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Optimality of the Least Sum of Logarithms in the Problem of Matching Map Recovery in the Presence of Noise and Outliers

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Abstract. We consider the problem of estimating the matching map between two sets of feature-vectors observed in a noisy environment and contaminated by outliers. It was already known in the literature that in the outlier-free setting, the least sum of squares (LSS) and the least sum of logarithms (LSL) are both minimax-rate-optimal. It has been recently proved that the optimality properties of the LSS continue to hold in the case the data sets contain outliers. In this work, we show that the same is true for the LSL as well. Therefore, LSL has the same desirable properties as the LSS, and, in addition, it is minimax-rate-optimal in the outlier-free setting with heteroscedastic noise.

Key Words: Multidimensional Statistics, Vector Matching, Separation Rate Mathematics Subject Classification 2010: 62H99

1 Introduction

The problem of detecting a one-to-one matching between two related datasets (e.g., keypoint descriptors from different pictures of the same scene, singlecell RNA sequencing data collected at different times, vector representation of texts, etc.) has been recently extensively studied [1, 2, 3, 5]. When only one dataset contains outliers, the optimality of the matching procedures was thoroughly studied in [3, 4] from a minimax statistical viewpoint. The main procedures that were shown to enjoy the optimality properties are the Least Sum of Logarithms (LSL) and the Least Sum of Squares (LSS). In the case of the LSS, Minasyan et al. [5] developed extensions to the setting in which both datasets may contain outliers, and the number of these outliers is unknown. In practice, however, it might be more suitable to use the LSL estimator, since it is known to be less sensitive to the heteroscedasticity of the noise, see [3] for details. Indeed, since there is no simple way of checking whether the noise is homoscedastic or not, LSL might be preferred to LSS.

The goal of the present work is to examine the properties of LSL as a solution to the problem of estimating the matching map between two point clouds, i.e., sets of observation vectors, in the presence of outliers. In particular, we investigate LSL through the lens of the minimax separation rate for detecting the matching map. Our main contribution shows that LSL can optimally handle outliers. More precisely, we prove that the separation rate for LSL is of order $(d \log n)^{1/4} \vee (\log n)^{1/2}$, which is known to be minimax optimal (see [5]).

2 Problem formulation and notations

In this section, we formally state the problem and define some key quantities. Initially, we have two sets of observations $\mathbf{X} = (X_1, \ldots, X_n)$ and $\mathbf{X}^{\#} = (X_1^{\#}, \ldots, X_m^{\#})$ that we want to match, given an underlying structure of the problem. Formally, we assume that

$$\begin{cases} X_i = \theta_i + \sigma \xi_i, \\ X_j^{\texttt{\#}} = \theta_j^{\texttt{\#}} + \sigma^{\texttt{\#}} \xi_j^{\texttt{\#}}, \end{cases} \quad i \in [n] \text{ and } j \in [m], \end{cases}$$

where $[n] = \{1, ..., n\}$, $\sigma, \sigma^{\#} > 0$ are noise magnitudes, $\boldsymbol{\theta} = (\theta_1, ..., \theta_n)$ and $\boldsymbol{\theta}^{\#} = (\theta_1^{\#}, ..., \theta_m^{\#})$ are sets of deterministic vectors with real coordinates, also known as feature-vectors, and $\xi_1, ..., \xi_n, \xi_1^{\#}, ..., \xi_m^{\#} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \mathbf{I}_d)$ are i.i.d. standard normal vectors. Notice that we only observe the noisy feature-vector sets \mathbf{X} and $\mathbf{X}^{\#}$. The goal is to recover the matching between original feature-vectors.

It is assumed that for some set $S^* \subset [n]$ of cardinality k^* , there exists an injective mapping $\pi^* : S^* \to [m]$ such that $\theta_i = \theta^{\#}_{\pi^*(i)}$ is true for all $i \in S^*$. We define the *signal-to-noise* ratio $\bar{\kappa}_{all}$, which plays a central role in the detection problem, by

$$\kappa_{i,j} \triangleq \|\theta_i - \theta_j^{\#}\|_2 / (\sigma^2 + \sigma^{\#2})^{1/2}, \qquad \bar{\kappa}_{\text{all}} \triangleq \min_{i \in [n]} \min_{j \in [m] \setminus \{\pi^*(i)\}} \kappa_{i,j}.$$

Here $\kappa_{i,j}$ is the signal-to-noise ratio of the difference of the noisy features X_i and X_j^{\sharp} . Note that for a pair i, j with $j = \pi^*(i)$, we have $\kappa_{i,j} = 0$ as $\theta_i = \theta_{\pi^*(i)}^{\sharp}$.

