Conformalized matrix completion

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Abstract

Matrix completion aims to estimate missing entries in a data matrix, using the assumption of a low-complexity structure (e.g., low rank) so that imputation is possible. While many effective estimation algorithms exist in the literature, uncertainty quantification for this problem has proved to be challenging, and existing methods are extremely sensitive to model misspecification. In this work, we propose a distribution-free method for predictive inference in the matrix completion problem. Our method adapts the framework of conformal prediction, which provides confidence intervals with guaranteed distribution-free validity in the setting of regression, to the problem of matrix completion. Our resulting method, conformalized matrix completion (cmc), offers provable predictive coverage regardless of the accuracy of the low-rank model. Empirical results on simulated and real data demonstrate that cmc is robust to model misspecification while matching the performance of existing model-based methods when the model is correct.

1 Introduction

Matrix completion, the task of filling in missing entries in a large data matrix, has a wide range of applications such as gene-disease association analysis in bioinformatics (Natarajan and Dhillon, 2014), collaborative filtering in recommender systems (Rennie and Srebro, 2005), and panel data prediction and inference in econometrics (Amjad et al., 2018; Bai and Ng, 2021; Athey et al., 2021). If the underlying signal is assumed to be low-rank, a range of estimation algorithms have been proposed in the literature, including approaches based on convex relaxations of rank (Candes and Plan, 2010; Candès and Tao, 2010; Koltchinskii et al., 2011; Foygel and Srebro, 2011; Negahban and Wainwright, 2012; Yang and Ma, 2022) and nonconvex optimization over the space of low-rank matrices (Keshavan et al., 2010; Jain et al., 2013; Sun and Luo, 2016; Ma et al., 2020).

While the problem of estimation has been explored through many different approaches in the literature, the question of uncertainty quantity for matrix completion remains challenging and underexplored. Cai et al. (2016) and Carpentier et al. (2018) construct confidence intervals for the missing entries using order-wise concentration inequalities, which could be extremely loose. Chen et al. (2019) proposes a de-biased estimator for matrix completion and characterizes its asymptotic distribution, which then yields entrywise confidence intervals are then derived for the underlying incoherent matrix with i.i.d. Gaussian noise. See also Xia and Yuan (2021); Farias et al. (2022) for related approaches.

The effectiveness of the aforementioned uncertainty quantification methods rely heavily on the exact low-rank structure as well as assumptions on the tail of the noise. In practice, the low-rank assumption can only be met approximately, and heavy-tailed noise is quite common in areas

such as macroeconomics and genomics (Nair et al., 2022). Without exact model specifications, the solution to the matrix completion algorithm is hard to interpret and the asymptotic distribution of the obtained estimator is no longer valid. The dependence of model-based approaches on exact model assumptions motivates us to answer the question: can we construct valid and short confidence intervals for the missing entries that are free of both model assumptions and of constraints on which estimation algorithms we may use?

1.1 Conformal prediction for distribution-free uncertainty quantification

Our proposed method is built on the idea of conformal prediction. The conformal prediction framework, developed by Vovk et al. (2005) and Shafer and Vovk (2008), has drawn significant attention in recent years in that it enables the construction of distribution-free confidence intervals that are valid with exchangeable data from any underlying distribution and with any "black-box" algorithm. To reduce computation in full conformal prediction, variants exist based on data splitting (Vovk et al., 2005; Lei et al., 2018), leave-one-out (Barber et al., 2021), cross-validation (Vovk, 2015; Barber et al., 2021), etc.

When distribution shift is present, with covariate shift as a special case, the exchangeability is violated, and Tibshirani et al. (2019) proposes a more general procedure called weighted conformal prediction that guarantees the validity under the weighted exchangeability of data. Barber et al. (2022) further relaxes the exchangeability assumption on the data and characterizes the robustness of a generalized weighted approach via an upper bound for the coverage gap. Other related works (Lei and Candès, 2020; Candès et al., 2021; Jin et al., 2023) adapt the conformal framework to applications in causal inference, survival analysis, etc., and study the robustness of weighted conformal prediction with estimated weights.

1.2 Main contributions

In this paper, we adapt the framework of conformal prediction for the problem of matrix completion, and make the following contributions:

- 1. We construct distribution-free confidence intervals for the missing entries in matrix completion via conformal prediction. The validity is free of any assumption on the underlying matrix and holds regardless of the choice of estimation algorithms practitioners use. To achieve this, we prove the (weighted) exchangeability of unobserved and observed units when they are sampled (possibly nonuniformly) without replacement from a finite population.
- 2. When the sampling mechanism is unknown, we develop a provable lower bound for the coverage rate which degrades gracefully as the estimation error of the sampling probability increases.
- 3. In addition, to improve computational efficiency when faced with a large number of missing entries, we propose a one-shot conformalized matrix completion approach that only computes the weighted quantile once for all missing entries.

2 Problem setup

In this section, we formulate the matrix completion problem and contrast our distribution-free setting with the model-based settings that are more common in the existing literature. For a partially-observed $d_1 \times d_2$ matrix, the subset $S \subseteq [d_1] \times [d_2]$ denotes the set of indices where data

is observed—that is, our observations consist of $(M_{ij})_{(i,j)\in\mathcal{S}}$. In much of the matrix completion literature, it is common to assume a signal-plus-noise model for the observations,

$$M_{ij} = M_{ij}^* + E_{ij},$$

where $\mathbf{M}^* = (M_{ij}^*)_{(i,j) \in [d_1] \times [d_2]}$ is the "true" underlying signal while $(E_{ij})_{(i,j) \in \mathcal{S}}$ denotes the (typically zero-mean) noise. Frequently, it is assumed that \mathbf{M}^* is low-rank, or follows some other latent low-dimensional structure, so that recovering \mathbf{M}^* from the observed data is an identifiable problem. In works of this type, the goal is to construct an estimator $\widehat{\mathbf{M}}$ that accurately recovers the underlying \mathbf{M}^* . In contrast, in a more model-free setting, we may no longer wish to hypothesize a signal-plus-noise model, and can instead assume that we are observing a random subset of entries of a deterministic matrix \mathbf{M} ; in this setting, estimating \mathbf{M} itself becomes the goal.

For both frameworks, many existing results focus on the problem of estimation (either of \mathbf{M}^* or of \mathbf{M}), with results establishing bounds on estimation errors under various assumptions. For instance, see Candes and Plan (2010); Candès and Tao (2010); Negahban and Wainwright (2012); Chen et al. (2020) for results on estimating \mathbf{M}^* (under stronger conditions, e.g., a low-rank and incoherent signal, and zero-mean sub-Gaussian noise), or Srebro and Shraibman (2005); Foygel and Srebro (2011) for results on estimating \mathbf{M} (under milder conditions); note that in the latter case, it is common to instead refer to predicting the entries of \mathbf{M} , e.g., temperature or stock market returns, since we often think of these as noisy observations of some underlying signal. On the other hand, relatively little is known about the problem of uncertainty quantification for these estimates: given some estimator $\widehat{\mathbf{M}}$, can we produce a confidence interval around each \widehat{M}_{ij} that is (asymptotically) quaranteed to contain the target with some minimum probability?

The results of Chen et al. (2019) address this question under strong assumptions, namely, a low-rank and incoherent signal \mathbf{M}^* , plus i.i.d. Gaussian noise $(E_{ij})_{(i,j)\in[d_1]\times[d_2]}$. In this work, we provide a complementary answer that instead addresses the model-free setting: without relying on assumptions, we aim to produce a provably valid confidence interval for the entries M_{ij} of \mathbf{M} (not of \mathbf{M}^* , because without assuming a low-rank model, there is no meaningful notion of an "underlying signal").

To do so, we will treat the matrix \mathbf{M} as deterministic, while the randomness arises purely from the random subset of entries that are observed. More specifically, we assume

$$Z_{ij} = \mathbb{1}\{(i,j) \text{ is observed}\} \sim \text{Bern}(p_{ij}), \text{ independently for all } (i,j) \in [d_1] \times [d_2],$$
 (1)

and let $S = \{(i,j) \in [d_1] \times [d_2] : Z_{ij} = 1\}$ be the subset of observed locations. After observing $\mathbf{M}_{S} = (M_{ij})_{(i,j) \in S}$, our goal is to provide confidence intervals $\{\widehat{C}(i,j)\}_{(i,j) \in S^c}$ for all unobserved entries, with $1 - \alpha$ coverage over the unobserved portion of the matrix—that is, we would like our confidence intervals to satisfy

$$\mathbb{E}\left[\operatorname{AvgCov}(\widehat{C}; \mathbf{M}, \mathcal{S})\right] \ge 1 - \alpha, \tag{2}$$

where

$$\operatorname{AvgCov}(\widehat{C}; \mathbf{M}, \mathcal{S}) = \frac{1}{|\mathcal{S}^c|} \sum_{(i,j) \in \mathcal{S}^c} \mathbb{1} \left\{ M_{ij} \in \widehat{C}(i,j) \right\}$$
(3)

measures the "average coverage rate" of the confidence intervals. The goal of this work is to provide an algorithm for constructing confidence intervals $\{\widehat{C}(i,j)\}_{(i,j)\in\mathcal{S}^c}$ based on the observed entries $\mathbf{M}_{\mathcal{S}}$,

¹To handle the degenerate case where $S = [d_1] \times [d_2]$ (i.e., we happen to have observed the entire matrix) and thus $S^c = \emptyset$, we simply define $AvgCov(\widehat{C}; \mathbf{M}, S) \equiv 1$.

satisfying (2) with no assumptions on \mathbf{M} . In particular, given the strong success of various matrix completion algorithms for the problem of estimation, we would like to be able to provide uncertainty quantification around any base estimator—i.e., given any algorithm for producing an estimate $\widehat{\mathbf{M}}$, our method constructs confidence intervals $\{\widehat{C}(i,j)\}_{(i,j)\in\mathcal{S}^c}$ around this initial estimate.

Notation. For a matrix $\mathbf{A} = (A_{ij}) \in \mathbb{R}^{m_1 \times m_2}$, we define $\|\mathbf{A}\|_{\infty} := \max_{(i,j) \in [m_1] \times [m_2]} |A_{ij}|$, and $\|\mathbf{A}\|_1 := \sum_{(i,j) \in [m_1] \times [m_2]} |A_{ij}|$. We use $\mathbf{A}_{i,}$ and $\mathbf{A}_{\cdot,j}$ to refer to the *i*th row and *j*th column of \mathbf{A} , respectively. For any $t \in \mathbb{R}$, δ_t denotes the distribution given by a point mass at t.

