ACTIVE COVARIANCE ESTIMATION BY RANDOM SUB-SAMPLING OF VARIABLES

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ABSTRACT

We study covariance matrix estimation for the case of partially observed random vectors, where different samples contain different subsets of vector coordinates. Each observation is the product of the variable of interest with a \(0 \rightarrow 1\) Bernoulli random variable. We analyze an unbiased covariance estimator under this model, and derive an error bound that reveals relations between the sub-sampling probabilities and the entries of the covariance matrix. We apply our analysis in an active learning framework, where the expected number of observed variables is small compared to the dimension of the vector of interest, and propose a design of optimal sub-sampling probabilities and an active covariance matrix estimation algorithm.

Index Terms — active covariance estimation, random sampling, missing data, graphical models, covariance matrix

1. INTRODUCTION

We study estimation of the covariance matrix of a random vector \(x\) from observations of the form \(y = [\delta_1 x_1, \delta_2 x_2, \cdots, \delta_n x_n]^\top\), where each component \(x_i\) is multiplied by a \(0 \rightarrow 1\) Bernoulli random variable \(\delta_i\). We assume the probabilities \(P(\delta_i = 1) = p_i\) are known, independent of each other, and of \(x\). Partial observations consistent with this model may arise when there are some physical limitations to the observation process (and thus there is missing data) or when the cost of observation needs to be reduced by selecting what to sample (i.e., active learning).

Applications where probabilistic models need to be constructed from observations with missing data include transportation networks [1] and sensor networks [2]. For example, different sensors in the network might have different capabilities, e.g., different reliability or number of samples per hour that can be acquired, and these can be captured by associating different sub-sampling probabilities \(p_i\) to each sensor.

For covariance estimation, or more generally graphical model estimation, active learning approaches have been considered where variables are observed in a sequential and adaptive manner to identify the graphical model with minimal number of observations. Active learning approaches for covariance estimation can be useful in distributed computation environments like sensor networks, where there are acquisition, processing or communication constraints, and there is a need for optimal resource allocation.

One critical difference between missing data and active covariance estimation scenarios is the control over the observation model. In the missing data case, the sub-sampling probabilities are a problem feature that is given or has to be estimated from data, while in active learning problems, the sampling probabilities are a design parameter. The results from this paper can be useful for analysis in the missing data case, as well as for designing active learning algorithms as we will discuss in more detail in Section 5.

In this work we analyze an unbiased covariance matrix estimator under sub-Gaussian assumptions on \(x\). Our main result is an error bound on the Frobenius norm that reveals the relation between number of observations, sub-sampling probabilities and entries of the true covariance matrix. We apply this error bound to the design of sub-sampling probabilities in an active covariance estimation scenario. An interesting conclusion from this work is that when the covariance matrix is approximately low rank, an active covariance estimation approach can perform almost as well as an estimator with complete observations. The paper is organized as follows, in Section 2 we review related work. Sections 3 and 4 introduce the problem and the main results respectively. In Section 5 we show an application of our bounds for optimal design of sampling probabilities for a batch based active covariance estimation algorithm. Proofs are presented in Section 6 and conclusion in Sections 7.

2. RELATED WORK

Lounici [3] studies covariance matrix estimation from missing data when all variables can be observed with the same probability. The focus of [3] is on estimation of approximately low rank covariance matrices with a matrix version of the lasso algorithm. In [4] the empirical covariance matrix under missing data is shown to be indefinite. Most recently Cai and Zhang [5] study the missing completely at random model (MCAR), which assumes arbitrary and unknown missing data probabilities. They show that a modified sample covariance matrix estimator, similar to ours but using the empirical estimation of probabilities \(p_i\), achieves optimal minimax rates in spectral norm for bandable and sparse covariance matrices. Compared to [3, 5], we allow all probabilities to be different and known, and we only study the unbiased sample covariance estimator. Moreover, all of the aforementioned papers consider estimation errors in spectral norm, while we consider errors in Frobenius norm, allowing us to derive error bounds with precise dependences between the entries of the true covariance matrix and the sampling probabilities \(p_i\). These bounds can then be applied to design the sampling distribution in an adaptive manner.

For distributed computing applications, the work of [6] studies covariance estimation from random subspace projections using dense matrices, which are generalized in [7] to sparse projection matrices. The same approach from [7] is used in [8] for memory and complexity reduced PCA. In all these works [6, 8, 7], each measurement is a (possibly sparse) linear combination of a few variables, and even though the designs are random, they have a fixed distribution for all observations.