Let \mathcal{P}_k be the set of all injective mappings of size k from $S \subset [n]$ to [m]

$$\mathcal{P}_k := \left\{ \pi : S \to [m] \text{ such, that } \begin{array}{c} S \subset [n], |S| = k, \\ \pi \text{ is injective} \end{array} \right\}.$$

We are now ready to define the LSL estimator $\hat{\pi}_k^{\text{LSL}}$ as follows:

$$\widehat{\pi}_k^{\text{LSL}} \in \underset{\pi \in \mathcal{P}_k}{\operatorname{arg\,min}} \sum_{i \in S_{\pi}} \log \|X_i - X_{\pi(i)}^{\sharp}\|_2^2.$$
(1)

Here and subsequently, by S_{π} we denote the support of the mapping π . We will denote by $\widehat{\Phi}(k)$ the error of $\widehat{\pi}_{k}^{\text{LSL}}$, that is,

$$\widehat{\Phi}(k) = \min_{\pi \in \mathcal{P}_k} \sum_{i \in S_{\pi}} \log \|X_i - X_{\pi(i)}^{\sharp}\|_2^2.$$

In the next section, we formulate and prove the main results of the present work. First, we show that for $k \leq k^*$, the estimator $\widehat{\pi}_k^{\text{LSL}}$ recovers a subset S^* of size k, and functions $\widehat{\pi}_k^{\text{LSL}}$ and π^* coincide on S^* .

3 Quality of LSL for $k \le k^*$

In the next theorem, we establish the quality of the $\widehat{\pi}_k^{\text{LSL}}$ estimator for $k \leq k^*$.

Theorem 1 Let $\widehat{S} = \operatorname{supp}(\widehat{\pi})$ for $\widehat{\pi} = \widehat{\pi}_k^{\operatorname{LSL}}$ defined by (1), $\alpha \in (0,1)$ and

$$\lambda_{n,d,\alpha} = 4 \Big(\Big(d \log(4n^2/\alpha) \Big)^{1/4} \vee \Big(8 \log(4n^2/\alpha) \Big)^{1/2} \Big).$$
 (2)

If $k \leq k^*$ and the signal-to-noise ratio satisfies the condition $\bar{\kappa}_{all} \geq \lambda_{n,d,\alpha}$, then, with probability at least $1-\alpha$, the support of the estimator $\hat{\pi}$ is included in S^* and $\hat{\pi}$ coincides with π^* on the set \hat{S} , that is,

$$\mathbf{P}(\widehat{S} \subset S^* \text{ and } \widehat{\pi}(i) = \pi^*(i) \text{ for all } i \in \widehat{S}) \ge 1 - \alpha.$$

Let us define some additional specific quantities used in the proofs. For any matching map π , we define its normalized LSL error as follows

$$L^{\text{LSL}}(\pi) = \sum_{i \in S_{\pi}} \log \frac{\|X_i - X_{\pi(i)}^{\#}\|_2^2}{\sigma^2 + \sigma^{\#2}}.$$

We also define η_{ij} and its associated quantities:

$$\eta_{ij} = \frac{\sigma\xi_i - \sigma^{\#}\xi_j^{\#}}{\sqrt{\sigma^2 + \sigma^{\#2}}}, \, \zeta_1 \triangleq \max_{i \neq j} \frac{|(\theta_i - \theta_j^{\#})^\top \eta_{ij}|}{\|\theta_i - \theta_j^{\#}\|_2}, \, \zeta_2 \triangleq d^{-1/2} \max_{i,j} \left| \|\eta_{ij}\|_2^2 - d \right|.$$
(3)

We start with upper and lower bounds on the squared norm of the quantity $\eta_{i,j}$. Using the standard concentration inequalities for χ^2_d distribution, it is straightforward to check that for any $i \in [n]$, the following holds:

$$d - \sqrt{d\zeta_2} \le \|\eta_{i,\pi(i)}\|_2^2 \le d + \sqrt{d\zeta_2}.$$

Next, we state auxiliary lemmas that we use for the proof of our main results. The first lemma states that the difference of normalized LSL error is bound from below for any π that cannot be obtained as a restriction of π^* .

