries in the \( j \)-th row of \( Q \) equals zero. One can verify that for any \( Q \in \mathbb{R}^{p \times p} \), \( \Pi_\mathcal{N}(Q) = Q - Q11^\top / p \). Let \( P = UDV^\top \) be the SVD of \( P \), where \( U, V \in \mathbb{R}^{p \times r} \) are orthonormal and the diagonals of \( D \) are in the non-increasing order. Define

\[
\mathcal{M} := \{ Q \in \mathbb{R}^{p \times p} \mid \text{row}(Q) \subseteq \text{col}(V), \text{col}(Q) \subseteq \text{col}(U) \},
\]

\[
\mathcal{M}^\perp := \{ Q \in \mathbb{R}^{p \times p} \mid \text{row}(Q) \perp \text{col}(V), \text{col}(Q) \perp \text{col}(U) \},
\]
where \( \text{col}(\cdot) \) and \( \text{row}(\cdot) \) denote the column space and row space respectively. We can write any \( \Delta \in \mathbb{R}^{p \times p} \) as
\[
\Delta = [U, U^\perp] \begin{bmatrix} \Gamma_{11} & \Gamma_{12} \\ \Gamma_{21} & \Gamma_{22} \end{bmatrix} [V, V^\perp]^T.
\]
Define \( \Delta_W \) as the projection of \( \Delta \) onto any Hilbert space \( W \subseteq \mathbb{R}^{p \times p} \). Then,
\[
\Delta_M = U\Gamma_{11}V^\top, \quad \Delta_M^\perp = U^\perp\Gamma_{22}(V^\perp)^\top, \quad \Delta_M = [U, U^\perp] \begin{bmatrix} \Gamma_{11} & \Gamma_{12} \\ \Gamma_{21} & 0 \end{bmatrix} [V, V^\perp]^T.
\]

The lemma below shows that \( \hat{\Delta} := \hat{P} - P \) falls in a nuclear-norm cone if \( \lambda \) is sufficiently large.

**Lemma 1.** If \( \lambda \geq 2\|\Pi_N(\nabla \ell_n(P))\|_2 \) in (2), then we have that
\[
\|\hat{\Delta}_M^\perp\|_* \leq 3\|\hat{\Delta}_M\|_* + 4\|P_M^\perp\|_*.
\]

In particular, when \( P \in \mathcal{M} \), \( \|P_M^\perp\|_* = 0 \) and
\[
\|\hat{\Delta}\|_* \leq \|\Delta_M^\perp\|_* + \|\Delta_M\|_* \leq 4\|\hat{\Delta}_M\|_* \leq 4(2r)^{1/2}\|\hat{\Delta}\|_F.
\]

Lemma 1 implies that the converting factor between the nuclear and Frobenius norms of \( \hat{\Delta} \) is merely \( 4(2r)^{1/2} \) when \( P \in \mathcal{M} \), which is much smaller than the worst-case factor \( p^{1/2} \) between nuclear and Frobenius norms of general \( p \)-by-\( p \) matrices. This property of \( \hat{\Delta} \) is one cornerstone for establishing Theorem 1 (see (EC.12) for details).

**Remark 5.** In Lemma 3, it holds with high probability that the loss function \( \ell_n(P + \Delta) \) is strongly convex with respect to \( \Delta \) if \( \Delta \) satisfies (5). Combining this with Lemma 1 one can bound \( \|\hat{\Delta}\|_F \) by \( \|\ell_n(\hat{P}) - \ell_n(P)\| \), which motivates the key step (EC.12) in the proof of Theorem 1.

Next, we derive the order of \( \|\Pi_N(\nabla \ell_n(P))\|_2 \) to determine the order of \( \lambda \) that ensures the condition of Lemma 1 to hold.

**Lemma 2.** Under Assumption 1 there exist \( C_1, C_2 > 0 \), depending only on \( \alpha \) and \( \beta \), such that for any \( \xi > 1 \),
\[
P\left\{ \|\Pi_N(\nabla \ell_n(P))\|_2 \geq \left( \frac{C_1 \xi^2 p \log p}{1 - \rho_+} \right)^{1/2} + \frac{C_2 \xi p \log p}{n} \right\} \leq 3p^{-(\xi-1)}.
\]
Remark 6. There are two main probabilistic tools we use to develop this lemma. One is the matrix Freedman inequality (Tropp 2011, Corollary 1.3) that characterizes concentration behavior of a matrix martingale (See (EC.2) for details); the other one is an variant of Bernstein’s inequality for general Markov chains (Jiang et al. 2018, Theorem 1.2), which we use to derive an exponential tail bound for the status counts of the Markov chain $X$ (See (EC.3) for details).

For any $R > 0$, define a constraint set $C(\beta, R, \kappa) := \{ \Delta \in \mathbb{R}^{p \times p} : \|\Delta\|_{\max} \leq \beta/p, \|\Delta\|_F \leq R, \|\Delta\|_* \leq \kappa r^{1/2}\|\Delta\|_F \}$. The final ingredient of our statistical analysis is the localized restricted strong convexity (Fan et al. 2018, Negahban and Wainwright 2011) of the loss function $\ell_n(P)$ near $P$. This property allows us to bound the distance in the parameter space by the difference in the objective function value. Define the first-order Taylor remainder term of the negative log-likelihood function $\ell_n(Q)$ around $P$ as

$$
\delta \ell_n(Q; P) := \ell_n(Q) - \ell_n(P) - \nabla \ell_n(P)^\top (Q - P).
$$

Lemma 3. Under Assumption 4, there exist a universal constant $K$ and $C > 0$ that depends only on $\alpha$ and $\beta$, such that for any $\xi > 1$, it holds with probability at least $1 - K \exp(-\xi)$ that for any $\Delta \in \mathcal{C}(\beta, R, \kappa)$,

$$
\delta \ell_n(P + \Delta; P) \geq \frac{\alpha^2}{8 \beta^2} \|\Delta\|_F^2 - 8R \left( \frac{3K \xi}{n} \right)^{1/2} - \frac{8K \xi \alpha^2 \log n}{\beta^2 n} - \frac{C \kappa K R r^{1/2}}{\beta} \left\{ \left( \frac{p \log p}{n(1 - p_+)} \right)^{1/2} + \frac{p \log p}{n} \right\}.
$$

Remark 7. One technical tool we use here is a tail bound for suprema of empirical processes due to Adamczak (2008). Specifically, we apply Adamczak (2008, Theorem 7) to derive a tail bound for $\delta \ell_n(P + \Delta; P)$ that holds uniformly with respect to $\Delta \in \mathcal{C}$. We refer the interested readers to (EC.6) for details.

Theorem 1 then follows immediately after combining Lemmas 1, 2 and 3. As for the rank-constrained MLE $\hat{P}^r$, let $\hat{\Delta}(r) := \hat{P}^r - P$. Note that the rank constraint in (3) implies that $\text{rank}(\hat{\Delta}(r)) \leq 2r$. Thus, $\|\hat{\Delta}(r)\|_* \leq (2r)^{1/2}\|\hat{\Delta}(r)\|_F$ and we can still apply Lemma 3 to bound $\|\hat{\Delta}(r)\|_F$ by $\ell_n(P + \hat{\Delta}(r)) - \ell_n(P)$ to achieve Theorem 2.
4. Computing the Markov models using low-rank optimization

In this section we develop efficient optimization methods to compute the proposed estimators for the low-rank Markov model.

4.1. Optimization methods for the nuclear-norm regularized likelihood problem

We first consider the nuclear-norm regularized likelihood problem (2). It is a special case of the following linearly constrained optimization problem:

\[
\min \{ g(X) + c\|X\|_* | A(X) = b \},
\]

where \( g : \mathbb{R}^{p \times p} \rightarrow (-\infty, +\infty] \) is a closed, convex, but possibly non-smooth function, \( A : \mathbb{R}^{p \times p} \rightarrow \mathbb{R}^m \) is a linear map, \( b \in \mathbb{R}^m \) and \( c > 0 \) are given data. If we take \( \alpha = 0, \beta = 1 \) in problem (2), it becomes a special case of the general problem (7) with \( g(X) = -\ell_n(X) + \delta(X \geq 0) \), \( A(X) = X1_p, b = 1_p \), and \( \delta(\cdot) \) being the indicator function.