The work of [9] considers the case when all \(p_i\) are unknown, and uses an unbiased covariance matrix estimator as an input to the graphical lasso algorithm [10] for inverse covariance matrix estimation. Other interesting active learning approaches for graphi-
In this section we present an error analysis of the covariance matrix estimators assuming the target covariance matrix is a linear combination of known covariance matrices, which leads to algorithms and theoretical analysis that are fundamentally different from ours.

3. PROBLEM FORMULATION

3.1. Notation

We denote scalars using regular font, while we use bold for vectors and matrices, e.g., \( a = (a_i) \), and \( A = (a_{ij}) \). The Hadamard product between matrices is defined as \( (A \odot B)_{ij} = a_{ij}b_{ij} \). We use \( || \cdot || \) for entry-wise matrix norms, with \( q = 2 \) corresponding to the Frobenius norm. \( || \cdot || \) denotes \( \ell_2 \) norm or spectral norm when applied to vectors or matrices respectively.

3.2. Unbiased estimation

Consider a random vector \( x \) taking values in \( \mathbb{R}^n \). We observe

\[
y = \delta \odot x,
\]

where \( \delta = (\delta_i) \) is a vector of Bernoulli \( 0 \)-\( 1 \) random variables. The probability of observing the \( i \)-th variable is given by \( P(\delta_i = 1) = p_i \). The vector of probabilities is denoted by \( p = [p_1, \cdots, p_n]^\top \), and \( P = \text{diag}(p) \) is a diagonal matrix. The average number of samples corresponds to \( \mathbb{E}(\sum_{i=1}^n \delta_i) = \sum_{i=1}^n p_i = m \). Given \( y^{(1)}, \ldots, y^{(T)} \), i.i.d. realizations of \( y \), the \( i \)-th variable will be sampled in average \( p_iT \) times, if all \( p_i = 1 \), then \( y = x \), and we have perfect observation of \( x \). We are interested in studying covariance estimation for \( x \) when \( m < n \) and \( 0 < p_i \) for all \( i \). Let \( \mu \) and \( \Sigma \) be the mean and covariance of \( x \), then

\[
\mathbb{E}(y) = \mathbf{P}\mu, \quad \text{Cov}(y) = \Sigma \odot \mathbf{E} + (\mathbf{P} - \mathbf{P}^2) \text{diag}(\mu \mu^\top),
\]

where \( \mathbf{E} = (\xi_{ij}) \) is defined as \( \xi_{ij} = p_i \) and \( \xi_{ij} = p_i p_j \) when \( i \neq j \).

For the rest of the paper we will assume \( \mu = 0 \). Given a set of i.i.d. samples \( \{y^{(k)}\}_{k=1}^T \) of the random vector \( y \), define

\[
\hat{\Sigma} = \frac{1}{T} \sum_{k=1}^T y^{(k)} y^{(k)^\top} \odot \mathbf{E}^\top,
\]

where \( \mathbf{E}^\top \) is the Hadamard (entry-wise) inverse of \( \mathbf{E} \). A simple calculation shows that \( \hat{\Sigma} \) is an unbiased estimator for \( \Sigma \). Indeed, \( \mathbb{E}(\hat{\Sigma}) = \frac{1}{T} \sum_{k=1}^T \mathbb{E}(y^{(k)} y^{(k)^\top} \odot \mathbf{E}^\top) = \Sigma \odot \mathbf{E} \odot \mathbf{E}^\top = \Sigma \). Because \( \mathbf{E}^\top \not= 0 \), the matrix \( \hat{\Sigma} \) might not be positive semi-definite (conditions for \( \hat{\Sigma} \) to be positive semi-definite are given in \( \text{(1)} \)).

4. ESTIMATION ERROR

In this section we present an error analysis of the covariance matrix estimator from \( \text{(2)} \) when \( x \) has sub-Gaussian entries. Sub-Gaussian random variables include Gaussian, Bernoulli and Bounded random variables. For more information see \( \text{[18]} \) and references therein.

**Definition 1 (\text{[18]}).** If \( \mathbb{E}[\exp(z^2/K^2)] \leq 2 \) holds for some \( K > 0 \), we say \( z \) is sub-Gaussian. If \( \mathbb{E}[\exp(|z|/K)] \leq 2 \) holds for some \( K > 0 \), we say \( z \) is sub-exponential.

**Definition 2 (\text{[18]}).** The sub-Gaussian and sub-exponential norms are defined as

\[
||z||_{\psi_2} = \inf\{u > 0 : \mathbb{E}[\exp(|z|^2/u^2)] \leq 2\},
\]

for \( \alpha = 2 \) and \( \alpha = 1 \) respectively.

Sub-Gaussian and sub-exponential random variables, and their norms, are related as follows.