3 Conformalized matrix completion

We next present our method, conformalized matrix completion (cmc). Our procedure adapts the split conformal prediction method (Vovk et al., 2005) to the problem at hand. As is standard in the conformal prediction framework, the goal of cmc is to provide uncertainty quantification (i.e., confidence intervals) around the output of any existing estimation procedure that the analyst chooses to use—this is a core strength of the conformal methodology, as it allows the analyst to use state-of-the-art estimation procedures without compromising on the validity of inference. At a high level, the cmc procedure will output a confidence interval of the form

$$\widehat{C}(i,j) = \widehat{M}_{ij} \pm \widehat{q} \cdot \widehat{s}_{ij}$$

for the matrix value M_{ij} at each unobserved entry (i,j). Here, after splitting the observed entries into a training set and a calibration set, the training set is used to produce \widehat{M}_{ij} (a point estimate for the target value M_{ij}) and \widehat{s}_{ij} (a scaling parameter that estimates our uncertainty for this point estimate); then, the calibration set is used to tune the scalar \widehat{q} , to adjust the width of these confidence intervals and ensure coverage at the desired level $1-\alpha$.

3.1 Exchangeability and weighted exchangeability

We split the set of observed indices S into a training and a calibration set $S = S_{\rm tr} \cup S_{\rm cal}$ as is shown in Algorithm 1. We should notice that the sampling without replacement may introduce implicit dependence as well as a distribution shift from the i.i.d. sampling. Thus the two sets are dependent, which is different from the split conformal methods in regression problems. Before we present the coverage guarantees for our method, we first examine the role of (weighted) exchangeability in this method, to build intuition for how the method is constructed.

3.1.1 Intuition: the uniform sampling case

First, for intuition, consider the simple case where the entries are sampled with constant probability, $p_{ij} \equiv p$. If this is the case, then the set of calibration samples and the test point are exchangeable—that is, for (i_*, j_*) denoting the test point that is drawn uniformly from \mathcal{S}^c , if we are told that the combined set $\mathcal{S}_{\text{cal}} \cup \{(i_*, j_*)\}$ is equal to $\{(i_1, j_1), \dots, (i_{n_{\text{cal}}+1}, j_{n_{\text{cal}}+1})\}$ in no particular order (where $n_{\text{cal}} = |\mathcal{S}_{\text{cal}}|$), then the test point location (i_*, j_*) is equally likely to be at any one of these $n_{\text{cal}} + 1$ locations. Consequently, by exchangeability, the calibration residuals $\{R_{ij} : (i, j) \in \mathcal{S}_{\text{cal}}\}$, defined

²More generally, cmc can be implemented with any choice of a nonconformity score that determines the shape of the resulting confidence intervals—and indeed, this generalization allows for categorical rather than real-valued matrix entries M_{ij} . We will address this extension in the Supplementary Material, as well as a version of cmc based on full conformal rather than split conformal, in order to avoid data splitting.

Algorithm 1 Conformalized matrix completion (cmc)

- 1: Input: target coverage level 1α ; data splitting proportion $q \in (0, 1)$; observed entries $\mathbf{M}_{\mathcal{S}}$.
- 2: Split the data: draw $W_{ij} \stackrel{\text{i.i.d.}}{\sim} \text{Bern}(q)$, and define training and calibration sets

$$S_{\text{tr}} = \{(i, j) \in S : W_{ij} = 1\}, \text{ and } S_{\text{cal}} = \{(i, j) \in S : W_{ij} = 0\}.$$

- 3: Using the training data $\mathbf{M}_{\mathcal{S}_{tr}}$ indexed by $\mathcal{S}_{tr} \subseteq [d_1] \times [d_2]$, compute:
 - An initial estimate $\widehat{\mathbf{M}}$ using any matrix completion algorithm (with \widehat{M}_{ij} estimating the target M_{ij});
 - Optionally, a local uncertainty estimate $\hat{\mathbf{s}}$ (with \hat{s}_{ij} estimating our relative uncertainty in the estimate \widehat{M}_{ij}), or otherwise set $\hat{s}_{ij} \equiv 1$;
 - An estimate $\widehat{\mathbf{P}}$ of the observation probabilities (with \widehat{p}_{ij} estimating p_{ij} , the probability of entry (i,j) being observed).
- 4: Compute normalized residuals on the calibration set, $R_{ij} = \frac{|M_{ij} \widehat{M}_{ij}|}{\widehat{s}_{ij}}, (i, j) \in \mathcal{S}_{\text{cal}}.$
- 5: Compute estimated odds ratios for the calibration set and test set, $\hat{h}_{ij} = \frac{1-\hat{p}_{ij}}{\hat{p}_{ij}}$, $(i,j) \in \mathcal{S}_{cal} \cup \mathcal{S}^c$, and then compute weights for the calibration set and test point,

$$\widehat{w}_{ij} = \frac{\widehat{h}_{ij}}{\sum_{(i',j')\in\mathcal{S}_{\text{cal}}} \widehat{h}_{i'j'} + \max_{(i',j')\in\mathcal{S}^c} \widehat{h}_{i'j'}}, \quad (i,j)\in\mathcal{S}_{\text{cal}}, \quad \widehat{w}_{\text{test}} = \frac{\max_{(i,j)\in\mathcal{S}^c} \widehat{h}_{ij}}{\sum_{(i',j')\in\mathcal{S}_{\text{cal}}} \widehat{h}_{i'j'} + \max_{(i',j')\in\mathcal{S}^c} \widehat{h}_{i'j'}}.$$

$$(4)$$

- 6: Compute threshold $\widehat{q} = \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}}} \widehat{w}_{ij} \cdot \delta_{R_{ij}} + \widehat{w}_{\text{test}} \cdot \delta_{+\infty} \right)$.
- 7: Output: confidence intervals $\widehat{C}(i,j) = \widehat{M}_{ij} \pm \widehat{q} \cdot \widehat{s}_{ij}$ for each unobserved entry $(i,j) \in \mathcal{S}^c$.

in Algorithm 1 above, are exchangeable with the test residual $R_{i_*j_*} = |M_{i_*j_*} - \widehat{M}_{i_*j_*}|/\widehat{s}_{i_*j_*}$; as a result, we can construct our confidence interval $\widehat{C}(i_*, j_*)$ with \widehat{q} determined by the $(1 - \alpha)$ -quantile of the calibration residuals $\{R_{ij} : (i, j) \in \mathcal{S}_{cal}\}$.

Indeed, this is exactly what cmc does in this case: if we are aware that sampling is uniform, it would naturally follow that we estimate $\hat{p}_{ij} \equiv \hat{p}_0$ by some (potentially data-dependent) scalar \hat{p}_0 ; consequently, all the weights are given by $\hat{w}_{ij} \equiv \frac{1}{n_{\rm cal}+1}$ and $\hat{w}_{\rm test} = \frac{1}{n_{\rm cal}+1}$, and thus \hat{q} is the (unweighted) $(1-\alpha)$ -quantile of the calibration residuals (with a small correction term, i.e., the term $+\hat{w}_{\rm test} \cdot \delta_{+\infty}$ appearing in the definition of \hat{q} , to ensure the correct probability of coverage at finite sample sizes).

3.1.2 Weighted exchangeability for the matrix completion problem

Next, we move to the general case, where now the sampling may be highly nonuniform. First suppose the sampling probabilities p_{ij} are known, and suppose again that we are told that the combined set $S_{\text{cal}} \cup \{(i_*, j_*)\}$ is equal to $\{(i_1, j_1), \dots, (i_{n_{\text{cal}}+1}, j_{n_{\text{cal}}+1})\}$ in no particular order. In this case, the test point (i_*, j_*) is not equally likely to be at any one of these $n_{\text{cal}} + 1$ locations. Instead, we have the following result:

Lemma 3.1. Following the notation defined above, if $(i_*, j_*) \mid \mathcal{S} \sim \text{Unif}(\mathcal{S}^c)$, it holds that

$$\mathbb{P}\{(i_*, j_*) = (i_k, j_k) \mid \mathcal{S}_{\text{cal}} \cup \{(i_*, j_*)\} = \{(i_1, j_1), \dots, (i_{n_{\text{cal}}+1}, j_{n_{\text{cal}}+1})\}, \mathcal{S}_{\text{tr}}\} = w_{i_k j_k},$$

where we define the weights $w_{i_k j_k} = \frac{h_{i_k j_k}}{\sum_{k'=1}^{n_{\text{cal}}+1} h_{i_{k'} j_{k'}}}$ for odds ratios given by $h_{ij} = \frac{1-p_{ij}}{p_{ij}}$.

Consequently, while the test point's residual $R_{i_*j_*} = |M_{i_*j_*} - \widehat{M}_{i_*j_*}| / \widehat{s}_{i_*j_*}$ is not exchangeable with the calibration set residuals $\{R_{ij}: (i,j) \in \mathcal{S}_{\text{cal}}\}$, the framework of weighted exchangeability (Tibshirani et al., 2019) tells us that we can view $R_{i_*j_*}$ as a draw from the weighted distribution that places weight $w_{i_kj_k}$ on each residual $R_{i_kj_k}$ —and in particular,

$$\mathbb{P}\left\{M_{i_*j_*} \in \widehat{M}_{i_*j_*} \pm q_{i_*,j_*}^* \cdot \widehat{s}_{i_*j_*}\right\} = \mathbb{P}\left\{R_{i_*j_*} \le q_{i_*,j_*}^*\right\} \ge 1 - \alpha,$$

where $q_{i_*,j_*}^* = \text{Quantile}_{1-\alpha} \left(\sum_{k=1}^{n_{\text{cal}}+1} w_{i_k j_k} \cdot \delta_{R_{i_k j_k}}\right)$. Noting that this threshold q_{i_*,j_*}^* may depend on the test location (i_*,j_*) , to accelerate the computation of prediction sets for all missing entries, we instead propose a one-shot weighted conformal approach by upper bounding the threshold uniformly over all test points: $q_{i_*,j_*}^* \leq q^* := \text{Quantile}_{1-\alpha} \left(\sum_{(i,j)\in\mathcal{S}_{\text{cal}}} w_{ij}^* \cdot \delta_{R_{ij}} + w_{\text{test}}^* \cdot \delta_{+\infty}\right)$, for $(i,j)\in\mathcal{S}_{\text{cal}}$,

$$w_{ij}^* = \frac{h_{ij}}{\sum_{(i',j')\in\mathcal{S}_{\text{cal}}} h_{i'j'} + \max_{(i',j')\in\mathcal{S}^c} h_{i'j'}}, \quad w_{\text{test}}^* = \frac{\max_{(i,j)\in\mathcal{S}^c} h_{ij}}{\sum_{(i',j')\in\mathcal{S}_{\text{cal}}} h_{i'j'} + \max_{(i',j')\in\mathcal{S}^c} h_{i'j'}}.$$
 (5)

Now the threshold q^* no longer depends on the location (i_*, j_*) of the test point. If the true probabilities p_{ij} were known, then, we could define "oracle" conformal confidence intervals

$$\widehat{C}^*(i,j) = \widehat{M}_{ij} \pm q^* \cdot \widehat{s}_{ij}, \quad (i,j) \in \mathcal{S}^c.$$

As we will see in the proofs below, weighted exchangeability ensures that, if we do have oracle knowledge of the p_{ij} 's, then these confidence intervals satisfy the goal (2) of $1 - \alpha$ average coverage. Since the p_{ij} 's are not known in general, our algorithm simply replaces the oracle weights \boldsymbol{w}^* in (5) with their estimates $\hat{\boldsymbol{w}}$ defined in (4), using \hat{p}_{ij} as a plug-in estimate of the unknown p_{ij} .