Despite its convexity, problem (7) is highly nontrivial due to the nonsmoothness of \( g \) and the presence of the nuclear norm regularizer. Here, we propose to solve it via the dual approach. The dual of problem (7) is

\[
\min g^*(-\Xi) - \langle b, y \rangle \\
\text{s.t.} \quad \Xi + A^*(y) + S = 0, \quad \|S\|_2 \leq c,
\]

where \( \| \cdot \|_2 \) denotes the spectral norm, and \( g^* \) is the conjugate function of \( g \) given by

\[
g^*(\Xi) = \sum_{(i,j) \in \Omega} \frac{n_{ij}}{n}(\log \frac{n_{ij}}{n} - 1 - \log(-\Xi_{ij})) + \delta(\Xi \leq 0) \quad \forall \Xi \in \mathbb{R}^{p \times p},
\]

where \( \Omega = \{(i, j) \mid n_{ij} \neq 0\} \) and \( \overline{\Omega} = \{(i, j) \mid n_{ij} = 0\} \). Given \( \sigma > 0 \), the augmented Lagrangian function \( L_\sigma \) associated with (8) is

\[
L_\sigma(\Xi, y, S; X) = g^*(-\Xi) - \langle b, y \rangle + \frac{\sigma}{2}\|\Xi + A^*(y) + S + X/\sigma\|^2 - \frac{1}{2\sigma}\|X\|^2.
\]

We consider popular ADMM type methods for solving problem (8) (A comprehensive numerical study has been conducted in [Li et al. 2016b] and justifies our procedure). Since there are three
separable blocks in (8) (namely $\Xi$, $y$, and $S$), the direct extended ADMM is not applicable. Indeed, it has been shown in (Chen et al. 2016) that the direct extended ADMM for multi-block convex minimization problem is not necessarily convergent. Fortunately, the functions corresponding to block $y$ in the objective of (8) is linear. Thus we can apply the multi-block symmetric Gauss-Sediel based ADMM (sGS-ADMM) (Li et al. 2016b). In literature (Chen et al. 2017, Ferreira et al. 2017, Lam et al. 2018, Li et al. 2016b, Wang and Zou 2018), extensive numerical experiments demonstrate that sGS-ADMM is not only convergent but also faster than the directly extended multi-block ADMM and its many other variants. Specifically, the algorithmic framework of sGS-ADMM for solving (8) is presented in Algorithm 1.

Algorithm 1: An sGS-ADMM for solving (8)

**Input:** initial point $(\Xi^0, y^0, S^0, X^0)$, penalty parameter $\sigma > 0$, maximum iteration number $K$, and the step-length $\gamma \in (0, (1 + \sqrt{5})/2)$

for $k = 0$ to $K$ do

$y^{k+\frac{1}{2}} = \text{arg min}_y \mathcal{L}_\sigma(\Xi^k, y, S^k; X^k)$

$\Xi^{k+1} = \text{arg min}_\Xi \mathcal{L}_\sigma(\Xi, y^{k+\frac{1}{2}}, S^k; X^k)$

$y^{k+1} = \text{arg min}_y \mathcal{L}_\sigma(\Xi^{k+1}, y, S^k; X^k)$

$S^{k+1} = \text{arg min}_S \mathcal{L}_\sigma(\Xi^{k+1}, y^{k+1}, S; X^k)$

$X^{k+1} = X^k + \gamma \sigma(\Xi^{k+1} + A^*(y^{k+1}) + S^{k+1})$

end for

Next, we discuss how the $k$-th iteration of Algorithm 1 are performed:

**Computation of** $y^{k+\frac{1}{2}}$ and $y^{k+1}$ Simple calculations show that $y^{k+\frac{1}{2}}$ and $y^{k+1}$ can be obtained by solving the following linear systems:

$$
\begin{align*}
&\begin{cases}
y^{k+\frac{1}{2}} = \frac{1}{\sigma}(AA^*)^{-1}(b - X^k - \sigma(\Xi^k + S^k)), \\
y^{k+1} = \frac{1}{\sigma}(AA^*)^{-1}(b - X^k - \sigma(\Xi^{k+1} + S^k))
\end{cases}
\end{align*}
$$
In our estimation problem, it is not difficult to verify that \( A^* y = py \) for any \( y \in \mathbb{R}^p \). Thanks to this special structure, the above formulas can be further reduced to

\[
y^{k+\frac{1}{2}} = \frac{1}{\sigma p} (b - X^k - \sigma (\Xi^k + S^k)) \quad \text{and} \quad y^{k+1} = \frac{1}{\sigma p} (b - X^k - \sigma (\Xi^{k+1} + S^k)).
\]

**Computation of \( \Xi^{k+1} \)** To compute \( \Xi^{k+1} \), we need to solve the following optimization problem:

\[
\min_{\Xi} \left\{ g^*(-\Xi) + \frac{\sigma}{2} \|\Xi + R^k\|^2 \right\},
\]

where \( R^k \in \mathbb{R}^{p \times p} \) is given. Careful calculations, together with the Moreau identity (Rockafellar 2015, Theorem 31.5), show that

\[
\Xi^{k+1} = \frac{1}{\sigma} [Z^k - \sigma R^k] \quad \text{and} \quad Z^k = \arg \min_Z \left\{ \sigma g(Z) + \frac{1}{2} \|Z - \sigma R^k\|^2 \right\}.
\]

For our estimation problem, i.e., \( g(X) = \ell_n(X) + \delta(X \geq 0) \), it is easy to see that \( Z^k \) admits the following form:

\[
Z_{ij}^k = \frac{\sigma R_{ij}^k + \sigma \sqrt{(R_{ij}^k)^2 + 4n_{ij}/(n\sigma)}}{2} \quad \text{if} \quad (i,j) \in \Omega \quad \text{and} \quad Z_{ij}^k = \sigma \max(R_{ij}^k, 0) \quad \text{if} \quad (i,j) \in \overline{\Omega}.
\]

**Computation of \( S^{k+1} \)** The computation of \( S^{k+1} \) can be simplified as:

\[
S^{k+1} = \arg \min_S \left\{ \frac{\sigma}{2} \|S + \Xi^{k+1} + A^* y^{k+1} + X^k/\sigma\|^2 \mid \|S\|_2 \leq c \right\}.
\]

Let \( W_k := - (\Xi^{k+1} + A^* y^{k+1} + X^k/\sigma) \) admit the following singular value decomposition (SVD)\( W_k = U_k \Sigma_k V_k^T \), where \( U_k \) and \( V_k \) are orthogonal matrices, \( \Sigma_k = \text{Diag}(\alpha_1^k, \ldots, \alpha_p^k) \) is the diagonal matrix of singular values of \( W_k \), with \( \alpha_1^k \geq \ldots \geq \alpha_p^k \geq 0 \). Then, by Lemma 2.1 in (Jiang et al. 2014), we know that

\[
S^{k+1} = U_k \min(\Sigma_k, c) V_k^T,
\]

where \( \min(\Sigma_k, c) = \text{Diag}(\min(\alpha_1^k, c), \ldots, \min(\alpha_p^k, c)) \). We also note that in the implementation, only partial SVD, which is much cheaper than full SVD, is needed as \( r \ll p \).

The nontrivial convergence results of Algorithm 1 can be obtained from Li et al. (2016b). We put the convergence theorem and a sketch of the proof in the supplementary material.
4.2. Optimization methods for the rank-constrained likelihood problem

Next we develop the optimization method for computing the rank-constrained likelihood maximizer from (3). In Subsection 4.2.1 a penalty approach is applied to transform the original intractable rank-constrained problem into a DC programming problem. Then we solve this problem by a proximal DC (PDC) algorithm in Subsection 4.2.2. We also discuss the solver for the subproblems involved in the proximal DC algorithm. Lastly, a unified convergence analysis of a class of majorized indefinite-proximal DC (Majorized iPDC) algorithms is provided in Subsection 4.2.3.

4.2.1. A penalty approach for problem (3) Recall (3) is intractable due to the non-convex rank constraint, we introduce a penalty approach to relax such a constraint, and particularly study the following optimization problem:

\[
\min \left\{ f(X) \mid A(X) = b, \text{rank}(X) \leq r \right\},
\]

where \( f : \mathbb{R}^{p \times p} \rightarrow (-\infty, +\infty] \) is a closed, convex, but possibly non-smooth function and \( r > 0 \) is given data. Comparing to problem (7), the nuclear norm regularizer now is replaced by a rank constraint. Here, we present a penalty approach to handle the rank constraint. Similar to the discussions in Section 4.1, the original rank-constraint maximum likelihood problem (3) can be viewed as a special case of the general model (9).

Given \( X \in \mathbb{R}^{p \times p} \), let \( \sigma_1(X) \geq \cdots \geq \sigma_p(X) \geq 0 \) be the singular values of \( X \). Since rank(\( X \)) \( \leq r \) if and only \( \sigma_{r+1}(X) + \cdots + \sigma_p(X) = \|X\|_* - \|X\|_{(r)} = 0 \), where \( \|X\|_{(r)} = \sum_{i=1}^{r} \sigma_i(X) \) is the Ky Fan \( r \)-norm of \( X \), (9) can be equivalently formulated as

\[
\min \left\{ f(X) \mid \|X\|_* - \|X\|_{(r)} = 0, A(X) = b \right\}.
\]

See also (Gao and Sun 2010, equation (29)). The penalized formulation of problem (9) is

\[
\min \left\{ f(X) + c(\|X\|_* - \|X\|_{(r)}) \mid A(X) = b \right\},
\]

where \( c > 0 \) is a penalty parameter. Since \( \| \cdot \|_{(r)} \) is convex, it is clear that the objective in problem (10) is a difference of two convex functions: \( f(X) + c\|X\|_* \) and \( c\|X\|_{(r)} \), i.e., (10) is a DC program.
Let $X^*_c$ be an optimal solution to the penalized problem (10). The following proposition shows that $X^*_c$ is also the optimizer to (9) when it is low-rank.