**Proposition 1 (\text{[18]}).** If \( z \) and \( w \) are sub-Gaussian, then \( z^2 \) and \( zw \) are sub-exponential with norms satisfying \( ||z||_{\psi_2} = ||z||_{\psi_1} \), and \( ||zw||_{\psi_1} \leq ||z||_{\psi_2} ||w||_{\psi_2} \).

We have that the following characterization of the product of sub-Gaussian and Bernoulli random variables.

**Lemma 1.** Let \( y_1 = \delta_1 x_1 \) and \( y_2 = \delta_2 x_2 \) be a product of Bernoulli \( \delta_1, \delta_2 \) and sub-Gaussian \( x_1, x_2 \) random variables with Bernoulli probabilities \( p_1 \) and \( p_2 \) respectively, the only dependent variables are \( x_1 \) and \( x_2 \), then

1. \( y_1 \) is sub-Gaussian and \( ||y_1||_{\psi_2} \leq ||x_1||_{\psi_2} \).
2. \( y_1 y_2 \) and \( y_1 y_2 \) are sub-exponential with norms satisfying \( ||y_1 y_2||_{\psi_1} \leq ||x_1||_{\psi_2} ||x_2||_{\psi_2} \).

The proof of Lemma \( \text{[1]} \) can be easily obtained from the definition of sub-Gaussian and sub-exponential norms. We omit it for space considerations. We also define the matrix \( H = (h_{ij}) \), with entries given by

\[
h_{ij} = \begin{cases} \frac{||x_i||_{\psi_1}}{p_i} & i \neq j \\ \frac{1}{p_i} & i = j. \end{cases}
\]

Now we state our main result, whose proof appears in Section\( \text{[6]} \).

**Theorem 1.** Let \( x \) be zero mean random vector in \( \mathbb{R}^n \) with sub-Gaussian entries and norm \( ||x||_{\psi_2} \). Let \( y = \delta \odot x \), where each \( \delta_i \) is a Bernoulli random variable with parameter \( 0 < p_i \leq 1 \), independent of each other and of \( x \). Given i.i.d. realizations \( \{y^{(k)}\}_{k=1}^T \), the estimator from \( \text{(2)} \) satisfies

\[
||\hat{\Sigma} - \Sigma||_q \leq ||H||_q \left\{ \sqrt{\frac{2 \log(n) + \log(\eta)}{T}} \vee \frac{\sqrt{2 \log(n) + \log(\eta)}}{T} \right\} + \gamma,
\]

with probability at least \( 1 - \tilde{\delta} \), where \( \gamma \) is an universal constant. Moreover if \( ||x||_{\psi_2} = \sigma \sqrt{\mathbb{E} x} \) and \( q \geq 2 \), then

\[
||H||_q \leq \frac{2\sigma^2}{\tilde{p}} r(\Sigma)/||\Sigma||,
\]

where \( \tilde{p} = \min_{i} p_i \), and \( r(\Sigma) = \text{tr}(\Sigma)/||\Sigma|| \) is the effective rank.

Theorem \( \text{[1]} \) shows that the estimation error \( ||\hat{\Sigma} - \Sigma||_q \to 0 \) in probability as the number of samples increases. More importantly, our result reveals that the sampling probabilities \( p_i \) are closely related to the sub-exponential norms of the variables \( x, x_1 \) through the matrix \( ||H||_q \). The bound from \( \text{(3)} \) suggests that distributions with smaller effective rank \( \text{[3]} \text{[18]} \) can tolerate a more aggressive sub-sampling factor (smaller \( m \)). This is not surprising since the effective rank \( r(\Sigma) \) is upper bounded by the actual rank, and can be significantly smaller for distributions whose energy concentrates in few principal components. We also note that the ratio \( r(\Sigma)/\tilde{p} \) appears in the bounds of \( \text{[3]} \) as well.
Algorithm 1 Covariance estimation with adaptive sampling

Require: initial distribution $p^{(0)}$, covariance $\Sigma^{(0)} = 0$, budget $1^T p^{(0)} = m$, and batch size $B$.
1: for $t = 0$ to $N - 1$ do
2: Sample $B$ i.i.d. realizations of $y = \delta(p^{(t)}) \circ x$
3: Estimate $\hat{\Sigma}^{(t+1)} = \frac{1}{t+1} \Sigma + \frac{t}{t+1} \hat{\Sigma}^{(t)}$
4: Update $p^{(t+1)}$ by solving (5) with $\hat{\Sigma}^{(t+1)}$ and budget $m$.
5: end for

5. ACTIVE COVARIANCE ESTIMATION

In this section we consider a scenario where we cannot observe (on average) more than $m$ variables at a time, but we have the freedom to choose the sub-sampling probability distribution.