3.2 Theoretical guarantee

In the setting where the p_{ij} 's are not known but instead are estimated, our cmc procedure simply repeats the procedure described above but with weights $\hat{\boldsymbol{w}}$ calculated using \hat{p}_{ij} 's in place of p_{ij} 's. Our theoretical results therefore need to account for the errors in our estimates \hat{p}_{ij} , to quantify the coverage gap of conformal prediction with the presence of these estimation errors. To do this, we define an estimation gap term

$$\Delta = \frac{1}{2} \sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} \left| \frac{\widehat{h}_{ij}}{\sum_{(i',j') \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} \widehat{h}_{i'j'}} - \frac{h_{ij}}{\sum_{(i',j') \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} h_{i'j'}} \right|, \tag{6}$$

where (i_*, j_*) denotes the test point. Effectively, Δ is quantifying the difference between the "oracle" weights, w_{ij}^* , defined in (5), and the estimated weights, \widehat{w}_{ij} , defined in (4), except that Δ is defined relative to a specific test point, while the weights $\widehat{\boldsymbol{w}}$ (and \boldsymbol{w}^* , for the oracle version) provide a "one-shot" procedure that is universal across all possible test points, and is thus slightly more conservative.

Theorem 3.2. Let $\widehat{\mathbf{M}}$, $\widehat{\mathbf{s}}$, and $\widehat{\mathbf{P}}$ be estimates constructed using any algorithms, which depend on the data only through the training samples $\mathbf{M}_{\mathcal{S}_{\mathrm{tr}}}$ at locations $\mathcal{S}_{\mathrm{tr}}$. Then, under the notation and definitions above, conformalized matrix completion (cmc) satisfies

$$\mathbb{E}\big[\mathrm{AvgCov}(\widehat{C};\mathbf{M},\mathcal{S})\big] \geq 1 - \alpha - \mathbb{E}[\Delta].$$

In the homogeneous case, where we are aware that sampling is uniform (i.e., $p_{ij} \equiv p$ for some potentially unknown $p \in (0,1)$), our error in estimating the weights is given by $\Delta \equiv 0$ (since h_{ij} is constant across all (i,j), and same for \hat{h}_{ij} —and therefore, the true and estimated weights are all equal to $\frac{1}{n_{\text{cal}}+1}$). In this setting, therefore, we would achieve the exact coverage goal (2), with $\mathbb{E}[\text{AvgCov}(\hat{C}; \mathbf{M}, \mathcal{S})]$ guaranteed to be at least $1-\alpha$.

3.3 Examples for missingness

To characterize the coverage gap explicitly, we present the following concrete examples for \mathbf{P} and show how the coverage gap Δ can be controlled. Technical details are shown in the Supplementary Material.

3.3.1 Logistic missingness

Suppose that the missingness follows a logistic model, with $\log(p_{ij}/(1-p_{ij})) = -\log(h_{ij}) = u_i + v_j$ for some $\boldsymbol{u} \in \mathbb{R}^{d_1}$ and $\boldsymbol{v} \in \mathbb{R}^{d_2}$, where we assume $\boldsymbol{u}^{\top} \mathbf{1} = 0$ for identifiability. This model is closely related to logistic regression with a diverging number of covariates (Portnoy, 1988; He and Shao, 2000; Wang, 2011). Following Chen et al. (2023), we estimate \boldsymbol{u} , \boldsymbol{v} via maximum likelihood,

$$\widehat{\boldsymbol{u}}, \widehat{\boldsymbol{v}} = \arg\max_{\boldsymbol{u}, \boldsymbol{v}} \ \mathcal{L}(\boldsymbol{u}, \boldsymbol{v})$$
 subject to $\mathbf{1}^{\top} \boldsymbol{u} = 0$.

Here the log-likelihood is defined by

$$\mathcal{L}(\boldsymbol{u}, \boldsymbol{v}) = \sum_{(i,j) \in [d_1] \times [d_2]} \{ -\log(1 + \exp(-u_i - v_j)) + \mathbf{1}_{(i,j) \in \mathcal{S}_{tr}^c} \log(1 - q + \exp(-u_i - v_j)) \}.$$

Consequently, we define the estimate of p_{ij} as $\widehat{p}_{ij} = (1 + \exp(-\widehat{u}_i - \widehat{v}_j))^{-1}$, for which one can show that $\mathbb{E}[\Delta] \lesssim \sqrt{\frac{\log(\max\{d_1,d_2\})}{\min\{d_1,d_2\}}}$.

3.3.2 Missingness with a general link function

More broadly, we can consider a general link function, where we assume $\log(p_{ij}/(1-p_{ij})) = -\log(h_{ij}) = \phi(A_{ij})$, where ϕ is a link function and $\mathbf{A} \in \mathbb{R}^{d_1 \times d_2}$ is the model parameter. The logistic model we introduced above corresponds to the case when ϕ is the identity function and $\mathbf{A} = \mathbf{u}\mathbf{1}^{\top} + \mathbf{1}\mathbf{v}^{\top}$ is a rank-2 matrix. In this general setup, if $\operatorname{rank}(\mathbf{A}) = k^*$ and $\|\mathbf{A}\|_{\infty} \leq \tau$, we can apply one-bit matrix completion (Davenport et al., 2014) to estimate $\{p_{ij}\}$. More precisely, we define the log-likelihood

$$\mathcal{L}_{\mathcal{S}_{tr}}(\mathbf{B}) = \sum_{(i,j) \in \mathcal{S}_{tr}} \log(\psi(B_{ij})) + \sum_{(i,j) \in \mathcal{S}_{tr}^c} \log(1 - \psi(B_{ij})),$$

where $\psi(t) = q(1+e^{-\phi(t)})^{-1}$ (here rescaling by the constant q is necessary to account for subsampling the training set $S_{\rm tr}$ from the observed data indices S), and solve the following optimization problem

$$\widehat{\mathbf{A}} = \arg \max_{\mathbf{B}} \ \mathcal{L}_{\mathcal{S}_{tr}}(\mathbf{B}) \qquad \text{subject to} \quad \|\mathbf{B}\|_* \le \tau \sqrt{k^* d_1 d_2}, \ \|\mathbf{B}\|_{\infty} \le \tau, \tag{7}$$

where $\|\mathbf{B}\|_*$ is the nuclear norm of **B**. Consequently, we let $\hat{h}_{ij} = \exp(-\phi(\hat{A}_{ij}))$, which leads to $\mathbb{E}[\Delta] \lesssim \min\{d_1, d_2\}^{-1/4}$.

4 Simulation studies

In this section, we conduct numerical experiments to verify the coverage guarantee of conformalized matrix completion (cmc) using both synthetic and real datasets. As the validity of cmc is independent of the choice of base algorithm, we choose alternating least squares (als) (Jain et al., 2013) as the base algorithm (results using a convex relaxation (Fazel et al., 2004; Candes and Recht, 2012; Chen et al., 2020) are shown in the Supplementary Material). We use cmc-als to refer to this combination. We use $\operatorname{AvgCov}(\widehat{C})$ (the average coverage, defined in (3)), and average confidence interval length, $\operatorname{AvgLength}(\widehat{C}) = \frac{1}{|S^c|} \sum_{(i,j) \in \mathcal{S}^c} \operatorname{length}(\widehat{C}(i,j))$, to evaluate the performance of different methods. The code for reproducing the simulations is publicly available at https://github.com/yugjerry/conf-mc.

4.1 Synthetic dataset

Throughout the experiments, we set the true rank $r^* = 8$, the desired coverage rate $1 - \alpha = 0.90$, and report the average results over 100 random trials.

Data generation. In the synthetic setting, we generate the data matrix by $\mathbf{M} = \mathbf{M}^* + \mathbf{E}$, where \mathbf{M}^* is a rank r^* matrix, and \mathbf{E} is a noise matrix (with distribution specified below). The low-rank component \mathbf{M}^* is generated by $\mathbf{M}^* = \kappa \mathbf{U}^* \mathbf{V}^{*\top}$, where $\mathbf{U}^* \in \mathbb{R}^{d_1 \times r^*}$ is the orthonormal basis of a random $d_1 \times r^*$ matrix consisting of i.i.d. entries from a certain distribution $\mathcal{P}_{u,v}$ (specified below) and $\mathbf{V}^* \in \mathbb{R}^{d_2 \times r^*}$ is independently generated in the same manner. In addition, the constant κ is chosen such that the average magnitude of the entries $|M_{ij}^*|$ is 2. Following the observation model (1), we only observe the entries in the random set \mathcal{S} .

Implementation. First, when implementing als, we adopt r as the hypothesized rank of the underlying matrix. For model-based methods, by the asymptotic distributional characterization $\widehat{M}_{ij} - M_{ij}^* \stackrel{d}{\to} \mathcal{N}(0, \theta_{ij}^2)$ and $E_{ij} \perp (\widehat{M}_{ij} - M_{ij}^*)$, one has $\widehat{M}_{ij} - M_{ij} \stackrel{d}{\to} \mathcal{N}(0, \theta_{ij}^2 + \sigma^2)$. Consequently, the confidence interval for the model-based methods can be constructed as $\widehat{M}_{ij} \pm q_{1-\alpha/2}(\widehat{\theta}_{ij}^2 + \widehat{\sigma}^2)^{1/2}$, where q_{β} is the β th quantile of $\mathcal{N}(0,1)$. The estimates are obtained via $\widehat{\sigma}^2 = \|\mathbf{M}_{\mathcal{S}_{tr}} - \widehat{\mathbf{M}}_{\mathcal{S}_{tr}}\|_F^2/|\mathcal{S}_{tr}|$ and $\widehat{\theta}_{ij}^2 = (\widehat{\sigma}^2/\widehat{p})(\|\widehat{\mathbf{U}}_{i,\cdot}\|^2 + \|\widehat{\mathbf{V}}_{j,\cdot}\|^2)$ with the SVD $\widehat{\mathbf{M}} = \widehat{\mathbf{U}}\widehat{\Sigma}\widehat{\mathbf{V}}^{\top}$. For cmc-als, we obtain $\widehat{\mathbf{M}}$, $\widehat{\mathbf{s}}$ from $\mathbf{M}_{\mathcal{S}_{tr}}$ by running als on this training set (and taking $\widehat{s}_{ij} = (\widehat{\theta}_{ij}^2 + \widehat{\sigma}^2)^{1/2}$). The probabilities \widehat{p}_{ij} 's are estimated via $\widehat{p}_{ij} \equiv (d_1 d_2 q)^{-1} |\mathcal{S}_{tr}|$ for this setting where the p_{ij} 's are homogeneous.