**Proposition 1.** If $\text{rank}(X^*_c) \leq r$, then $X^*_c$ is also an optimal solution to the original problem (9).

In practice, one can gradually increase the penalty parameter $c$ to obtain a sufficient low rank solution $X^*_c$. In our numerical experiments, we can obtain solutions with the desired rank with a properly chosen parameter $c$.

**4.2.2. A PDC algorithm for the penalized problem (10)** The central idea of the DC algorithm (Pham Dinh and Le Thi 1997) is as follows: at each iteration, one approximates the concave part of the objective function by its affine majorant, then solves the resulting convex optimization problem. In this subsection, we present a variant of the classic DC algorithm for solving (10). For the execution of the algorithm, we recall that the sub-gradient of Ky Fan $r$-norm at a point $X \in \mathbb{R}^{p \times p}$ (Watson 1993) is

$$\partial \|X\|_{(r)} = \{ U \text{Diag}(q^*) V^T | q^* \in \Delta \},$$

where $U$ and $V$ are the singular vectors of $X$, and $\Delta$ is the optimal solution set of the following problem

$$\max_{q \in \mathbb{R}^p} \left\{ \sum_{i=1}^p \sigma_i(X) q_i | \langle 1_p, q \rangle \leq r, 0 \leq q \leq 1 \right\}.$$

Note that one can efficiently obtain a component of $\partial \|X\|_{(r)}$ by computing the SVD of $X$ and picking up the SVD vectors corresponding to the $r$ largest singular values. After these preparations, we are ready to state the PDC algorithm for problem (10). Different from the classic DC algorithm, an additional proximal term is added to ensure the existence of solutions of subproblems (11) and the convergence of the difference of two consecutive iterations generated by the algorithm. See Theorem 5 and Remark 8 for more details.

We say that $X$ is a critical point of problem (10) if

$$\partial(f(X) + c\|X\|_*, + \delta(A(X) = b)) \cap (c\partial\|X\|_{(r)}) \neq \emptyset.$$ 

Now, we are ready to state the following convergence results for Algorithm 2.
Algorithm 2 A PDC algorithm for solving problem (10)

Given $c > 0$, $\alpha \geq 0$, and the stopping tolerance $\eta$, choose initial point $X^0 \in \mathbb{R}^{p \times p}$. Iterate the following steps for $k = 0, 1, \ldots$:

1. Choose $W_k \in \partial \|X_k\|_r$. Compute

$$X^{k+1} = \arg\min_{X} f(X) + c\left(\|X\|_* - (W_k, X - X^k) - \|X_k\|_r\right) + \frac{\alpha}{2}\|X - X^k\|_F^2$$

subject to $A(X) = b$. (11)

2. If $\|X^{k+1} - X^k\|_F \leq \eta$, stop.

**Theorem 5 (Convergence of Algorithm 2).** Let $\{X^k\}$ be the sequence generated by Algorithm 2 and $\alpha \geq 0$. Then $\{f(X^k) + c(\|X^k\|_* - \|X^k\|_r)\}$ is a non-increasing sequence. If $X^{k+1} = X^k$ for some integer $k \geq 0$, then $X^k$ is a critical point of (10). Otherwise, it holds that

$$(f(X^{k+1}) + c(\|X^{k+1}\|_* - \|X^{k+1}\|_r)) - (f(X^k) + c(\|X^k\|_* - \|X^k\|_r)) \leq -\frac{\alpha}{2}\|X^{k+1} - X^k\|_F^2.$$  

Moreover, any accumulation point of the bounded sequence $\{X^k\}$ is a critical point of problem (10). In addition, if $\alpha > 0$, it holds that $\lim_{k \to \infty} \|X^{k+1} - X^k\|_F = 0$.

**Remark 8 (Adjusting Parameters).** In practice, a small $\alpha > 0$ is suggested to ensure strict decrease of the objective value and convergence of $\{\|X^{k+1} - X^k\|_F\}$; if $f$ is strongly convex, one achieves these nice properties even if $\alpha = 0$ based on the results of Theorem 6. The penalty parameter $c$ can be adaptively adjusted according to the rank of the sequence generated by Algorithm 2.

Next, we discuss how the subproblems (11) can be solved. A careful observation shows that (11) is again a nuclear norm penalized convex optimization problem and is in fact a special case of model (7) but with a new function $g$ as $g(X) = f(X) + \langle W, X \rangle + \frac{\sigma}{2}\|X\|_F^2$. Here, $W \in \mathbb{R}^{p \times p}$ and $\alpha \geq 0$ are given. Hence, Algorithm 1 can be directly used to handle these subproblems efficiently. Moreover, when Algorithm 1 is executed with this new function $g$, in each iteration, only the computation associated with $\Xi$ needs special attention while all the other computations have already been discussed in detail in the previous section. Indeed, given $R \in \mathbb{R}^{p \times p}$ and $\sigma > 0$, in the process of
execution of Algorithm 1 for solving (11) with \( g(X) = \ell_n(X) + \delta(X \geq 0) + \langle W, X \rangle + \frac{\alpha}{2}\|X\|_F^2 \), to perform the update of obtaining \( \Xi \), we need to solve the following minimization problem

\[
Z^* = \arg \min_Z \left\{ \sigma g(Z) + \frac{1}{2}\|Z - \sigma R\|_2^2 \right\}.
\]

Without much difficulty, we observe that \( Z^* \) can be obtained via:

\[
Z_{ij}^* = \begin{cases} 
\frac{(\sigma R_{ij} - W_{ij}) + \sigma \sqrt{(R_{ij} - W_{ij})^2 + 4(\alpha + 1)n_{ij} / (n\sigma)}}{2(\alpha + 1)} & \text{if } (i, j) \in \Omega, \\
\sigma \max(R_{ij} - W_{ij} / \sigma, 0) & \text{if } (i, j) \in \overline{\Omega}.
\end{cases}
\]

### 4.2.3. A unified analysis for the majorized iPDC algorithm

Due to the presence of the proximal term \( \frac{\alpha}{2}\|X - X^k\|_2^2 \) in Algorithm 2, the classical DC analyses cannot be applied directly. Hence, in this subsection, we provide a unified convergence analysis for the majorized indefinite-proximal DC (majorized iPDC) algorithm which includes Algorithm 2 as a special instance. Let \( X \) be a finite-dimensional real Euclidean space endowed with inner product \( \langle \cdot, \cdot \rangle \) and induced norm \( \| \cdot \| \). Consider the following optimization problem

\[
\min_{x \in \mathbb{X}} \theta(x) \triangleq g(x) + p(x) - q(x),
\]

where \( g: \mathbb{X} \to \mathbb{R} \) is a continuously differentiable function (not necessarily convex) with a Lipschitz continuous gradient and Lipschitz modulus \( L_g > 0 \), i.e.,

\[
\|\nabla f(x) - \nabla f(x')\| \leq L_g \|x - x'\| \quad \forall x, x' \in \mathbb{X},
\]

\( p: \mathbb{X} \to (-\infty, +\infty] \) and \( q: \mathbb{X} \to (-\infty, +\infty] \) are two proper closed convex functions. It is not difficult to observe that penalized problem (10) is a special instance of problem (12). For general model (12), one can only expect the DC algorithm converges to a critical point \( \bar{x} \in \mathbb{X} \) of (12) satisfying

\[
(\nabla g(\bar{x}) + \partial p(\bar{x})) \cap \partial q(\bar{x}) \neq \emptyset.
\]

Since \( g \) is continuously differentiable with Lipschitz continuous gradient, there exists a self-adjoint positive semidefinite linear operator \( \mathcal{G} : \mathbb{X} \to \mathbb{X} \) such that for any \( x, x' \in \mathbb{X} \),

\[
g(x) \leq \tilde{g}(x; x') \triangleq g(x') + \langle \nabla g(x'), x - x' \rangle + \frac{1}{2}\|x - x'\|^2_\mathcal{G}.
\]
Algorithm 3 A majorized indefinite-proximal DC algorithm for solving problem (12)

Given initial point $x^0 \in \mathbb{X}$ and stopping tolerance $\eta$, choose a self-adjoint, possibly indefinite, linear operator $\mathcal{T}: \mathbb{X} \rightarrow \mathbb{X}$. Iterate the following steps for $k = 0, 1, \ldots$:

1. Choose $\xi^k \in \partial q(x^k)$. Compute

   $$x^{k+1} \in \arg \min_{x \in \mathbb{X}} \left\{ \hat{\theta}(x; x^k) + \frac{1}{2} \|x - x^k\|_T^2 \right\},$$  

   where $\hat{\theta}(x; x^k) \triangleq \hat{g}(x; x^k) + p(x) - (g(x^k) + \langle x - x^k, \xi^k \rangle)$.

2. If $\|x^{k+1} - x^k\| \leq \eta$, stop.

The majorized iPDC algorithm for solving (12) is presented in Algorithm 3. We further provide the following convergence results.