Lemma 1 Let π be any matching map that cannot be obtained as a restriction of π^* on a subset of [n]. Let $S_0 \subset S^*$ be an arbitrary set satisfying $|S_0| \leq |S_{\pi}|$ and $\{i \in S_{\pi} \cap S^* : \pi(i) = \pi^*(i)\} \subset S_0$, and let π_0 be the restriction of π^* to S_0 . On the event $\Omega_0 = \{8\zeta_1 \leq \bar{\kappa}_{all}; 4\sqrt{d}\zeta_2 \leq \bar{\kappa}_{all}^2\}$, we have

$$L^{\text{LSL}}(\pi) - L^{\text{LSL}}(\pi_0) \ge \log\left(1 + \frac{\bar{\kappa}_{\text{all}}^2}{\bar{\kappa}_{\text{all}}^2 + 4d}\right) + (|S_{\pi}| - |S_0|) \log\left(\frac{\bar{\kappa}_{\text{all}}^2}{2} + d\right).$$

Proof. Let $S_{\pi}^+ \triangleq \{i \in S_{\pi} \cap S_{\pi^*} : \pi(i) = \pi^*(i)\}$ and $S_{\pi}^- \triangleq S_{\pi} \setminus S_{\pi}^+, S_0^- \triangleq S_0 \setminus S_{\pi}^+$. Without loss of generality, we enumerate the index sets $S_{\pi}^- = \{t_1, t_2, \ldots, t_k\}$ and $S_0^- = \{p_1, p_2, \ldots, p_r\}$, where $k = |S_{\pi}^-| \ge |S_0^-| = r$. Let

$$L_i(\pi) \triangleq \frac{\|X_i - X_{\pi(i)}^{\#}\|_2^2}{\sigma^2 + \sigma^{\#2}}.$$

On the event Ω_0 , for any $t \in S_{\pi}^-$, we have

$$L_{t}(\pi) = \frac{\|X_{t} - X_{\pi(t)}^{\sharp}\|_{2}^{2}}{\sigma^{2} + \sigma^{\sharp 2}}$$

$$= \frac{\|\theta_{t} - \theta_{\pi(t)}^{\sharp}\|_{2}^{2}}{\sigma^{2} + \sigma^{\sharp 2}} + 2\frac{(\theta_{t} - \theta_{\pi(t)}^{\sharp})^{\top}\eta_{t,\pi(t)}}{\sqrt{\sigma^{2} + \sigma^{\sharp 2}}} + \|\eta_{t,\pi(t)}\|_{2}^{2}$$

$$\geq \frac{\|\theta_{t} - \theta_{\pi(t)}^{\sharp}\|_{2}^{2}}{\sigma^{2} + \sigma^{\sharp 2}} - 2\zeta_{1}\frac{\|\theta_{t} - \theta_{\pi(t)}^{\sharp}\|_{2}}{\sqrt{\sigma^{2} + \sigma^{\sharp 2}}} + \|\eta_{t,\pi(t)}\|_{2}^{2}$$

$$= \kappa_{t,\pi(t)}^{2} - 2\zeta_{1}\kappa_{t,\pi(t)} + \|\eta_{t,\pi(t)}\|_{2}^{2}$$

$$\geq \kappa_{t,\pi(t)}^{2} - 2\zeta_{1}\kappa_{t,\pi(t)} + d - \sqrt{d}\zeta_{2}$$

$$\geq d + \bar{\kappa}_{all}^{2}/2.$$
(4)