4.1.1 Homogeneous missingness

In the homogeneous case, we consider the following four settings with $d_1 = d_2 = 500$:

- Setting 1: large sample size + Gaussian noise. p = 0.8, $\mathcal{P}_{u,v} = \mathcal{N}(0,1)$, and $E_{ij} \sim \mathcal{N}(0,1)$.
- Setting 2: small sample size + Gaussian noise. p = 0.2, $\mathcal{P}_{u,v} = \mathcal{N}(0,1)$, and $E_{ij} \sim \mathcal{N}(0,1)$.

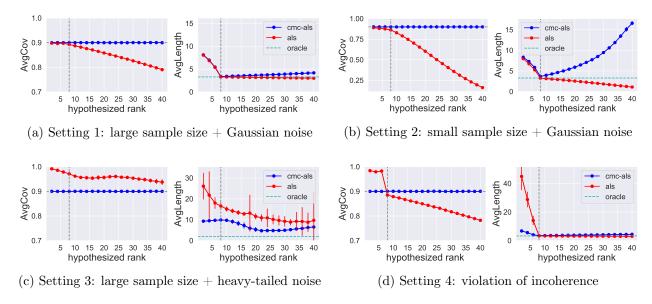


Figure 1: Comparison between cmc-als and als.

- Setting 3: large sample size + heavy-tailed noise. p = 0.8, $\mathcal{P}_{u,v} = \mathcal{N}(0,1)$, and $E_{ij} \sim 0.2 \, \mathrm{t}_{1.2}$, where t_{ν} denotes the t distribution with ν degrees of freedom.
- Setting 4: violation of incoherence. p = 0.8, $\mathcal{P}_{u,v} = t_{1.2}$, and $E_{ij} \sim \mathcal{N}(0,1)$.

Figure 1 displays the results (i.e., the coverage rate and the interval length) for both cmc-als and als when we vary the hypothesized rank r from 2 to 40. The oracle length is the difference between the $(1 - \alpha/2)$ -th and $(\alpha/2)$ -th quantiles of the underlying distribution for E_{ij} . As can be seen, cmc-als achieves nearly exact coverage regardless of the choice of r across all four settings. When the hypothesized rank r is chosen well, cmc-als is often able to achieve an average length similar to that of the oracle.

For the model-based method als, when we underestimate the true rank $(r < r^*)$, we may still see adequate coverage since $\hat{\sigma}$ tends to over-estimate σ by including the remaining r^*-r factors as noise. However, if we overestimate the rank $(r > r^*)$, then als tends to overfit the noise with additional factors and under-estimate σ regardless of the choice of r, leading to significant undercoverage in Settings 1, 2 and 4. In Setting 3 with heavy-tailed noise, als tends to be conservative due to overestimating σ . Overall, Figure 1 confirms our expectation that the validity of the model-based estimates relies crucially on a well specified model, and it fails to hold when sample size is small (cf. Figure 1b), when noise is heavy tailed (cf. Figure 1c), and when the underlying matrix is not incoherent (cf. Figure 1d).

4.1.2 Heterogeneous missingness

Now we move on to the case with heterogeneous missingness, where the observed entries are no longer sampled uniformly. To simulate this setting, we draw $\{a_{il}: i \leq d_1, l \leq k^*\}$ i.i.d. from Unif(0,1) and $\{b_{lj}: l \leq k^*, j \leq d_2\}$ i.i.d. from Unif(-0.5, 0.5), and define sampling probabilities by

$$\log(p_{ij}/(1-p_{ij})) = \sum_{l=1}^{k^*} a_{il}b_{lj}.$$
 (8)

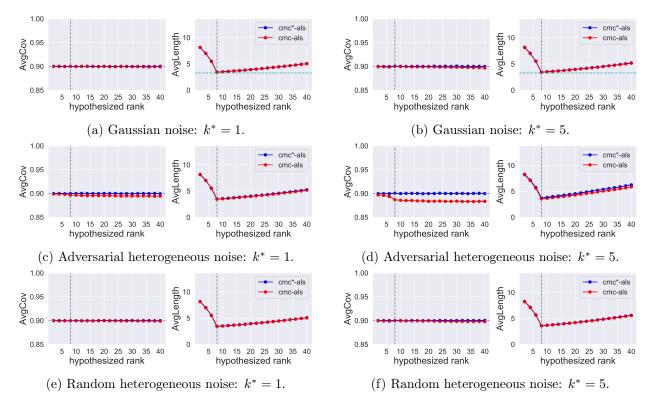


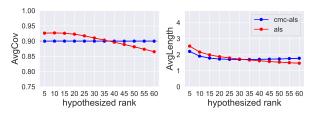
Figure 2: Comparison under heterogeneous missingness.

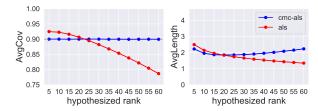
We consider two settings with $k^* = 1$ and $k^* = 5$, respectively. In both settings, \hat{p}_{ij} is constructed by estimating \hat{a}_{il} and \hat{b}_{lj} via constrained maximum likelihood estimation as is shown in Example 3.3.2.

To analyze the effect of estimation error predicted by Theorem 3.2, we consider three matrix generation processes for each choice of k^* , where \mathbf{M}^* is generated in the same way as in Section 4.1.1 with $d_1 = d_2 = d = 500$, $\mathcal{P}_{u,v} = \mathcal{N}(0,1)$:

- Gaussian homogeneous noise: $E_{ij} \sim \mathcal{N}(0,1)$ independently.
- Adversarial heterogeneous noise: $E_{ij} \sim \mathcal{N}(0, \sigma_{ij}^2)$ independently, where we take $\sigma_{ij} = 1/2p_{ij}$. For this setting, note that the high-noise entries (i.e., those entries that are hardest to predict) occur in locations (i, j) that are least likely to be observed during training.
- Random heterogeneous noise: $E_{ij} \sim \mathcal{N}(0, \sigma_{ij}^2)$ independently, where $(\sigma_{ij})_{(i,j) \in [d_1] \times [d_2]}$ is drawn from the same distribution as $(1/2p_{ij})_{(i,j) \in [d_1] \times [d_2]}$.

We write cmc^* -als to denote the conformalized method (with als as the base algorithm) where we use oracle knowledge of the true p_{ij} 's for weighting, while cmc-als uses estimates \widehat{p}_{ij} . The results are shown in Figures 2, for the settings $k^* = 1$ and $k^* = 5$ (i.e., the rank of **P**). Under both homogeneous noise and random heterogeneous noise, both cmc^* -als and cmc-als achieve the correct coverage level, with nearly identical interval length. For adversarial heterogeneous noise, on the other hand, cmc^* -als achieves the correct coverage level as guaranteed by the theory, but cmc-als shows some undercoverage due to the errors in the estimates \widehat{p}_{ij} (since now the variance of the noise is adversarially aligned with these errors); nonetheless, the undercoverage is mild.





- (a) als vs cmc-als: homogeneous missingness.
- (b) als vs cmc-als: logistic missingness.

Figure 3: Comparison between conformalized and model-based matrix completion with sales dataset.

4.2 Real data application

We also compare conformalized approaches with model-based approaches using the Rossmann sales dataset³ (Farias et al., 2022). This real data provides the underlying fixed matrix \mathbf{M} ; the missingness pattern is generated artificially, as detailed below. We focus on daily sales (the unit is 1K dollar) of 1115 drug stores on workdays from Jan 1, 2013 to July 31, 2015 and hence the underlying matrix has dimension 1115×780 . The hypothesized rank r is varied from 5 to 60 with step size 5 and we set the target level to be $1 - \alpha = 0.9$. We apply random masking for 100 independent trials and report the average for AvgCov and AvgLength in Figure 3.

- Homogeneous p_{ij} . For each entry, we first apply random masking $1 Z_{ij} \sim \text{Bern}(0.2)$ independently. In Figure 3a, conformalized approach has exact coverage at 1α but als tends to be conservative when r is small and loses coverage when r increases to 50.
- Heterogeneous p_{ij} . After drawing p_{ij} 's from model (8) in Section 4.1.2 with $k^* = 1$, $\widehat{\mathbf{P}}$ is obtained via the constrained maximum likelihood estimator in Example 3.3.2. In Figure 3b, cmc-als has coverage around 1α and in comparison, when r is greater than 40, als fails to guarantee the coverage and AvgCov decreases to 0.75.

5 Discussion

In this paper, we introduce the conformalized matrix completion method cmc, which offers a finite-sample coverage guarantee for all missing entries on average and requires no assumptions on the underlying matrix or any specification of the algorithm adopted, relying only on an estimate of the entrywise sampling probabilities. Given an estimate of the entrywise sampling probability, we provide an upper bound for the coverage gap and give the explicit form with examples of the logistic as well as the general one-bit low-rank missingness. In the implementation, an efficient one-shot weighted conformal approach is proposed with the provable guarantee and achieves nearly exact coverage.

We can compare our findings to a few related results in the literature. The work of Chernozhukov et al. (2021) applies conformal prediction to counterfactual and synthetic control methods, where they include matrix completion as an example with a regression-type formulation. However, their approach relies on a test statistic that is a function of estimated residuals. Consequently, their method requires the assumption of stationarity and weak dependence of errors. Furthermore, the validity of their approach is contingent upon the estimator being either consistent or stable. Additionally, Wieczorek (2023) studies conformal prediction with samples from a deterministic and finite

https://www.kaggle.com/c/rossmann-store-sales

population, but the validity under the sampling without replacement remains an open question in their work.

Our results suggest a number of questions for further inquiry. In the setting of matrix completion, while the results are assumption-free with regard to the matrix **M** itself, estimating the sampling probabilities **P** that determine which entries are observed remains a key step in the procedure; while our empirical results suggest the method is robust to estimation error in this step, studying the robustness properties more formally is an important open question. More broadly, our algorithm provides an example of how the conformal prediction framework can be applied in a setting that is very different from the usual i.i.d. sampling regime, and may lend insights for how to develop conformal methodologies in other applications with non-i.i.d. sampling structure.

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A Proofs

The section collects the proofs for the technical results in the main text. Section A.1 and A.2 are devoted to the proof of Lemma 3.1 and Theorem 3.2, respectively. In the end, Section A.3 provides proofs for the coverage gap bounds in the two examples in Section 3.3.