**Theorem 6 (Convergence of iPDC).** Assume that $\inf_{x \in \mathbb{X}} \theta(x) > -\infty$. Let $\{x^k\}$ be the sequence generated by Algorithm 3. If $x^{k+1} = x^k$ for some $k \geq 0$, then $x^k$ is a critical point of (12). If $\mathcal{G} + 2\mathcal{T} \succeq 0$, then any accumulation point of $\{x^k\}$, if exists, is a critical point of (12). In addition, if $\mathcal{G} + 2\mathcal{T} > 0$, it holds that $\lim_{i \to \infty} \|x^{k+1} - x^k\| = 0$.

The proof of Theorem 6 is provided in the supplementary material.

Here, we shall discuss the roles of linear operators $\mathcal{G}$ and $\mathcal{T}$. The majorization technique of handling the smooth function $g$ and the presence of $\mathcal{G}$ are used to make the subproblems (13) in Algorithm 3 more amenable to efficient computations. As can be observed in Theorem 6, the algorithm is convergent if $\mathcal{G} + 2\mathcal{T} \succeq 0$. This indicates that instead of adding the commonly used positive semidefinite or positive definite proximal terms, we allow $\mathcal{T}$ to be indefinite for better practical performance. Indeed, the computational benefit of using indefinite proximal terms has been observed in [Gao and Sun 2010, Li et al. 2016a]. In fact, the introduction of indefinite proximal terms in the DC algorithm is motivated by these numerical evidence. As far as we know, Theorem 6 provides the first rigorous convergence proof of the introduction of the indefinite proximal terms in the DC algorithms. The presence of $\mathcal{G}$ and $\mathcal{T}$ also helps to guarantee the existence of solutions for the subproblems (13). Since $\mathcal{G} + 2\mathcal{T} \succeq 0$ and $\mathcal{G} \succeq 0$, we have that $2\mathcal{G} + 2\mathcal{T} \succeq 0$, i.e., $\mathcal{G} + \mathcal{T} \succeq 0$. 
(the reverse direction holds when $T \succeq 0$). Hence, $G + 2T \succeq 0$ ($G + 2T > 0$) implies that subproblems (13) are (strongly) convex problems. Meanwhile, the choices of $G$ and $T$ are very much problem dependent. The general principle is that $G + T$ should be as small as possible while $x^{k+1}$ is still relatively easy to compute.

5. Simulation results

In this section, we conduct numerical experiments to assess our theoretical results. We first compare the proposed nuclear-norm regularized estimator and the rank-constrained estimator with previous methods in literature using synthetic data. We then use the rank-constrained method to analyze a public data set of Manhattan taxi trips to reveal citywide traffic patterns. All of our computational results are obtained by running MATLAB (version 9.5) on a windows workstation (8-core, Intel Xeon W-2145 at 3.70GHz, 64 G RAM).

5.1. Experiments with simulated data

We randomly draw the transition matrix $P$ as follows. Let $U_0, V_0 \in \mathbb{R}^{p \times r}$ be random matrices with i.i.d. standard normal entries and let

$$
\tilde{U}_{[i,:]} = (U_0 \circ U_0)_{[i,:]} / \| (U_0)_{[i,:]} \|^2_2 \quad \text{and} \quad \tilde{V}_{[:,j]} = (V_0 \circ V_0)_{[:,j]} / \| (V_0)_{[:,j]} \|^2_2, \quad i = 1, \ldots, p, j = 1, \ldots, r,
$$

where $\circ$ is the Hadamard product and $\tilde{U}_{[i,:]}$ denotes the $i$-th row of $\tilde{U}$. The transition matrix $P$ is obtained via $P = \tilde{U} \tilde{V}^\top$. Then we simulate a Markov chain trajectory of length $n = \text{round}(krp \log(p))$ on $p$ states, $\{X_0, \ldots, X_n\}$, with varying values of $k$.

We compare the performance of four procedures: the nuclear norm penalized MLE, rank-constrained MLE, empirical estimator and spectral estimator. Here, the empirical estimator is the empirical count distribution matrix defined as follows:

$$
\hat{P} = \left(\hat{P}_{ij}\right)_{1 \leq i,j \leq p}, \quad \hat{P}_{ij} = \begin{cases} \frac{\sum_{k=1}^n 1\{X_{k-1} = i, X_k = j\}}{\sum_{k=1}^n 1\{X_{k-1} = i\}}, & \text{when } \sum_{k=1}^n 1\{X_{k-1} = i\} \geq 1; \\ \frac{1}{p}, & \text{when } \sum_{k=1}^n 1\{X_{k-1} = i\} = 0. \end{cases}
$$

The empirical estimator is in fact the unconstrained maximum likelihood estimator without taking into account the low-rank structure. The spectral estimator [Zhang and Wang 2017] Algorithm
1) is based on a truncated SVD. In the implementation of the nuclear norm penalized estimator, the regularization parameter $\lambda$ in (2) is set to be $C\sqrt{p\log p/n}$ with constant $C$ selected by cross-validation. For each method, let $\hat{U}$ and $\hat{V}$ be the leading $r$ left and right singular vectors of the resulting estimator $\hat{P}$. We measure the statistical performance of $\hat{P}$ through three quantities:

$$\eta_F := \|P - \hat{P}\|_F^2, \quad \eta_{KL} := D_{KL}(P, \hat{P}), \quad \text{and} \quad \eta_{UV} := \max\{\|\sin \Theta(\hat{U}, U)\|_F^2, \|\sin \Theta(\hat{V}, V)\|_F^2\}.$$  

We consider the following setting with $p = 1000$, $r = 10$, and $k \in [10, 100]$. The results are plotted in Figure 1. One can observe from these results that for rank-constrained, nuclear norm penalized and spectral methods, $\eta_F, \eta_{KL}$ and $\eta_{UV}$ converge to zero quickly as the number of the state transitions $n$ increases, while the statistical error of the empirical estimator decreases in a much slower rate. Among the three estimators in the zoomed plots (second rows of Figure 1), the rank constrained estimator slightly outperforms the nuclear norm penalized estimator and the spectral estimator. This observation is consistent with our algorithmic design: the nuclear norm minimization procedure is actually the initial step of Algorithm 2; thus the rank-constrained estimator can be seen as a refined version of the nuclear norm regularized estimator.

We also consider the case where the invariant distribution $\pi$ is “imbalanced”, i.e., we construct $P$ such that $\min_{i=1,\ldots,p} \pi_i$ is quite small and the appearance of some states is significantly less than the others. Specifically, given $\gamma_1, \gamma_2 > 0$, we generate a diagonal matrix $D$ with i.i.d. beta-distributed ($\text{Beta}(\gamma_1, \gamma_2)$) diagonal elements. After obtaining $\tilde{U}$ and $\tilde{V}$ in the same way as in the beginning of this subsection, we compute $\tilde{P} = \tilde{U}\tilde{V}^T D$. The ground truth transition matrix $P$ is obtained after a normalization of $\tilde{P}$. Then, we simulate a Markov chain trajectory of length $n = \text{round}(kRp\log(p))$ on $p$ states. In our experiment, we set $p = 1000$, $r = 10$, $k \in [10, 100]$, and $\gamma_1 = \gamma_2 = 0.5$. The detailed results are plotted in Figure 2. As can be seen from the figure, under the imbalanced setting, the rank-constrained, nuclear norm penalized and spectral methods perform much better than the empirical approach in terms of all the three statistical performance measures ($\eta_F$, $\eta_{KL}$ and $\eta_{UV}$). In addition, the rank-constrained estimator exhibits a clear advantage over two other approaches.
Figure 1  The first row compares the rank-constrained estimator, nuclear norm penalized estimator, spectral method, and empirical estimator in terms of $\eta_F = \|P - \hat{P}\|_F^2, \eta_{KL} = D_{KL}(P, \hat{P})$, and $\eta_{UV} = \max\{\|\sin \Theta(\hat{U}, U)\|_F^2, \|\sin \Theta(\hat{V}, V)\|_F^2\}$. The second row provides the zoomed plots of the first row without the empirical estimator. Here, $n = \text{round}(k r p \log p)$ with $p=1,000$, $r=10$ and $k$ ranging from 10 to 100.

Figure 2  The first row compares the rank-constrained estimator, nuclear norm penalized estimator, spectral method, and empirical estimator in terms of $\eta_F = \|P - \hat{P}\|_F^2, \eta_{KL} = D_{KL}(P, \hat{P})$, and $\eta_{UV} = \max\{\|\sin \Theta(\hat{U}, U)\|_F^2, \|\sin \Theta(\hat{V}, V)\|_F^2\}$ with imbalanced invariant distribution. The second row provides the zoomed plots of the first row without the empirical estimator. Here, $n = \text{round}(k r p \log p)$ with $p=1,000$, $r=10$ and $k$ ranging from 10 to 100.
5.2. Experiments with Manhattan Taxi data

In this experiment, we analyze a real dataset of $1.1 \times 10^7$ trip records of NYC Yellow cabs (Link: https://s3.amazonaws.com/nyc-tlc/trip+data/yellow_tripdata_2016-01.csv) in January 2016. Our goal is to partition the Manhattan island into several areas, in each of which the taxi customers share similar destination preference. This can provide guidance for balancing the supply and demand of taxi service and optimizing the allocation of traffic resources.