5.1. Sub-sampling distribution for true covariance matrix

Based on the error bound from Theorem 1 we propose designing the sub-sampling distribution by approximately minimizing $\| H \|_2$. Theorem 1 suggests that $p_i$ should be large whenever the sub-Gaussian norm of $x_i$ is large, but also the product $p_i p_j$ should be large when the sub-exponential norm of $x_i x_j$ is large. We assume that $\| x_i \|_2 = \sigma \sqrt{\Sigma x_i}$. The bounds for $h_{ii}$ and $h_{ij}$ from (6) and (7) respectively suggest the approximation $p_i \sim \Sigma x_i$. Given a sampling budget $m$, we estimate the sub-sampling probability vector $p$ by solving the following scaled projection problem

$$\min_{p \geq 0} \frac{1}{2} \| p - \rho \text{diag}(\Sigma)^{\frac{1}{2}} \|_2^2, \quad \text{s.t.} \quad 1^T p = m, \quad 0 \leq p \leq 1.$$  \hspace{0.5cm} (4)

5.2. Sub-sampling distribution for empirical covariance matrix

Since the true covariance matrix is unknown, (4) does not lead to a practical estimator. Instead, we consider a batch-based algorithm that for a given budget $m$, and a starting sub-sampling distribution, it iteratively refines the sub-sampling probability distribution as a function of previous observations. We show the pseudo code for such procedure in Algorithm 2 which can be summarized in the following steps: observation with variable sub-sampling, covariance estimation, and sub-sampling distribution update. At the $t$-th iteration, $B$ i.i.d. realizations are observed according to (4) with sub-sampling probabilities $p^{(t)}$. The covariance estimator is a convex combination of the estimator at the previous iteration, and the estimator for the current batch. Finally, the new covariance matrix estimator is used to update the sub-sampling probabilities as

$$p^{(t)} = \arg \min_{p \geq 0} \frac{1}{2} \| p - \rho \text{diag}(\hat{\Sigma}^{(t)})^{\frac{1}{2}} \|_2^2, \quad \text{s.t.} \quad 1^T p = m, \quad 0 \leq p \leq 1.$$  \hspace{0.5cm} (5)

Proposition 2. Algorithm 2 produces an unbiased estimator for $\Sigma$.

Proof. We will proceed by induction. For the first iteration we have used uniform sampling, thus we have $\mathbb{E}(\hat{\Sigma}^{(1)}) = \Sigma$. Now assume $\mathbb{E}(\hat{\Sigma}^{(t)}) = \Sigma$, then at the $(t + 1)$-th iteration, the covariance of the new data satisfies $\mathbb{E}(\hat{\Sigma}) = \Sigma$, which implies $\mathbb{E}(\hat{\Sigma}^{(t+1)}) = \frac{1}{t+1} \mathbb{E}(\hat{\Sigma}) + \frac{t}{t+1} \mathbb{E}(\hat{\Sigma}^{(t)}) = \Sigma$. \qed

5.3. Numerical evaluation

In this section we evaluate our proposed method using the MNIST [19] dataset, which consists of $28 \times 28$ images of scanned digits from 0 to 9. In our experiments we consider $N = 5851$ images of the digit 8. The vectorized, and mean removed images are denoted by $\{x_i\}_{i=1}^N$ with covariance matrix $C$. We consider estimation of the the covariance matrix of $x_i = x_i + \epsilon/\sqrt{|C|}$, where $\epsilon$ is zero mean Gaussian noise with unit variance, therefore $\Sigma = C + \epsilon/\sqrt{|C|}$.

To draw i.i.d. realizations of $x_i$, we sample images $x_i$ without replacement and add Gaussian noise with variance $\epsilon/\sqrt{|C|}$. The effective rank of $\Sigma$ is controlled by the parameter $\theta$ and satisfies