A.1 Proof of Lemma 3.1

Fix a set of locations $\mathcal{B} := \{(i_1, j_1), \dots, (i_{n_{\text{cal}}+1}, j_{n_{\text{cal}}+1})\}$, and an index $1 \leq m \leq n_{\text{cal}} + 1$. By the definition of conditional probability, we have

$$\mathbb{P}((i_{*}, j_{*}) = (i_{m}, j_{m}) \mid \mathcal{S}_{cal} \cup \{(i_{*}, j_{*})\} = \mathcal{B}, \ \mathcal{S}_{tr} = \mathcal{S}_{0})
= \frac{\mathbb{P}((i_{*}, j_{*}) = (i_{m}, j_{m}), \mathcal{S}_{cal} = \mathcal{B} \setminus \{(i_{m}, j_{m})\} \mid \mathcal{S}_{tr} = \mathcal{S}_{0}, \ |\mathcal{S}| = n)}{\mathbb{P}(\mathcal{S}_{cal} \cup \{(i_{*}, j_{*})\} = \mathcal{B} \mid \mathcal{S}_{tr} = \mathcal{S}_{0}, \ |\mathcal{S}| = n)}
= \frac{\mathbb{P}((i_{*}, j_{*}) = (i_{m}, j_{m}), \mathcal{S}_{cal} = \mathcal{B} \setminus \{(i_{m}, j_{m})\} \mid \mathcal{S}_{tr} = \mathcal{S}_{0}, \ |\mathcal{S}| = n)}{\sum_{l=1}^{n_{cal}+1} \mathbb{P}((i_{*}, j_{*}) = (i_{l}, j_{l}), \mathcal{S}_{cal} = \mathcal{B} \setminus \{(i_{l}, j_{l})\} \mid \mathcal{S}_{tr} = \mathcal{S}_{0}, \ |\mathcal{S}| = n)}.$$

It then boils down to computing $\mathbb{P}\left(\mathcal{S}_{\text{cal}} = \mathcal{S}_1, (i_*, j_*) = (i_l, j_l) \mid \mathcal{S}_{\text{tr}} = \mathcal{S}_0, |\mathcal{S}| = n\right)$ for any fixed set \mathcal{S}_1 and fixed location $(i_l, j_l) \notin \mathcal{S}_0 \cup \mathcal{S}_1$. To this end, we have the following claim (we defer its proof to the end of this section)

$$\mathbb{P}\left(S_{\text{cal}} = S_{1}, (i_{*}, j_{*}) = (i_{l}, j_{l}) \mid S_{\text{tr}} = S_{0}, |S| = n\right)
= \frac{1}{d_{1}d_{2} - n} \cdot \frac{\prod_{(i,j) \in S_{1}} \frac{p_{i,j}}{1 - p_{i,j}}}{\sum_{A \in \Omega_{S_{\text{tr}},n}} \prod_{(i',j') \in A} \frac{p_{i',j'}}{1 - p_{i',j'}}},$$
(9)

where $\Omega_{\mathcal{S}_{tr},n} = \{ \mathcal{A} \subseteq [d_1] \times [d_2] : |\mathcal{A}| = n - |\mathcal{S}_{tr}|, \ \mathcal{A} \cap \mathcal{S}_{tr} = \emptyset \}.$ As a result, we obtain

$$\mathbb{P}\left((i_{*}, j_{*}) = (i_{m}, j_{m}) \mid \mathcal{S}_{\text{cal}} \cup \{(i_{*}, j_{*})\} = \mathcal{B}, \; \mathcal{S}_{\text{tr}} = \mathcal{S}_{0}\right) \\
= \frac{\prod_{(i,j) \in \mathcal{B} \setminus \{(i_{m}, j_{m})\}} \frac{p_{ij}}{1 - p_{ij}}}{\sum_{l=1}^{n_{\text{cal}} + 1} \prod_{(i,j) \in \mathcal{B} \setminus \{(i_{l}, j_{l})\}} \frac{p_{ij}}{1 - p_{ij}}} \\
= \frac{h_{i_{m}, j_{m}}}{\sum_{l=1}^{n_{\text{cal}} + 1} h_{i_{l}, j_{l}}}, \tag{10}$$

where $h_{ij} = (1 - p_{ij})/p_{ij}$. This finishes the proof.

Proof of Equation (9). Fix any two disjoint subsets $S_0, S_1 \subseteq [d_1] \times [d_2]$ with $|S_0| + |S_1| = n$. We have

$$\mathbb{P}\left(\mathcal{S}_{\text{cal}} = \mathcal{S}_{1}, \mathcal{S}_{\text{tr}} = \mathcal{S}_{0} \mid |\mathcal{S}| = n\right)$$

$$= \mathbb{P}\left(\text{supp}(\mathbf{Z}) = \mathcal{S}_{0} \cup \mathcal{S}_{1}, \mathcal{S}_{0} \subseteq \text{supp}(\mathbf{W}), \mathcal{S}_{1} \subseteq \text{supp}(\mathbf{W})^{c} \mid |\mathcal{S}| = n\right).$$

Since W and Z are independent, one further has

$$\mathbb{P}\left(\operatorname{supp}(\mathbf{Z}) = \mathcal{S}_{0} \cup \mathcal{S}_{1}, \mathcal{S}_{0} \subseteq \operatorname{supp}(\mathbf{W}), \mathcal{S}_{1} \subseteq \operatorname{supp}(\mathbf{W})^{c} \mid |\mathcal{S}| = n\right)
= \mathbb{P}\left(\mathcal{S}_{0} \subseteq \operatorname{supp}(\mathbf{W}), \mathcal{S}_{1} \subseteq \operatorname{supp}(\mathbf{W})^{c}\right) \cdot \mathbb{P}\left(\operatorname{supp}(\mathbf{Z}) = \mathcal{S}_{0} \cup \mathcal{S}_{1} \mid |\mathcal{S}| = n\right)
= q^{|\mathcal{S}_{0}|} (1 - q)^{|\mathcal{S}_{1}|} \cdot \mathbb{P}\left(\operatorname{supp}(\mathbf{Z}) = \mathcal{S}_{0} \cup \mathcal{S}_{1} \mid |\mathcal{S}| = n\right)
= \frac{q^{|\mathcal{S}_{0}|} (1 - q)^{|\mathcal{S}_{1}|}}{\mathbb{P}(|\mathcal{S}| = n)} \prod_{(i',j') \in [d_{1}] \times [d_{2}]} (1 - p_{i'j'}) \prod_{(i,j) \in \mathcal{S}_{0} \cup \mathcal{S}_{1}} \frac{p_{ij}}{1 - p_{ij}}, \tag{11}$$

where the last two identities are based on direct computations.

Based on (11), one can further compute

$$\mathbb{P}\left(\mathcal{S}_{\text{tr}} = \mathcal{S}_{0} \mid |\mathcal{S}| = n\right) \\
= \sum_{\mathcal{A} \in \Omega_{\mathcal{S}_{\text{tr}},n}} \mathbb{P}\left(\mathcal{S}_{\text{cal}} = \mathcal{A}, \mathcal{S}_{\text{tr}} = \mathcal{S}_{0} \mid |\mathcal{S}| = n\right) \\
= \frac{q^{|\mathcal{S}_{0}|} (1 - q)^{n - |\mathcal{S}_{0}|}}{\mathbb{P}(|\mathcal{S}| = n)} \sum_{\mathcal{A} \in \Omega_{\mathcal{S}_{\text{tr}},n}} \prod_{(i',j') \in [d_{1}] \times [d_{2}]} (1 - p_{i'j'}) \prod_{(i,j) \in \mathcal{S}_{0} \cup \mathcal{A}} \frac{p_{ij}}{1 - p_{ij}}, \tag{12}$$

where the last identity uses Equation (11).

Now we are ready to prove (9). Recall that the new data point $(i_*, j_*) \mid \mathcal{S}$ is drawn uniformly from Unif (\mathcal{S}^c) . Therefore one has

$$\mathbb{P}\left(S_{\text{cal}} = S_{1}, (i_{*}, j_{*}) = (i_{n+1}, j_{n+1}) \mid S_{\text{tr}} = S_{0}, |S| = n\right)
= \frac{\mathbb{P}\left(S_{\text{cal}} = S_{1}, S_{\text{tr}} = S_{0}, (i_{*}, j_{*}) = (i_{n+1}, j_{n+1}) \mid |S| = n\right)}{\mathbb{P}\left(S_{\text{tr}} = S_{0} \mid |S| = n\right)}
= \frac{\mathbb{P}\left((i_{*}, j_{*}) = (i_{n+1}, j_{n+1}) \mid S = S_{1} \cup S_{0}\right) \mathbb{P}\left(S_{\text{cal}} = S_{1}, S_{\text{tr}} = S_{0} \mid |S| = n\right)}{\mathbb{P}\left(S_{\text{tr}} = S_{0} \mid |S| = n\right)}
= \frac{1}{d_{1}d_{2} - n} \cdot \frac{\prod_{(i, j) \in S_{1}} \frac{p_{i, j}}{1 - p_{i, j}}}{\sum_{A \in \Omega_{S_{\text{tr}}, n}} \prod_{(i', j') \in A} \frac{p_{i', j'}}{1 - p_{i', j'}}}, \tag{13}$$

where the last line follows from (11) and (12).

A.2 Proof of Theorem 3.2

First, fix any $a \in [0, 1]$. Lemma 3.1, together with the weighted conformal prediction framework of Tibshirani et al. (2019), implies that

$$\mathbb{P}\left(M_{i_*j_*} \in \widehat{M}_{i_*j_*} \pm q_{i_*j_*}^*(a) \cdot \widehat{s}_{i_*j_*} \middle| \mathcal{S}_{tr}, \mathcal{S}_{cal} \cup \{(i_*, j_*)\}\right) \ge 1 - a,$$

where

$$q_{i_*j_*}^*(a) = \text{Quantile}_{1-a} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} w_{ij} \cdot \delta_{R_{ij}} \right),$$

and

$$w_{ij} = \frac{h_{ij}}{\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} h_{i'j'}}.$$

Indeed, here a can be any function of the random variables we are conditioning on—that is, a may depend on n, on \mathcal{S}_{tr} , and on $\mathcal{S}_{cal} \cup \{(i_*, j_*)\}$.