We discretize the Manhattan island into a fine grid and model each cell of the grid as a state of the Markov chain; each taxi trip can thus be viewed as a state transition of this Markov chain (Yang et al. 2017, Benson et al. 2017, Liu et al. 2012). For stability concerns, our model ignores the cells that have fewer than 1,000 taxi visits. Given that the traffic dynamics typically vary over time, we fit the MC under three periods of a day, i.e., 06:00 ~ 11:59 (morning), 12:00 ~ 17:59 (afternoon) and 18:00 ~ 23:59 (evening), where the number of the active states $p = 803,999$ and 1,079 respectively. We apply the rank-constrained likelihood approach to obtain the estimator $\hat{P}^r$ of the transition matrix, and then apply $k$-means to the left singular subspaces of $\hat{P}^r$ to classify all the states into several clusters. Figure 3 presents the clustering result with $r = 4$ and $k = 4$ for the three periods of a day.

First of all, we notice that the locations within the same cluster are close with each other in geographical distance. This is non-trivial: we do not have exposure to GPS location in the clustering analysis. This implies that taxi customers in neighboring locations have similar destination preference, which is consistent with common sense. Furthermore, to track the variation of the traffic dynamics over time, Figure 4 visualizes the distribution of the destination choice that is correspondent to the center of the green cluster in the morning, afternoon and evening respectively. We identify the varying popular destinations in different periods of the day and provide corresponding explanations in the following table:
The meta-states compression of Manhattan traffic network via rank-constrained approach with $r = 4$: mornings (left), afternoons (middle) and evenings (right). Each color or symbol represents a meta-state. One can see the day-time state aggregation results differ significantly from that of the evening time.

| Time      | Popular Destinations                                      | Explanation                      |
|-----------|-----------------------------------------------------------|----------------------------------|
| Morning   | New York–Presbyterian Medical Center, 42–59 St. Park Ave, Penn Station | hospitals, workplaces, the train station |
| Afternoon | 66 St. Broadway                                           | lunch, afternoon break, short trips |
| Evening   | Penn Station                                              | go home                           |

6. Conclusion

This paper studies the recovery and state compression of low-rank Markov chains from empirical trajectories via a rank-constrained likelihood approach. We provide statistical upper bounds for the $\ell_2$ risk and Kullback-Leiber divergence between the estimator and the true probability transition matrix for the proposed estimator. Then, a novel DC programming algorithm is developed to
solve the associated rank-constrained optimization problem. The proposed algorithm non-trivially combines several recent optimization techniques, such as the penalty approach, the proximal DC algorithm, and the multi-block sGS-ADMM. We further study a new class of majorized indefinite-proximal DC algorithms for solving general non-convex non-smooth DC programming problems and provide a unified convergence analysis. Experiments on simulated data illustrate the merits of our approach.

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Proofs of Theorems

**EC.1. Proof of Lemma 1**

By the inequality (52) in Lemma 3 in the Appendix of [Negahban and Wainwright (2012)](Negahban2012), we have for any $\Delta \in \mathbb{R}^{p \times p}$,

$$
\|P + \Delta\|_* - \|P\|_* \geq \|\Delta_{\mathcal{M}^\perp}\|_* - \|\Delta_{\mathcal{N}^\perp}\|_* - 2\|P_{\mathcal{M}^\perp}\|_* .
$$

Thus it holds that

$$
\ell_n(P + \Delta) - \ell_n(P) \geq \langle \nabla \ell_n(P), \Delta \rangle = \langle \Pi_{\mathcal{N}}(\nabla \ell_n(P)), \Delta \rangle \geq -\langle \Pi_{\mathcal{N}}(\nabla \ell_n(P)), \Delta \rangle \geq -\frac{\lambda}{2}(\|\Delta_{\mathcal{M}}\|_* + \|\Delta_{\mathcal{N}^\perp}\|_*).
$$

By the optimality of $\hat{P}$, we have

$$
\ell_n(\hat{P}) + \lambda\|\hat{P}\|_* \leq \ell_n(P) + \lambda\|P\|_* .
$$

Therefore,

$$
\lambda(\|\Delta_{\mathcal{M}}\|_* + 2\|P_{\mathcal{M}^\perp}\|_* - \|\Delta_{\mathcal{N}^\perp}\|_* ) \geq \lambda(\|P\|_* - \|\hat{P}\|_* ) \geq -\frac{\lambda}{2}(\|\hat{\Delta}_{\mathcal{M}}\|_* + \|\hat{\Delta}_{\mathcal{N}^\perp}\|_* ),
$$

which further delivers that

$$
\|\hat{\Delta}_{\mathcal{N}^\perp}\|_* \leq 3\|\hat{\Delta}_{\mathcal{M}}\|_* + 4\|P_{\mathcal{M}^\perp}\|_* .
$$

**EC.2. Proof of Lemma 2**

Some algebra yields that

$$
\nabla \ell_n(Q) = \frac{1}{n} \sum_{i=1}^{n} -\frac{X_i}{(Q, X_i)}. \tag{EC.1}
$$

For ease of notation, write $Z_i := -X_i / \langle P, X_i \rangle$. Note that

$$
\mathbb{E}(Z_i | Z_{i-1}) = \mathbb{E}(Z_i | X_{i-1}) = \sum_{j=1}^{p} -\frac{e_{X_{i-1}j}e_j^\top}{P_{X_{i-1},j}}P_{X_{i-1},j} = -e_{X_{i-1}1}1^\top .
$$
Thus \( \|Z_i - \mathbb{E}(Z_i|Z_{i-1})\|_2 \leq p/\alpha + \sqrt{p} =: R < \infty \). Define \( S_k := \sum_{i=1}^k Z_i - \mathbb{E}(Z_i|Z_{i-1}) \), then \( \{S_k\}_{k=1}^n \) is a matrix martingale. In addition,

\[
\mathbb{E}\{(Z_i - \mathbb{E}(Z_i|Z_{i-1}))^T(Z_i - \mathbb{E}(Z_i|Z_{i-1}))\mid \{S_k\}_{k=1}^{i-1}\} = \mathbb{E}\{(Z_i - \mathbb{E}(Z_i|Z_{i-1}))^T(Z_i - \mathbb{E}(Z_i|Z_{i-1}))\mid Z_{i-1}\}
\]

and similarly,

\[
\mathbb{E}\{(Z_i - \mathbb{E}(Z_i|Z_{i-1}))(Z_i - \mathbb{E}(Z_i|Z_{i-1}))^T\mid \{S_k\}_{k=1}^{i-1}\} = \sum_{j=1}^p \frac{e_{j}^T}{P_{X_{i-1},j}} - 11^T =: \mathbf{W}_i^{(1)},
\]

Write \( \|\sum_{i=1}^n \mathbf{W}_i^{(1)}\|_2 \) as \( W_n^{(1)} \), \( \|\sum_{i=1}^n \mathbf{W}_i^{(2)}\|_2 \) as \( W_n^{(2)} \) and \( \max(W_n^{(1)}, W_n^{(2)}) \) as \( W_n \). By the matrix Freedman inequality (Tropp 2011, Corollary 1.3), for any \( t \geq 0 \) and \( \sigma^2 > 0 \),

\[
P(\|S_n\|_2 \geq t, W_n \leq \sigma^2) \leq 2p \exp\left(-\frac{t^2/2}{\sigma^2 + Rt/3}\right). \tag{EC.2}
\]

Now we need to choose an appropriate \( \sigma^2 \) so that \( W_n \leq \sigma^2 \) holds with high probability. Note that \( W_n^{(1)} \leq np(\alpha^{-1} + 1) \) and \( W_n^{(2)} \leq (p^2\alpha^{-1} - p) \sup_{j \in [p]} \sum_{i=1}^n 1_{\{X_i = s_j\}} \). In the following we derive a bound for \( \sup_{j \in [p]} \sum_{i=1}^n 1_{\{X_i = s_j\}} \). For any \( j \in [p] \), by Jiang et al. (2018 Theorem 1.2), which is a variant of Bernstein’s inequality for Markov chains, we have that

\[
P\left\{ \frac{1}{n} \sum_{i=1}^n (1_{\{X_i = s_j\}} - \pi_j) > \epsilon \right\} \leq \exp\left(-\frac{n\epsilon^2}{2(A_1\beta/p + A_2\epsilon)}\right), \tag{EC.3}
\]

where

\[
A_1 = \frac{1 + \max(\rho_+, 0)}{1 - \max(\rho_+, 0)} \quad \text{and} \quad A_2 = \frac{1}{3}1_{\{\rho_+ \leq 0\}} + \frac{5}{1 - \rho_+}1_{\{\rho_+ > 0\}}.
\]

Some algebra yields that for any \( \xi > 0 \),

\[
P\left\{ \frac{1}{n} \sum_{i=1}^n 1_{\{X_i = s_j\}} - \pi_j > \left(\frac{4A_1\xi}{np}\right)^{1/2} + \frac{4A_2\xi}{n}\right\} \leq \exp(-\xi).
\]