$$r(\Sigma) = \frac{r(C) + n\theta}{1 + \theta}.$$  \hspace{0.5cm}

We first compare uniform sub-sampling with non uniform sub-sampling for estimation of $\Sigma$ with $\theta = 1/n$. We designed the non uniform sub-sampling distribution using (4) with the true covariance matrix. We report relative errors in Frobenius norm as a function of $T/n$ in Figure 1a. Each point in the plot is an average over 50 independent trials. We observe that when $m = 0.75n$ the non uniform sampling distribution matches closely the performance of the estimator with full data. It is clear that when $m = 0.50n$ and $m = 0.25n$ performance decreases (for uniform and non uniform sampling) as $m$ decreases, and non uniform sampling always out-performs uniform sampling. In Figure 1b we evaluate our active method from Algorithm 2 with batch size $B = 300$. We consider the same scenario as in Figure 1a for $m = 0.5n$ and $m = 0.25n$. The proposed active covariance estimation method quickly learns the optimal sub-sampling distribution, is always better than uniform sampling, and matches the performance of the non uniform sub-sampling method obtained from the true covariance matrix. Finally we show in Figure 1c the same experiment shown in Figure 1b, but now with covariance matrix with parameter $\theta = 10/n$, which changes the effective rank from $r(\Sigma) = 9.08$ with $\theta = 1/n$ to $r(\Sigma) = 17.86$. We observe that the problem becomes more difficult since the estimation errors are larger. There is no major difference between uniform, and non uniform sampling, thus the advantages of the proposed active covariance estimation method are limited. This might be due to various effects including, relative magnitudes of diagonal entries of $\Sigma$, sampling budget $m$, effective rank, and probability update algorithm. Moreover, since the effective rank did not change much (compared with $n$), this experiment suggests the effective rank does not quantify effectively the problem difficulty. Also, a more precise method to update the probabilities $p_i$ might help improving the performance of the active covariance estimation algorithm.

6. PROOF OF THEOREM 1

We first need the following concentration bounds

**Lemma 2.** Under the same assumptions of Theorem 4 for any $\nu > 0$ we have

$$\mathbb{P}(|\hat{\Sigma}_{ij} - \Sigma_{ij}| > \nu) \leq 2 \exp\left\{-c_1 T \min\{\nu^2/h_{ij}^2, \nu/h_{ij}\}\right\},$$  \hspace{0.5cm}

$$\mathbb{P}(|\hat{\Sigma}_{ii} - \Sigma_{ii}| > \nu) \leq 2 \exp\left\{-c_2 T \min\{\nu^2/h_{ii}^2, \nu/h_{ii}\}\right\},$$  \hspace{0.5cm}

for off-diagonal and diagonal entries respectively.

**Proof.** The error events for off-diagonal entries satisfy

$$|\hat{\Sigma}_{ij} - \Sigma_{ij}| > \nu \iff \left| \sum_{k=1}^T (y_i^{(k)} y_j^{(k)} - p_i p_j \Sigma_{ij}) \right| > \nu T p_i p_j.$$  \hspace{0.5cm}
We apply Bernstein’s inequality \[18\] for sums of independent zero mean sub-exponential random variables, which combined with the bound from Lemma \[1\] leads to the desired bound. The proof for diagonal terms follows almost the same procedure.

We also need the following geometric result which we state without proof.

**Lemma 3.** Let \( A = \{ x \in \mathbb{R}^n : \|x\|_1 > c \} \), and \( B_i = \{ x \in \mathbb{R}^n : |x_i| > \alpha_i c \} \), then for all \( c > 0 \), and \( \alpha_i \in (0, 1) \) that satisfy \( \sum_{i=1}^n \alpha_i = 1 \), have that \( A \subset \bigcup_{i=1}^n B_i \).

The proof of Theorem \[1\] starts by bounding the probability of the event \( \| \hat{\Sigma} - \Sigma \|_q > \epsilon \| \Sigma \|_q \). Pick a set of \( \alpha_{ij} \in (0, 1) \) such that \( \sum_{i,j} \alpha_{ij} = 1 \), and apply Lemma \[3\] and the union bound to get

\[
P(\| \hat{\Sigma} - \Sigma \|_q > \epsilon \| \Sigma \|_q) = \mathbb{P}(\sum_{i,j} |\hat{\Sigma}_{ij} - \Sigma_{ij}|^q > \epsilon^q \| \Sigma \|_q^q) \\
\leq \sum_{i,j} \mathbb{P}(\|\hat{\Sigma}_{ij} - \Sigma_{ij}\|_q > \alpha_{ij} \epsilon \| \Sigma \|_q) \\
= \sum_{i,j} \mathbb{P}(\|\hat{\Sigma}_{ij} - \Sigma_{ij}\|_q > \alpha_{ij}^{1/q} \| \Sigma \|_q) \\
\leq \sum_{i=1}^n 2 \exp \left( -c_2 T \min \left( \frac{2^{q/2} \| \Sigma \|_q^2}{\| \hat{\Sigma} \|_q}, \frac{1}{\epsilon \| \Sigma \|_q} \right) \right) + \sum_{i,j=1}^n 2 \exp \left( -c_3 T \min \left( \frac{2^{q/2} \| \Sigma \|_q^2}{\| \hat{\Sigma} \|_q}, \frac{1}{\epsilon \| \Sigma \|_q} \right) \right) 
\]
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