Next define $a = \alpha + \Delta$ where Δ is defined as in (6). We observe that, since each \hat{h}_{ij} is a function of \mathcal{S}_{tr} , then Δ (and thus also a) can therefore be expressed as a function of n, \mathcal{S}_{tr} , and $\mathcal{S}_{cal} \cup \{(i_*, j_*)\}$. Therefore, applying the work above, we have

$$\mathbb{P}\left(M_{i_*j_*} \in \widehat{M}_{i_*j_*} \pm q_{i_*j_*}^*(\alpha + \Delta) \cdot \widehat{s}_{i_*j_*} \,\middle|\, \mathcal{S}_{\mathrm{tr}}, \mathcal{S}_{\mathrm{cal}} \cup \{(i_*, j_*)\}\right) \ge 1 - \alpha - \Delta$$

and thus, after marginalizing,

$$\mathbb{P}\left(M_{i_*j_*} \in \widehat{M}_{i_*j_*} \pm q_{i_*j_*}^*(\alpha + \Delta) \cdot \widehat{s}_{i_*j_*}\right) \ge 1 - \alpha - \mathbb{E}[\Delta].$$

Next, we verify that

$$\widehat{q} \ge q_{i_*j_*}^*(\alpha + \Delta)$$

holds almost surely—if this is indeed the case, then we have shown that

$$\mathbb{P}\left(M_{i_*j_*} \in \widehat{M}_{i_*j_*} \pm \widehat{q} \cdot \widehat{s}_{i_*j_*}\right) \ge 1 - \alpha - \mathbb{E}[\Delta],$$

which establishes the desired result. Thus we only need to show that $\widehat{q} \geq q_{i_*j_*}^*(\alpha + \Delta)$, or equivalently,

$$\operatorname{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\operatorname{cal}}} \widehat{w}_{ij} \cdot \delta_{R_{ij}} + \widehat{w}_{\operatorname{test}} \cdot \delta_{+\infty} \right) \ge \operatorname{Quantile}_{1-\alpha-\Delta} \left(\sum_{(i,j) \in \mathcal{S}_{\operatorname{cal}} \cup \{(i_*,j_*)\}} w_{ij} \cdot \delta_{R_{ij}} \right).$$

Define

$$w'_{ij} = \frac{\hat{h}_{ij}}{\sum_{(i',j')\in\mathcal{S}_{cal}\cup\{(i_*,j_*)\}} \hat{h}_{i'j'}}$$
(14)

for all $(i,j) \in \mathcal{S} \cup \{(i_*,j_*)\}$. Then by definition of $\widehat{\boldsymbol{w}}$, we see that $w'_{ij} \geq \widehat{w}_{ij}$ for $(i,j) \in \mathcal{S}$, and therefore,

$$\begin{aligned} & \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}}} \widehat{w}_{ij} \cdot \delta_{R_{ij}} + \widehat{w}_{\text{test}} \cdot \delta_{+\infty} \right) \\ & \geq \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}}} w'_{ij} \cdot \delta_{R_{ij}} + w'_{(i_*,j_*)} \cdot \delta_{+\infty} \right) \geq \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} w'_{ij} \cdot \delta_{R_{ij}} \right) \end{aligned}$$

holds almost surely. Therefore it suffices to show that

$$\text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} w'_{ij} \cdot \delta_{R_{ij}} \right) \ge \text{Quantile}_{1-\alpha-\Delta} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} w_{ij} \cdot \delta_{R_{ij}} \right)$$

holds almost surely. Indeed, we have

$$\mathsf{d}_{\mathsf{TV}}\left(\sum_{(i,j) \in \mathcal{S}_{\mathsf{cal}} \cup \{(i_*,j_*)\}} w'_{ij} \cdot \delta_{R_{ij}}, \sum_{(i,j) \in \mathcal{S}_{\mathsf{cal}} \cup \{(i_*,j_*)\}} w_{ij} \cdot \delta_{R_{ij}}\right) \leq \frac{1}{2} \sum_{(i,j) \in \mathcal{S}_{\mathsf{cal}} \cup \{(i_*,j_*)\}} |w'_{ij} - w_{ij}| = \Delta,$$

where d_{TV} denotes the total variation distance. This completes the proof.

A.3 Proofs for examples in Section 3.3

Recall the definition of Δ :

$$\Delta = \frac{1}{2} \sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} \left| \frac{\widehat{h}_{ij}}{\sum_{(i',j') \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} \widehat{h}_{i'j'}} - \frac{h_{ij}}{\sum_{(i',j') \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} h_{i'j'}} \right|.$$

Note that $\Delta \leq 1$ by definition. We start with stating a useful lemma to bound the coverage gap Δ using the estimation error of \hat{h}_{ij} .

Lemma A.1. By the definition of the coverage gap Δ , we have

$$\Delta \le \frac{\sum_{(i,j)\in\mathcal{S}_{\text{cal}}\cup\{(i_*,j_*)\}}|\widehat{h}_{ij} - h_{ij}|}{\sum_{(i',j')\in\mathcal{S}_{\text{cal}}}\widehat{h}_{i'j'}}.$$
(15)

A.3.1 Proof for Example 3.3.1

Under the logistic model, one has for any (i, j)

$$\mathbb{P}((i,j) \in \mathcal{S}_{tr}) = q \cdot p_{ij} = \frac{q \cdot \exp(u_i + v_j)}{1 + \exp(u_i + v_j)}.$$

In this case, if \hat{u} and \hat{v} are the constrained maximum likelihood estimators in Example 3.3.1, Theorem 6 in Chen et al. (2023) implies that

$$\|\widehat{\mathbf{u}} - \mathbf{u}\|_{\infty} = O_{\mathbb{P}}\left(\sqrt{\frac{\log d_1}{d_2}}\right), \qquad \|\widehat{\mathbf{v}} - \mathbf{v}\|_{\infty} = O_{\mathbb{P}}\left(\sqrt{\frac{\log d_2}{d_1}}\right),$$

with the proviso that $\|\boldsymbol{u}\|_{\infty} + \|\boldsymbol{v}\|_{\infty} \leq \tau < \infty$, $d_2 \gg \sqrt{d_1} \log d_1$ and $d_1 \gg (\log d_2)^2$. Then for $h_{ij} = \exp(-u_i - v_j)$ and $\hat{h}_{ij} = \exp(-\hat{u}_i - \hat{v}_j)$, we have

$$\max_{i,j} |\widehat{h}_{ij} - h_{ij}| = \max_{i,j} e^{-u_i - v_j} \left(e^{-(\widehat{u}_i - u_i) - (\widehat{v}_j - v_j)} - 1 \right) = O_{\mathbb{P}} \left(\sqrt{\frac{\log d_1}{d_2}} + \sqrt{\frac{\log d_2}{d_1}} \right).$$

Further, as $\min_{i,j} h_{i,j} = \min_{i,j} \exp(-u_i - v_j) \ge e^{-\tau}$, then with probability approaching one, for every $(i,j) \in [d_1] \times [d_2]$, one has $\hat{h}_{i,j} \ge h_{i,j} - |h_{ij} - \hat{h}_{ij}| \ge e^{-\tau}/2 =: h_0$. By the upper bound (15), we have

$$\Delta \lesssim \sqrt{\frac{\log d_1}{d_2}} + \sqrt{\frac{\log d_2}{d_1}} \asymp \sqrt{\frac{\log \max\{d_1, d_2\}}{\min\{d_1, d_2\}}}.$$

Further, as $\Delta \leq 1$, we have $\mathbb{E}[\Delta] \lesssim \sqrt{\frac{\log \max\{d_1, d_2\}}{\min\{d_1, d_2\}}}$

A.3.2 Proof of Example 3.3.2

Define the link function $\psi(t) = q(1 + e^{-\phi(t)})$, where ϕ is monotonic. Applying Theorem 1 in the paper (Davenport et al., 2014), we obtain that with probability at least $1 - C_1/(d_1 + d_2)$

$$\frac{1}{d_1 d_2} \|\widehat{\mathbf{A}} - \mathbf{A}\|_{\mathrm{F}}^2 \le \sqrt{2} \widetilde{C}_{\tau} \sqrt{\frac{k(d_1 + d_2)}{d_1 d_2}},\tag{16}$$

with the proviso that $d_1 d_2 \ge (d_1 + d_2) \log(d_1 d_2)$. Here $\widetilde{C}_{\tau} = 2^{39/4} e^{9/4} (1 + \sqrt{6}) \tau L_{\tau} \beta_{\tau}$ with

$$L_{\tau} = \sup_{-\tau < t \le \tau} \frac{|\psi'(t)|}{\psi(t)(1 - \psi(t))}, \quad \text{and} \quad \beta_{\tau} = \sup_{-\tau \le t \le \tau} \frac{\psi(t)(1 - \psi(t))}{|\psi'(t)|^2}.$$
 (17)

Denote this high probability event to be \mathcal{E}_0 . Since $\|\mathbf{A}\|_1 \leq \sqrt{d_1 d_2} \|\mathbf{A}\|_F$, on this event \mathcal{E}_0 , we further have

$$\frac{1}{d_1 d_2} \|\widehat{\mathbf{A}} - \mathbf{A}\|_1 \le C_\tau \left(\frac{k(d_1 + d_2)}{d_1 d_2} \right)^{1/4},$$

where $C_{\tau} = \zeta \sqrt{L_{\tau} \beta_{\tau}}$ and ζ is a universal constant.

Recall that $h_{ij} = \exp(-\phi(A_{ij}))$ and $\|\mathbf{A}\|_{\infty} \leq \tau$. On the same event \mathcal{E}_0 , we further have

$$\frac{1}{d_1 d_2} \|\widehat{\mathbf{H}} - \mathbf{H}\|_1 \le C_\tau' \left(\frac{k(d_1 + d_2)}{d_1 d_2} \right)^{1/4}, \tag{18}$$

where $C'_{\tau} = 2e^{\phi(\tau)}\sqrt{\widetilde{C}_{\tau}}$.

By the feasibility of the minimizer $\widehat{\mathbf{A}}$ and the fact that $\widehat{h}_{ij} = \exp(-\phi(\widehat{A}_{ij}))$, we have $\widehat{h}_{ij} \geq h_0 = e^{-\phi(\tau)}$ for all (i,j). This together with the upper bound (15) implies that

$$\Delta \leq \frac{1}{h_0 n_{\text{cal}}} \sum_{(i,j) \in \mathcal{S}_{\text{cal}} \cup \{(i_*,j_*)\}} |h_{ij} - \widehat{h}_{ij}| \leq \frac{1}{h_0 n_{\text{cal}}} ||\widehat{\mathbf{H}} - \mathbf{H}||_1.$$

Define a second high probability event $\mathcal{E}_1 = \{n_{\text{cal}} \geq (1-c)(1-q) || \mathbf{P} ||_1 \}$. Using the Chernoff bound, we have $\mathbb{P}(\mathcal{E}_1) \geq 1 - C_0(d_1d_2)^{-5}$. Therefore, on the event $\mathcal{E}_0 \cap \mathcal{E}_1$, we have

$$\Delta \le \frac{d_1 d_2}{c h_0 (1 - q) \|\mathbf{P}\|_1} C_{\tau}' \left(\frac{k(d_1 + d_2)}{d_1 d_2} \right)^{1/4}.$$

Under the assumptions that $p_{ij} = 1/(1 + e^{-\phi(A_{ij})})$, and that $\|\mathbf{A}\|_{\infty} \leq \tau$, we know that $p_{ij} \geq C_2$ for some constant that only depends on τ . As a result, we have $\|\mathbf{P}\|_1 \geq C_2 d_1 d_2$, which further leads to the conclusion that

$$\Delta \le \frac{1}{cC_2h_0(1-q)}C_{\tau}'\left(\frac{k(d_1+d_2)}{d_1d_2}\right)^{1/4}.$$

on the event $\mathcal{E}_0 \cap \mathcal{E}_1$. In addition, on the small probability event $(\mathcal{E}_0 \cap \mathcal{E}_1)$, one trivially has $\Delta \leq 1$. Therefore simple combinations of the cases yields the desired bound on $\mathbb{E}[\Delta]$.