By the union bound over \( j \in [p] \),

\[
P\left\{ \sup_{j \in [p]} \frac{1}{n} \sum_{i=1}^n (1_{\{X_i = s_j\}} - \pi_j) > \left(\frac{4A_1\xi \log p}{np}\right)^{1/2} + \frac{4A_2\xi \log p}{n}\right\} \leq p^{-\xi}.
\]
Since $\pi_j \leq \beta/p$ for all $j \in [p]$, we have
\[
P\left\{ \sup_{j \in [p]} \frac{1}{n} \sum_{i=1}^{n} 1_{X_i = s_j} > \frac{\beta}{p} + \left( \frac{4 A_1 \xi \log p}{np} \right)^{1/2} + \frac{4 A_2 \xi \log p}{n} \right\} \leq p^{-(\xi-1)}.
\]
Given that $n \geq cp \log p$ for some universal constant $c > 0$, we can find $C_1 > 0$ that depends on $\alpha, \beta$ such that for any $\xi > 1$,
\[
P\left( \sup_{j \in [p]} \frac{1}{n} \sum_{i=1}^{n} 1_{X_i = s_j} > \frac{C_1 \xi}{p(1-\rho_+)} \right) \leq p^{-(\xi-1)}, \quad \text{(EC.4)}
\]
which further implies that there exists a $C_2 > 0$ depending on $\alpha, \beta$ such that
\[
P\left( W_n > C_2 \xi np \right) \leq p^{-(\xi-1)}.
\]
Now choosing $\sigma^2 = C_2 \xi np/(1-\rho_+)$, we deduce that
\[
P\left( \left\| S_n \right\|_2 \geq \frac{C_2 \xi \log p}{n(1-\rho_+)} \right) \leq 3p^{-(\xi-1)}.
\]
Equivalently,
\[
P\left( \left\| \frac{1}{n} S_n \right\|_2 \geq \left( \frac{C_2 \xi^2 p \log p}{n(1-\rho_+)} \right)^{1/2} + \frac{C_4 \xi p \log p}{n} \right) \leq 3p^{-(\xi-1)}.
\]
Finally, observe that for any $i \in [n]$, $\Pi_N(\mathbb{E}(Z_i|Z_{i-1})) = \Pi_N(-e_{X_i-1}1^T) = 0$. Therefore, $\Pi_N(\nabla \ell_n(P)) = n^{-1}S_n$ and the final conclusion follows.

**EC.3. Proof of Lemma 3**

Given any $\Delta \in C$, it holds that for some $0 \leq v \leq 1$ that
\[
\delta \ell_n(P + \Delta; P) = \frac{1}{2} \text{vec}(\Delta)^T H_n(P + v \Delta) \text{vec}(\Delta) = \frac{1}{2n} \sum_{i=1}^{n} \frac{(X_i, \Delta)^2}{(P + v \Delta, X_i)^2} \geq \frac{1}{2n} \sum_{i=1}^{n} \frac{p^2}{4\beta^2} \langle \Delta, X_i \rangle^2. \quad \text{(EC.5)}
\]
Define
\[
\Gamma_n := \sup_{\Delta \in C(\beta, R, \kappa)} \left| \frac{1}{n} \sum_{i=1}^{n} \langle \Delta, X_i \rangle^2 - \mathbb{E}(\langle \Delta, X_i \rangle^2) \right|.
\]
We first bound the deviation of $\Gamma_r$ from its expectation $\mathbb{E}\Gamma_r$. Note that $\{X_i\}_{i=1}^n$ is a Markov chain on $\mathcal{M} := \{e_je_k^\top\}_{j,k=1}^p$. Here we apply a tail inequality for suprema of unbounded empirical processes due to [Adamczak (2008) Theorem 7]. To apply this result, we need to verify that $\{X_i\}_{i=1}^n$ satisfies the “minorization condition” as stated in Section 3.1 of Adamczak (2008). Below we characterize a specialized version of this condition.

**Condition 1 (Minorized Condition).** We say that a Markov chain $X$ on $S$ satisfies the minorized condition if there exist $\delta > 0$, a set $C \subset S$ and a probability measure $\nu$ on $S$ for which $\forall x \in C\nu(A) \geq \delta \nu(A)$ and $\forall x \in S\exists n \in \mathbb{N}\nu^n(x, C) > 0$.

One can verify that the Markov chain $\{X_i\}_{i=1}^n$ satisfies Condition 1 with $\delta = 1/2$, $C = \{e_1e_2^\top\}$ and $\nu(e_je_k^\top) = P_{jk}1_{\{j=2\}}$ for $j, k \in [p]$.

Now consider a new Markov chain $\{(\tilde{X}, R_i)\}_{i=1}^n$ constructed as follows. Let $\{R_i\}_{i=1}^n$ be i.i.d. Bernoulli random variables with $\mathbb{E}R_1 = \delta$. For any $i \in \{0, \ldots, n-1\}$, at step $i$, if $X_i \notin C$, we sample $\tilde{X}_{i+1}$ according to $\mathbb{P}(\tilde{X}_i, \cdot)$; otherwise, the distribution of $\tilde{X}_i$ depends on $R_i$: if $R_i = 1$, the chain regenerates in the sense that we draw $\tilde{X}_i$ from $\nu$, and if $R_i = 0$, we draw $\tilde{X}_i$ from $(\mathbb{P}(X_i, \cdot) - \delta \nu(\cdot))/(1-\delta)$. One can verify that the sequence $\{\tilde{X}_i\}_{i=1}^n$ has exactly the same distribution as the original Markov chain $\{X_i\}_{i=1}^n$. Define $T_1 := \inf\{n > 0 : R_n = 1\}$ and $T_i+1 := \inf\{n > 0 : R_{T_1} + \ldots + R_{T_i} + T = 1\}$ for $i \geq 0$. Note that $\{T_i\}_{i \geq 0}$ are i.i.d. Geometric random variables with $\mathbb{E}T_1 = 2$ and $\|T_1\|_{\nu_1} \leq 4$. Let $S_0 = -1$, $S_j := T_1 + \ldots + T_j$ and $Y_j := \{\tilde{X}_i\}_{i=S_{j-1}+1}^{S_j}$ for $j \geq 1$. Based on our construction, we deduce that $\{Y_j\}_{j \geq 1}$ are independent. Thus we chop the original Markov chain $\{X_i\}_{i \in [n]}$ into independent sequences. Finally, Adamazak’s bound entails the following asymptotic weak variance

$$\sigma^2 := \sup_{\Delta \in C(\beta, R, \kappa)} \operatorname{Var}\left\{ \sum_{i=S_{1}+1}^{S_2} \langle \Delta, X_i \rangle^2 - \mathbb{E}(\langle \Delta, X_i \rangle^2) \right\}/\mathbb{E}T_2.$$

We have

$$\sigma^2 \leq \sup_{\Delta \in C(\beta, R, \kappa)} \mathbb{E}\left[ \left\{ \sum_{i=S_{1}+1}^{S_2} \langle \Delta, X_i \rangle^2 - \mathbb{E}(\langle \Delta, X_i \rangle^2) \right\}^2 \right]/\mathbb{E}T_2$$

$$= \frac{1}{2} \sup_{\Delta \in C(\beta, R, \kappa)} \sum_{j=1}^{\infty} \mathbb{E}\left[ \left\{ \sum_{i=S_{1}+1}^{S_2} \langle \Delta, X_i \rangle^2 - \mathbb{E}(\langle \Delta, X_i \rangle^2) \right\}^2 1_{\{T_2 = j\}} \right]$$

$$\leq \frac{1}{2} \sum_{j=1}^{\infty} \frac{j^2 R^2 \beta^4}{p^4} \mathbb{P}(T_2 = j) = \frac{R^2 \beta^4 \mathbb{E}(T_2^2)}{2p^4} = \frac{3\beta^4 R^2}{p^4}.$$
By Adamczak (2008) Theorem 7), there exists a universal constant $K$ such that for any $\xi > 0$,

$$\mathbb{P}\left\{ |\Gamma_n - \mathbb{E}\Gamma_n| \geq K\Gamma_n + \frac{R\beta^2}{p^2}\left( \frac{3K\xi}{n} \right)^{1/2} + \frac{64K\xi^2\log n}{np^2} \right\} \leq K\exp(-\xi). \quad \text{(EC.6)}$$