A.3.3 Proof of Lemma A.1

Reusing the definition of w' (14), one has

$$\Delta = \frac{1}{2} \sum_{(i,j) \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} |w_{ij} - w'_{ij}|
= \frac{1}{2} \sum_{(i,j) \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \frac{|h_{ij} \sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \hat{h}_{i'j'} - \hat{h}_{ij} \sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} h_{i'j'}|}{\left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \hat{h}_{i'j'}\right) \left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} h_{i'j'}\right)}
\leq \frac{1}{2} \sum_{(i,j) \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \left\{ \frac{h_{ij} |\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \hat{h}_{i'j'}}{\left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \hat{h}_{i'j'}\right) \left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} h_{i'j'}\right)} + \frac{|\hat{h}_{ij} - h_{ij}| \sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \hat{h}_{i'j'}}{\left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} \hat{h}_{i'j'}\right) \left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} h_{i'j'}\right)} + \frac{1}{2} \frac{\sum_{(i,j) \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} |\hat{h}_{ij} - h_{ij}|}{\left(\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} |\hat{h}_{i'j'}\right)}$$

$$\leq \frac{\sum_{(i,j) \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} |\hat{h}_{ij} - h_{ij}|}{\sum_{(i',j') \in \mathcal{S}_{cal} \cup \{(i_*,j_*)\}} |\hat{h}_{i'j'}}.$$
(19)

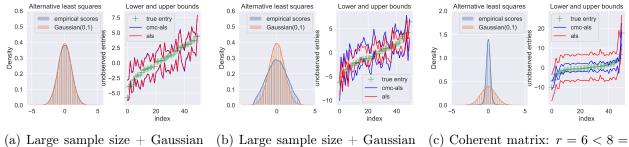
This completes the proof.

B Additional numerical experiments

In this section, we provide additional simulation results. In Section B.1, the confidence intervals are visualized. We also present the simulation results for the convex relaxation (cvx) and the conformalized convex method (cmc-cvx) in both settings with homogeneous and heterogeneous missingness in Section B.2 and B.4.

B.1 Illustration of confidence intervals and normalized scores

In Figure 4, we present the histogram of standardized scores $(\widehat{M}_{ij} - M_{ij})/\sqrt{\widehat{\theta}_{ij}^2 + \widehat{\sigma}^2}$ and the plot of the upper and lower bounds for three settings. In Figure 4a, when the model assumptions are met and $r = r^*$, the scores match well with the standard Gaussian and the prediction bounds produced by als and cmc-als are similar. With the same data generating process, when the rank is overparametrized, the distribution of scores cannot be captured by the standard Gaussian, thus the quantiles are misspecified. As we can see from the confidence intervals, als tends to have smaller intervals which lead to the undercoverage. In the last setting, the underlying matrix is no longer incoherent. When the rank is underestimated, the $r^* - r$ factors will be captured by the noise term and the high heterogeneity in the entries will further lead to overestimated noise level. As a result, the intervals by als are much larger while the conformalized intervals are more adaptive to the magnitude of entries.



noise: $r = r^* = 8$ noise: $r^* = 8 < 50 = r$

Figure 4: Histogram of standardized scores for als and prediction lower and upper bounds for 50 distinct unobserved entries.

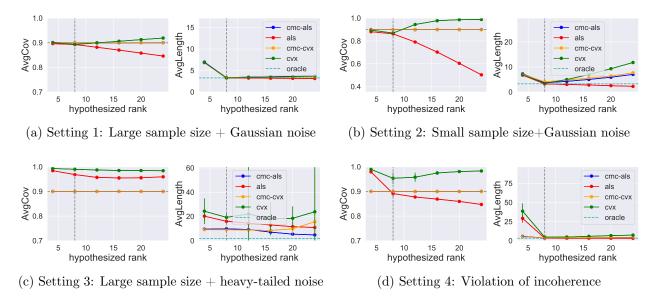


Figure 5: Comparison between conformalized and model-based matrix completion approaches.

B.2 Additional results for homogeneous misingness

In this section, we present the results for synthetic simulation with the convex relaxation cvx and the conformalized convex matrix completion method cmc-cvx. Setting 1, 2, 3, 4 are the same as introduced in Section 4.1. The true rank is $r^* = 8$ and the hypothesized rank varies from 4 to 24 with the stepsize 4.

The conformalized methods, regardless of the based algorithm adopted, have nearly exact coverage around $1-\alpha$. But we can observe different behaviors between als and cvx since the convex relaxation is free of the choice of r until the projection of $\widehat{\mathbf{M}}_{\text{cvx}}$ onto the rank-r subspace (Chen et al., 2020). As a result, when $r > r^*$, cvx tends to overestimate the strength of the noise. In Figure 5a, 5b and 5d, when $r > r^*$, cvx has coverage rate higher than the target level and the confidence interval is more conservative than conformalized methods. Since the accuracy of cvx is based on the large sample size, in Figure 5b, when the effective sample size is insufficient with small p_{ij} , the residuals from cvx have a large deviation from the standard distribution and the intervals are much larger than the oracle ones. Besides, in Figure 5c, when the noise has heavy tails than Gaussian variables, cvx overestimates the noise strength similar to als and is conservative in

coverage. When the incoherence condition is violated in Figure 5d, if $r < r^*$, both cvx and als fit the missed factor by overestimating the noise strength and produce extremely large intervals.

B.3 Estimation error for one-bit matrix estimation

The estimation error in \hat{p}_{ij} can be visualized from the following heatmaps comparing **P** and **P**. Here the entries are sorted by the order of p_{ij} for each row and each column.

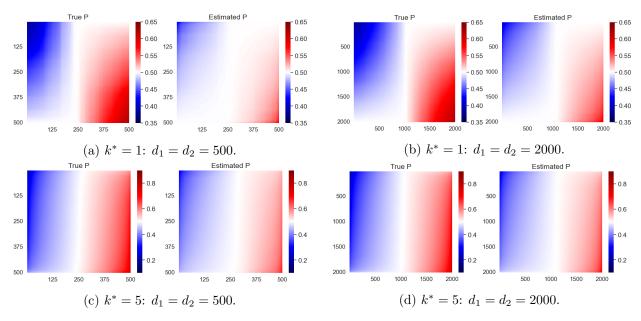


Figure 6: Heatmaps for \mathbf{P} and $\hat{\mathbf{P}}$.

B.4 Additional results for heterogeneous missingness

In Figure 7, we present the results for synthetic simulation with the convex relaxation cvx as the base algorithm, where we denote cmc-cvx and cmc*-cvx as the conformalized matrix completion method with estimated weights and true weights, respectively. Three settings with heterogeneous missingness are the same as Figure 2.

B.5 Additional plots for the sales dataset

Denote **M** the underlying matrix in the sales dataset. In Figure 8a, we plot singular values of **M** and top-5 singular values contain a large proportion of the information. In Figure 8b, we plot the histogram of entries M_{ij} 's of the underlying matrix, and the sales dataset has the range from 0 to over 20 thousand with a heavy tail.

In Figure 9, cmc-cvx has nearly exact coverage at $1-\alpha$, but cvx tends to have higher coverage than the target level. Besides, the convex approach has much larger intervals when r is large, which can be caused by the overfitting of the observed entries. As conformalized approach leaves out a proportion of observed entries as the training set, intervals produced by cmc-cvx are less accurate than cvx due to the poorly behaved base algorithm.

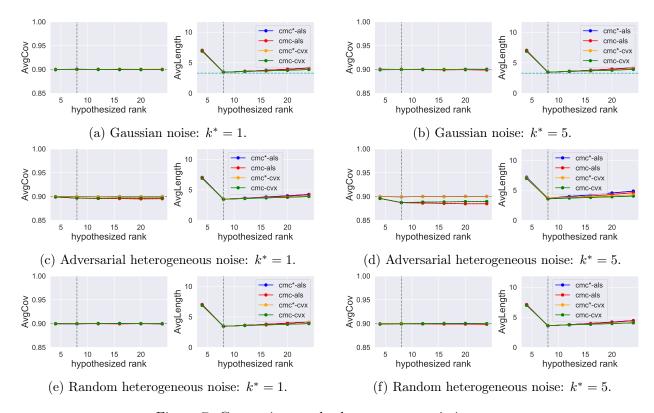


Figure 7: Comparison under heterogenous missingness.

C Additional details of algorithms and extensions

C.1 Extension to likelihood-based scores and categorical matrices

We will show in this section that cmc can also be applied to categorical matrix completion (Cao and Xie, 2015) or a more general setting in (20), the validity of which is also guaranteed by the presented theorem.

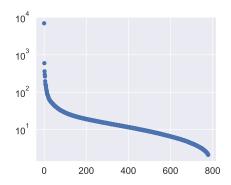
Setup To formulate the problem, consider an underlying parameter matrix $\mathbf{M}^* \in [d_1] \times [d_2]$ and the observations $\{M_{ij}: i \in [d_1], j \in [d_2]\}$ are drawn from the distribution

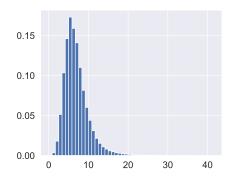
$$M_{ij} \mid M_{ij}^* \sim \mathcal{P}_{M_{ij}^*}, \tag{20}$$

where $\{\mathcal{P}_{\theta}\}_{\theta\in\Theta}$ can be a family of parametric distributions with probability density p_{θ} . The categorical matrix completion is a specific example where the support of M_{ij} is finite or countable. For example, a Poisson matrix is generated by $M_{ij} \sim \operatorname{Pois}(M_{ij}^*)$, where M_{ij}^* is the Poisson mean. Similar to the previous setup, we treat \mathbf{M} as deterministic, and entries in the subset $\mathcal{S} \subseteq [d_1] \times [d_2]$ are available. Here \mathcal{S} is sampled in the same manner as before with the matrix $\mathbf{P} \in [d_1] \times [d_2]$.

Split conformal approach Consider the split approach with the partition $S = S_{tr} \cup S_{cal}$ as in Algorithm 1. With the training set \mathbf{M}_{tr} , we obtain an estimated likelihood function $\widehat{\pi}(m; i, j)$ such that

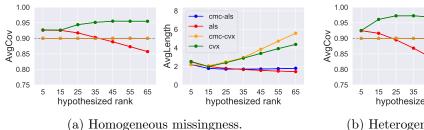
$$\widehat{\pi}(m; i, j) = \widehat{p}_{M_{ij}^*}(m),$$





- (a) Singular values of the underlying matrix **M**.
- (b) Histogram of entries in M.