Next, by the symmetrization argument and Ledoux-Talagrand contraction inequality (Ledoux and Talagrand 2013), for $n$ independent and identically distributed Rademacher variables $\{\gamma_i\}_{i=1}^n$,

$$\mathbb{E}\Gamma_n \leq 2\mathbb{E} \sup_{\|\Delta\|_{C(\beta, R, \kappa)} \leq R} \left\| \frac{1}{n} \sum_{i=1}^n \gamma_i \langle \Delta, X_i \rangle^2 \right\| \leq \frac{8\beta}{p} \mathbb{E} \sup_{\|\Delta\|_{C(\beta, R, \kappa)} \leq R} \left\| \frac{1}{n} \sum_{i=1}^n \gamma_i X_i, \Delta \right\| \leq \frac{8\beta}{p} \mathbb{E} \left\| \frac{1}{n} \sum_{i=1}^n \gamma_i X_i \right\|_2,$$

where the last inequality is due to the fact that $\Delta \in C(\beta, R, \kappa)$. Here we apply the matrix Freedman inequality (Tropp 2011 Corollary 1.3) to bound $\mathbb{E}\|n^{-1} \sum_{i=1}^n \gamma_i X_i\|_2$. Define $S_k := \sum_{i=1}^k \gamma_i X_i$. Since $\gamma_i \perp X_i$ and $\gamma_i$ is a Rademacher random variable, $\{S_k\}_{k=1}^n$ is a matrix martingale. In addition,

$$\mathbb{E}(\gamma_i^2 X_{i+1}^\top X_{i+1} | \{S_k\}_{k \leq i}) = \mathbb{E}(X_{i+1}^\top X_{i+1} | \{S_k\}_{k \leq i}) = \sum_{j \in [p]} P_{X_{i,j}} e_j e_j^\top$$

and

$$\mathbb{E}(\gamma_i^2 X_{i+1}^\top X_{i+1} | \{S_k\}_{k \leq i}) = \mathbb{E}(X_{i+1}^\top X_{i+1} | \{S_k\}_{k \leq i}) = \left( \sum_{j \in [p]} P_{X_{i,j}} \right) e_{X_i} e_{X_i}^\top = e_{X_i} e_{X_i}^\top.$$
where $C_2$ is a constant that depends only on $\alpha$ and $\beta$. Therefore,

$$\mathbb{E} \Gamma_r \leq \frac{32C_2(2r)^{1/2}\beta R}{p}\left\{ \left( \frac{\log p}{np(1-\rho_+)} \right)^{1/2} + \frac{\log p}{n} \right\}.$$  \hspace{1cm} (EC.9)

Finally,

$$\mathbb{E}(\Delta, X) = \sum_{1 \leq j, k \leq d} \pi_j P_{jk} \Delta_{jk} \geq \frac{\alpha^2}{p^2} \|\Delta\|_F^2.$$  \hspace{1cm} (EC.10)

Combining all the bounds above, we have for any $\xi > 1$, with probability at least $1 - K \exp(-\xi),$

$$\delta \ell_n(P + \Delta; P) \geq \frac{\alpha^2}{8\beta^2} \|\Delta\|_F^2 - 8R \left( \frac{3K\xi}{n} \right)^{1/2} - \frac{8K\xi^2 \log n}{\beta^2 n} - 4(2r)^{1/2} KC_2 R \left\{ \left( \frac{p\log p}{n(1-\rho_+)} \right)^{1/2} + \frac{p\log p}{n} \right\}.$$  \hspace{1cm} (EC.11)

### EC.4. Proof of Theorem [1]

For a specific $R$ whose value will be determined later, we construct an intermediate estimator

$$\hat{P}_\eta = P + \eta(\hat{P} - P),$$

where $\eta = 1$ if $\|\hat{P} - P\|_F \leq R$ and $\eta = R/\|\hat{P} - P\|_F$ if $\|\hat{P} - P\|_F > R$. Choose

$$\lambda = \left( \frac{C_1\xi^2 p \log p}{1-\rho_+} \right)^{1/2} + \frac{C_2\xi p \log p}{n},$$

where $\xi$ is the same as in Lemma [2]. By Lemmas [3] and [2], it holds with probability at least $1 - K \exp(-\xi) - 3p^{-(\xi-1)},$

$$\frac{\alpha^2}{8\beta^2} \|\hat{\Delta}_\eta\|_F^2 - \frac{R}{8\alpha} \left( \frac{K\xi(2-\alpha)}{n} \right)^{1/2} - \frac{K\xi^2 \log n}{8\beta^2 n} - \frac{KCR}{\beta} \left\{ \left( \frac{p\log p}{n(1-\rho_+)} \right)^{1/2} + \frac{p\log p}{n} \right\}$$

$$\leq \delta \ell_n(\hat{P}_\eta; P) \leq -\langle \Pi_\alpha(\nabla \mathcal{L}_n(P)), \hat{\Delta}_\eta \rangle + \lambda(\|P\|_* - \|\hat{P}_\eta\|_*)$$

$$\leq -(\Pi_\alpha(\nabla \mathcal{L}_n(P)), \hat{\Delta}_\eta) + \lambda\|\hat{\Delta}_\eta\|_* \leq (\|\Pi_\alpha(\nabla \mathcal{L}_n(P))\|_2 + \lambda)\|\hat{\Delta}_\eta\|_* \leq 8\lambda\|\hat{\Delta}_\eta\|_* \leq 8\lambda\sqrt{r}\|\hat{\Delta}_\eta\|_F.$$  \hspace{1cm} (EC.12)

which, given Lemma [2], further implies that there exists a constant $C_3$ depending on $\alpha$ and $\beta$ such that

$$\|\hat{\Delta}_\eta\|_F^2 \leq C_3 \max\left\{ \lambda^2 r, R \left( \frac{\xi}{n} \right)^{1/2}, \xi p \log n, R \left( \frac{r p \log p}{n(1-\rho_+)} \right)^{1/2}, \frac{R p^{1/2} \log p}{n} \right\}.$$  \hspace{1cm} (EC.13)
Letting $R$ be greater than the RHS of the inequality above, we can find $C_4$ depending on $\alpha$ and $\beta$ such that

$$R \geq C_4 \xi \left( \frac{r \log p}{(1 - \rho_+) n} \right)^{1/2} =: R_0.$$  

Choose $R = R_0$. Therefore, $\|\hat{\Delta}_\eta\|_F \leq R$ and $\hat{\Delta}_\eta = \hat{\Delta}$. We can thus reach the conclusion. As to the KL-Divergence, by Zhang and Wang (2017, Lemma 4), we deduce that

$$D_{KL}(\hat{P}, P) = \sum_{j=1}^{p} \pi_j D_{KL}(P_{j}, \hat{P}_{j}) \leq \sum_{j=1}^{p} \beta^2 2\alpha^2 \|P_j - \hat{P}_j\|^2 = \frac{\beta^2}{2\alpha^2} \|\hat{P} - P\|^2_F, \quad (EC.14)$$

from which we attain the conclusion.

**EC.5. Proof of Theorem 2**

Define $\hat{\Delta}(r) := \hat{P}^r - P$. Since rank($P$) $\leq r$ and rank($\hat{P}^r$) $\leq r$, rank($\hat{\Delta}(r)$) $\leq 2r$. Thus $\|\hat{\Delta}(r)\|_F \leq (2r)^{1/2} \|\hat{\Delta}(r)\|_*$. Now we follow the proof strategy of Theorem 1 to establish the statistical error bound for $\hat{P}^r$. Similarly, for a specific $R > 0$ whose value will be determined later, we can construct an intermediate estimator $\hat{P}^r_\eta$ between $\hat{P}^r$ and $P$:

$$\hat{P}^r_\eta = P + \eta(\hat{P}^r - P),$$

where $\eta = 1$ if $\|\hat{P}^r - P\|_F \leq R$ and $\eta = R/\|\hat{P}^r - P\|_F$ if $\|\hat{P}^r - P\|_F > R$. Let $\hat{\Delta}_\eta(r) := \hat{P}^r_\eta - P$. Since $\hat{\Delta}_\eta(r) \in C(\beta, R, \sqrt{2})$, applying Lemma 3 yields that

$$\alpha^2 8\beta^2 \|\hat{\Delta}_\eta(r)\|_F^2 - \frac{R}{8\alpha} \left( \frac{K \xi (2 - \alpha)}{n} \right)^{1/2} - \frac{K \xi \alpha^2 \log n}{8\beta^2 n} - \frac{KCR \sqrt{2}r}{\beta} \left\{ \left( \frac{p \log p}{n(1 - \rho_+)} \right)^{1/2} + \frac{p \log p}{n} \right\} \leq \delta \ell_n(\hat{P}^r_\eta; P) \leq -\langle \Pi_N(\nabla \ell_n(P)), \hat{\Delta}_\eta(r) \rangle \leq \|\Pi_N(\nabla \ell_n(P))\|_2 \|\hat{\Delta}_\eta(r)\|_* \leq \sqrt{2r}\|\Pi_N(\nabla \ell_n(P))\|_2 \|\hat{\Delta}_\eta(r)\|_F, \quad (EC.15)$$

which further implies that there exists $C_1$ depending only on $\alpha$ and $\beta$ such that

$$\|\hat{\Delta}_\eta(r)\|_F^2 \leq C_1 \max \left\{ r\|\Pi_N(\nabla \ell_n(P))\|_2^2, R \left( \frac{\xi}{n} \right)^{1/2}, \frac{\xi \log n}{n}, R \left( \frac{r \log p}{n(1 - \rho_+)} \right)^{1/2}, \frac{R \log p r^{1/2}}{n} \right\}.$$

By a contradiction argument as in the proof of Theorem 1, we can choose an appropriate $R$ large enough such that $\hat{P}^r_\eta = \hat{P}^r$ and attain the conclusion.
EC.6. Proof of Theorem 3

Based on the proof of Theorem 1 in [Zhang and Wang (2017)], one has
\[
\inf_{\hat{P}} \sup_{P \in \bar{\Theta}} \frac{1}{p} \sum_{i=1}^{p} \mathbb{E} \| \hat{P}_i - P_i \|_1 \geq c \min \left( \left( \frac{r^p}{n} \right)^{1/2}, 1 \right),
\]
where \( \bar{\Theta} = \{ P \in \Theta : 1/(2p) \leq P_{ij} \leq 3/(2p) \} \subseteq \Theta \). By the Cauchy–Schwarz inequality,
\[
\sum_{i=1}^{p} \| \hat{P}_i - P_i \|_1 = \sum_{i,j=1}^{p} | \hat{P}_{ij} - P_{ij} | \leq p \left\{ \sum_{i,j=1}^{p} (\hat{P}_{ij} - P_{ij})^2 \right\}^{1/2}.
\]
Thus,
\[
\inf_{\hat{P}} \sup_{P \in \bar{\Theta}} \sum_{i=1}^{p} \| \hat{P}_i - P_i \|_2^2 \geq \left( \inf_{\hat{P}} \sup_{P \in \bar{\Theta}} \sum_{i=1}^{p} \| \hat{P}_i - P_i \|_1 \right)^2 \geq c^2 \left( \frac{r^p}{n} \wedge 1 \right) \geq \frac{c^2 p^r}{n}.
\]
The lower bound for KL divergence essentially follows due to the inequalities between \( \ell_2 \) and KL-divergence for bounded vectors in Lemma 5 of [Zhang and Wang (2017)].

EC.7. Proof of Theorem 4

Let \( \hat{U}_\perp, \hat{V}_\perp \in \mathbb{R}^{p \times (p-r)} \) be the orthogonal complement of \( \hat{U} \) and \( \hat{V} \). Since \( U, V, \hat{U}, \) and \( \hat{V} \) are the leading left and right singular vectors of \( P \) and \( \hat{P} \), we have
\[
\| \hat{P} - P \|_F \geq \| \hat{U}_\perp^\top (\hat{P} - UU^\top P) \|_F = \| \hat{U}_\perp^\top UU^\top P \|_F \geq \| \hat{U}_\perp^\top U \|_F \sigma_r(U^\top P) = \| \Theta(\hat{U}, U) \|_F \sigma_r(P).
\]
Similar argument also applies to \( \| \sin \Theta(\hat{V}, V) \|_F \). Thus,
\[
\max(\| \sin \Theta(\hat{U}, U) \|_F, \| \sin \Theta(\hat{V}, V) \|_F) \leq \min \left( \frac{\| \hat{P} - P \|_F}{\sigma_r(P)}, r^{1/2} \right).
\]
The rest of the proof immediately follows from Theorem 1.

EC.8. Proof of Proposition 2

Since \( \text{rank}(X^*_c) \leq r \), we know that \( X^*_c \) is in fact a feasible solution to the original problem (5) and \( \| X^*_c \|_\ast - \| X^*_c \|_{(r)} = 0 \). Therefore, for any feasible solution \( X \) to (5), it holds that
\[
f(X^*_c) = f(X^*_c) + c(\| X^*_c \|_\ast - \| X^*_c \|_{(r)})
\]
\[
\leq f(X) + c(\| X \|_\ast - \| X \|_{(r)}) = f(X).
\]
This completes the proof of the proposition.
EC.9. Theorem 5 (Convergence of sGS-ADMM) and its proof

**Theorem EC.1.** Suppose that the solution sets of (7) and (8) are nonempty. Let $\{(\Xi^k, y^k, S^k, X^k)\}$ be the sequence generated by Algorithm 1. If $\tau \in (0, (1 + \sqrt{5})/2)$, then the sequence $\{(\Xi^k, y^k, S^k)\}$ converges to an optimal solution of (8) and $\{X^k\}$ converges to an optimal solution of (7).

In order to use (Li et al. 2016b, Theorem 3), we need to write problem (8) as following:

$$\min g^*(-\Xi) - \langle b, y \rangle + \delta(S | \|S\|_2 \leq c)$$

s.t. $\mathcal{F}(\Xi) + A^*_1(y) + \mathcal{G}(S) = 0$,

where $\mathcal{F}, A_1$ and $\mathcal{G}$ are linear operators such that for all $(\Xi, y, S) \in \mathbb{R}^{p \times p} \times \mathbb{R}^n \times \mathbb{R}^{p \times p}$, $\mathcal{F}(\Xi) = \Xi$, $A^*_1(y) = A^*(y)$ and $\mathcal{G}(S) = S$. Clearly, $\mathcal{F} = \mathcal{G} = \mathcal{I}$ where $\mathcal{I} : \mathbb{R}^{p \times p} \rightarrow \mathbb{R}^{p \times p}$ is the identity map. Therefore, we have $A_1A^*_1 > 0$ and $\mathcal{F}\mathcal{F}^* = \mathcal{G}\mathcal{G}^* = \mathcal{I} > 0$. Hence, the assumptions and conditions in (Li et al. 2016b, Theorem 3) are satisfied. The convergence results thus follow directly.

EC.10. Proof of Theorems 4 and 6

We only need to prove Theorem 6 as Theorem 4 is a special incidence. To prove Theorem 6, we first introduce the following lemma.

**Lemma EC.1.** Suppose that $\{x^k\}$ is the sequence generated by Algorithm 3. Then $\theta(x^{k+1}) \leq \theta(x^k) - \frac{1}{2}\|x^{k+1} - x^k\|_\Omega^2 + 2\tau$.

For any $k \geq 0$, by the optimality condition of problem (10) at $x^{k+1}$, we know that there exist $\eta^{k+1} \in \partial p(x^{k+1})$ such that

$$0 = \nabla g(x^k) + (\mathcal{G} + \mathcal{T})(x^{k+1} - x^k) + \eta^{k+1} - \xi^k.$$ 

Then for any $k \geq 0$, we deduce

$$\theta(x^{k+1}) - \theta(x^k) \leq \widetilde{\theta}(x^{k+1}; x^k) - \theta(x^k)$$

$$= p(x^{k+1}) - p(x^k) + \langle x^{k+1} - x^k, \nabla g(x^k) - \xi^k \rangle + \frac{1}{2}\|x^{k+1} - x^k\|_\mathcal{G}^2$$

$$\leq \langle \nabla g(x^k) + \eta^{k+1} - \xi^k, x^{k+1} - x^k \rangle + \frac{1}{2}\|x^{k+1} - x^k\|_\mathcal{G}^2$$

$$= -\frac{1}{2}\|x^{k+1} - x^k\|_\mathcal{G}^2 + 2\tau.$$
This completes the proof of this lemma.

Now we are ready to prove Theorem 6.

From the optimality condition at \( x^{k+1} \), we have that

\[
0 \in \nabla g(x^k) + (\mathcal{G} + \mathcal{T})(x^{k+1} - x^k) + \partial p(x^{k+1}) - \xi^k.
\]

Since \( x^{k+1} = x^k \), this implies that

\[
0 \in \nabla g(x^k) + \partial p(x^k) - \partial q(x^k),
\]

i.e., \( x^k \) is a critical point. Observe that the sequence \( \{\theta(x^k)\} \) is non-increasing since

\[
\theta(x^{k+1}) \leq \hat{\theta}(x^{k+1}; x^k) \leq \hat{\theta}(x^k; x^k) = \theta(x^k), \quad k \geq 0.
\]

Suppose that there exists a subsequence \( \{x^{kj}\} \) that converging to \( \bar{x} \), i.e., one of the accumulation points of \( \{x^k\} \). By Lemma EC.1 and the assumption that \( \mathcal{G} + 2\mathcal{T} \succeq 0 \), we know that for all \( x \in \mathbb{X} \)

\[
\hat{\theta}(x^{kj+1}; x^{kj+1}) = \theta(x^{kj+1})
\]

\[
\leq \theta(x^{kj+1}) \leq \hat{\theta}(x^{kj+1}; x^{kj}) \leq \hat{\theta}(x; x^{kj}).
\]

By letting \( j \to \infty \) in the above inequality, we obtain that

\[
\hat{\theta}(\bar{x}; \bar{x}) \leq \hat{\theta}(x; \bar{x}).
\]

By the optimality condition of \( \hat{\theta}(x; \bar{x}) \), we have that there exists \( \bar{u} \in \partial p(\bar{x}) \) and \( \bar{v} \in \partial q(\bar{x}) \) such that

\[
0 \in \nabla g(\bar{x}) + \bar{u} - \bar{v}
\]

This implies that \( (\nabla g(\bar{x}) + \partial p(\bar{x})) \cap \partial q(\bar{x}) \neq \emptyset \). To establish the rest of this proposition, we obtain from Lemma 1 that

\[
\lim_{t \to +\infty} \frac{1}{2} \sum_{i=0}^{t} \|x^{k+1} - x^k\|_G^2 + 2\mathcal{T}
\]

\[
\leq \liminf_{t \to +\infty} (\theta(x^0) - \theta(x^{k+1})) \leq \theta(x^0) < +\infty,
\]

which implies \( \lim_{t \to +\infty} \|x^{k+1} - x^i\|_G + 2\mathcal{T} = 0 \). The proof of this theorem is thus complete by the positive definiteness of the operator \( \mathcal{G} + 2\mathcal{T} \).