Figure 8: Descriptive plots for the underlying matrix M.





us missingness. (b) Heterogeneous missingness with $k^* = 1$.

Figure 9: Comparison between conformalized and model-based matrix completion with sales dataset.

which is an estimate for the true likelihood of M_{ij} at m. The estimation can be feasible given certain low-complexity structures. For example, if a hypothesized distribution family $\{Q_{\theta}\}_{{\theta}\in\Theta}$ with probability density q_{θ} is given and the underlying mean matrix \mathbf{M}^* is assumed to be low-rank. Then, \mathbf{M} can be viewed as a perturbation of \mathbf{M}^* and we can estimate \mathbf{M}^* via matrix completion algorithms with entries in \mathbf{M}_{tr} . Denote $\widehat{\mathbf{M}}$ as the estimate for \mathbf{M}^* , then we have the estimated likelihood

$$\widehat{\pi}(m; i, j) = q_{\widehat{M}_{ij}}(m).$$

The odds ratios are also estimated from the training set, i.e. \hat{h}_{ij} , from which we compute the weights

$$\widehat{w}_{ij} = \frac{\widehat{h}_{ij}}{\sum_{(i',j') \in \mathcal{S}_{cal}} \widehat{h}_{i'j'} + \max_{(i',j') \in \mathcal{S}^c} \widehat{h}_{i'j'}}, \ (i,j) \in \mathcal{S}_{cal}, \ \widehat{w}_{test} = \frac{\widehat{h}_{i*j*}}{\sum_{(i',j') \in \mathcal{S}_{cal}} \widehat{h}_{i'j'} + \max_{(i',j') \in \mathcal{S}^c} \widehat{h}_{i'j'}}.$$

For each $(i, j) \in \mathcal{S}_{cal}$, calculate the likelihood-based nonconformity score

$$R_{ij} = -\widehat{\pi}(M_{ij}; i, j).$$

Then, for any test point $(i_*, j_*) \in \mathcal{S}^c$, we can construct the confidence interval

$$\widehat{C}(i_*, j_*) = \{ m \in [K] : \widehat{\pi}(m; i_*, j_*) \le \widehat{q} \},$$

where \widehat{q} is the weighted quantile

$$\widehat{q} = \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}}} \widehat{w}_{ij} \cdot \delta_{R_{ij}} + \widehat{w}_{\text{test}} \cdot \delta_{+\infty} \right).$$

More examples of conformal methods for classification are shown in Romano et al. (2020), Angelopoulos et al. (2020), etc.

C.2 Full conformalized matrix completion

In Algorithm 2, the procedure of the full conformalized matrix completion (full-cmc) is presented. This full conformal version of cmc offers the same coverage guarantee as given in Theorem 3.2 for the split version of cmc (except with the entire observed set S in place of S_{cal} , when defining $\Delta(\widehat{\boldsymbol{w}})$; the formal proof of this bound for full conformal is very similar to the proof of Theorem 3.2, using an analogous weighted exchangeability argument as in Lemma 3.1, and so we omit it here.

To define this algorithm, we need some notation: given the observed data $\mathbf{M}_{\mathcal{S}}$, plus a test point location (i_*, j_*) and a hypothesized value m for the test point $M_{i_*j_*}$, define a matrix $\mathbf{M}^{(m)}$ with entries

$$M_{ij}^{(m)} = \begin{cases} M_{ij}, & (i,j) \in \mathcal{S}, \\ m, & (i,j) = (i_*, j_*), \\ \emptyset, & \text{otherwise,} \end{cases}$$

$$(21)$$

where, abusing notation, " $M_{ij} = \emptyset$ " denotes that no information is observed in this entry.

We note that, when $\mathcal{M} = \mathbb{R}$ (or an infinite subset of \mathbb{R}), the computation of the prediction set is impossible in most of the cases. In that case, our algorithm can be modified via a trimmed or discretized approximation; these extensions are presented for the regression setting in the work of Chen et al. (2016, 2018), and can be extended to the matrix completion setting in a straightforward way.

C.3 Exact split conformalized matrix completion

In Algorithm 3, we present the exact split approach, which is less conservative than our one-shot approach given in Algorithm 1, but may be less computationally efficient. In this version of the algorithm, the quantile $\hat{q} = \hat{q}(i_*, j_*)$ needs to be computed for each missing entry since the weight vector $\hat{\boldsymbol{w}}$ depends on the value of \hat{p}_{i_*,j_*} .

Algorithm 2 full-cmc: full conformalized matrix completion

- 1: Input: target level 1α ; partially observed matrix $\mathbf{M}_{\mathcal{S}}$.
- 2: Using the training data $\mathbf{M}_{\mathcal{S}}$, compute an estimate $\widehat{\mathbf{P}}$ of the observation probabilities (with \widehat{p}_{ij} estimating p_{ij} , the probability of entry (i,j) being observed).
- 3: for (i_*, j_*) in S^c do
- 4: for $m \in \mathcal{M}$ do
- 5: Augment $\mathbf{M}_{\mathcal{S}}$ with one additional hypothesized entry, $\{M_{i_*,j_*}=m\}$, to obtain $\mathbf{M}^{(m)}$ defined as in (21).
- 6: Using the imputed matrix $\mathbf{M}_{\mathcal{S}}^{(m)}$, compute:
 - An initial estimate $\widehat{\mathbf{M}}^{(m)}$ using any matrix completion algorithm (with $\widehat{M}_{ij}^{(m)}$ estimating the target M_{ij});
 - Optionally, a local uncertainty estimate $\widehat{\mathbf{s}}^{(m)}$ (with $\widehat{s}_{ij}^{(m)}$ estimating our relative uncertainty in the estimate $\widehat{M}_{ij}^{(m)}$), or otherwise set $\widehat{s}_{ij}^{(m)} \equiv 1$;
 - An estimate $\widehat{\mathbf{P}}$ of the observation probabilities (with \widehat{p}_{ij} estimating p_{ij} , the probability of entry (i,j) being observed).
- 7: Compute normalized residuals for $(i, j) \in \mathcal{S} \cup \{(i_*, j_*)\},\$

$$R_{ij}^{(m)} = \frac{|M_{ij} - \widehat{M}_{ij}^{(m)}|}{\widehat{s}_{ij}^{(m)}}.$$

8: Compute weights

$$\widehat{w}_{ij} = \frac{\widehat{h}_{ij}}{\sum_{(i',j') \in \mathcal{S} \cup \{(i_*,j_*)\}} \widehat{h}_{i'j'}}, \qquad \widehat{h}_{ij} = \frac{1 - \widehat{p}_{ij}}{\widehat{p}_{ij}}, \qquad (i,j) \in \mathcal{S} \cup \{(i_*,j_*)\}.$$

9: Compute the weighted quantile

$$\widehat{q}^{(m)}(i_*, j_*) = \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}} \widehat{w}_{ij} \delta_{R_{ij}^{(m)}} + \widehat{w}_{i_*j_*} \delta_{+\infty} \right)$$
(22)

- 10: end for
- 11: end for
- 12: Output: $\left\{ \widehat{C}(i_*, j_*) = \left\{ m \in \mathcal{M} : R_{i_*j_*}^{(m)} \leq \widehat{q}^{(m)}(i_*, j_*) \right\} : (i_*, j_*) \in \mathcal{S}^c \right\}$

Algorithm 3 split-cmc: split conformalized matrix completion

- 1: **Input**: target coverage level 1α ; data splitting proportion $q \in (0, 1)$; observed entries $\mathbf{M}_{\mathcal{S}}$.
- 2: Split the data: draw $W_{ij} \stackrel{\text{i.i.d.}}{\sim} \text{Bern}(q)$, and define training and calibration sets,

$$S_{\text{tr}} = \{(i, j) \in S : W_{ij} = 1\}, \quad S_{\text{cal}} = \{(i, j) \in S : W_{ij} = 0\}.$$

- 3: Using the training data $\mathbf{M}_{\mathcal{S}_{tr}}$ indexed by $\mathcal{S}_{tr} \subseteq [d_1] \times [d_2]$, compute:
 - An initial estimate $\widehat{\mathbf{M}}$ using any matrix completion algorithm (with \widehat{M}_{ij} estimating the target M_{ij});
 - Optionally, a local uncertainty estimate $\hat{\mathbf{s}}$ (with \hat{s}_{ij} estimating our relative uncertainty in the estimate \widehat{M}_{ij}), or otherwise set $\hat{s}_{ij} \equiv 1$;
 - An estimate $\widehat{\mathbf{P}}$ of the observation probabilities (with \widehat{p}_{ij} estimating p_{ij} , the probability of entry (i, j) being observed).
- 4: Compute normalized residuals on the calibration set,

$$R_{ij} = \frac{\left| M_{ij} - \widehat{M}_{ij} \right|}{\widehat{s}_{ij}}, \ (i, j) \in \mathcal{S}_{\text{cal}}.$$

5: Compute estimated odds ratios for the calibration set and test set,

$$\widehat{h}_{ij} = \frac{\widehat{p}_{ij}}{1 - \widehat{p}_{ij}}, \ (i, j) \in \mathcal{S}_{\text{cal}} \cup \mathcal{S}^c,$$

- 6: for $(i_*, j_*) \in \mathcal{S}^c$ do
- 7: Compute weights for the calibration set and test point,

$$\widehat{w}_{ij} = \frac{\widehat{h}_{ij}}{\sum_{(i',j') \in \mathcal{S}_{\text{cal}}} \widehat{h}_{i'j'} + \widehat{h}_{i_*j_*}}, \ (i,j) \in \mathcal{S}_{\text{cal}}, \ \ \widehat{w}_{\text{test}} = \frac{\widehat{h}_{i_*j_*}}{\sum_{(i',j') \in \mathcal{S}_{\text{cal}}} \widehat{h}_{i'j'} + \widehat{h}_{i_*j_*}}.$$

8: Compute threshold

$$\widehat{q}(i_*, j_*) = \text{Quantile}_{1-\alpha} \left(\sum_{(i,j) \in \mathcal{S}_{\text{cal}}} \widehat{w}_{ij} \cdot \delta_{R_{ij}} + \widehat{w}_{\text{test}} \cdot \delta_{+\infty} \right),$$

where δ_t denotes the point mass at t.

- 9: end for
- 10: **Output**: confidence intervals

$$\widehat{C}(i_*, j_*) = \widehat{M}_{i_*j_*} \pm \widehat{q}(i_*, j_*) \cdot \widehat{s}_{i_*j_*}$$

for each unobserved entry $(i_*, j_*) \in \mathcal{S}^c$.