On the same event, we have

$$L_p(\pi_0) = \|\eta_{p,\pi_0(p)}\|_2^2 \le d + \sqrt{d\zeta_2} \le d + \bar{\kappa}_{all}^2/4$$

as π_0 is a restriction of π^* . Combining this with equation (4), on the event Ω_0 , for any $t \in S_{\pi}^-$ and $p \in S_0^-$, we obtain

$$L_t(\pi) - L_p(\pi_0) \ge d + \bar{\kappa}_{all}^2 / 2 - d - \bar{\kappa}_{all}^2 / 4 \ge \bar{\kappa}_{all}^2 / 4$$

For any $t \in S_{\pi}^{-}$ and $p \in S_{0}^{-}$, on the event Ω_{0} , direct computations lead to the following relation

$$\log(L_t(\pi)) - \log(L_p(\pi_0)) \ge \log \frac{L_p(\pi_0) + \bar{\kappa}_{all}^2/4}{L_p(\pi_0)}$$
$$= \log \left(1 + \frac{\bar{\kappa}_{all}^2/4}{L_p(\pi_0)}\right)$$
$$\ge \log \left(1 + \frac{\bar{\kappa}_{all}^2}{4d + \bar{\kappa}_{all}^2}\right)$$

Putting things together, we take the corresponding sums over S_{π} and S_0 , and combining with the inequality from the last display, we have

$$\begin{split} L^{\text{LSL}}(\pi) - L^{\text{LSL}}(\pi_0) &= \sum_{i \in S_{\pi}} \log L_i(\pi) - \sum_{i \in S_0} \log L_i(\pi_0) \\ &= \sum_{t \in S_{\pi}^-} \log L_t(\pi) - \sum_{p \in S_0^-} \log L_p(\pi_0) \\ &= \sum_{1 \le i \le r} \left(\log L_{t_i}(\pi) - \log L_{p_i}(\pi_0) \right) + \sum_{r+1 \le i \le k} \log L_{t_i}(\pi) \\ &\geq \sum_{1 \le i \le r} \log \left(1 + \frac{\bar{\kappa}_{\text{all}}^2}{4d + \bar{\kappa}_{\text{all}}^2} \right) + \sum_{r+1 \le i \le k} \log(\bar{\kappa}_{\text{all}}^2/2 + d) \\ &\geq \log \left(1 + \frac{\bar{\kappa}_{\text{all}}^2}{\bar{\kappa}_{\text{all}}^2 + 4d} \right) + (|S_{\pi}| - |S_0|) \log(\bar{\kappa}_{\text{all}}^2/2 + d). \end{split}$$

on Ω_0 , which concludes the proof of the lemma. \Box

For the proof of Theorem 1, we also use Lemma 2 of [5] which is restated below.

Lemma 2 [Galstyan et al. [5], Lemma 2] Let $\Omega_{0,x} = \{8\zeta_1 \leq x\} \cap \{4\sqrt{d}\zeta_2 \leq x^2\}$ with ζ_1, ζ_2 defined as in (3). Then for every x > 0, $\mathbf{P}(\Omega_{0,x}^{\complement})$ is upper bounded by

$$2n^{2} \Big(\exp\left\{-\frac{x^{2}}{128}\right\} + \exp\left\{-\frac{x^{2}}{128d}(x^{2} \wedge 4d)\right\} \Big).$$
 (5)

We are now ready to prove Theorem 1.

Proof of Theorem 1 Let $\hat{\pi}$ be a matching map that cannot be obtained as a restriction of π^* . Using Lemma 1 on Ω_0 , we have $L^{\text{LSL}}(\hat{\pi}) - L^{\text{LSL}}(\pi_0) \geq \log(\bar{\kappa}_{\text{all}}^2/2 + d) > 0$ for some π_0 which is a restriction of π^* . Therefore, $\hat{\pi}$ cannot be a minimizer of $\hat{\Phi}(k)$, hence a minimizer of $L^{\text{LSL}}(\cdot)$ over \mathcal{P}_k must be a restriction of π^* , and consequentially, $\hat{S} \subset S^*$. According to Lemma 2, a sufficient condition for $\mathbf{P}(\Omega_0) \geq 1 - \alpha$ to hold can be the following:

$$\begin{cases} 2n^2 \exp\left\{-\bar{\kappa}_{\rm all}^2/128\right\} \le \alpha/2,\\ 2n^2 \exp\left\{-\frac{(\bar{\kappa}_{\rm all}/16)^2}{d} \left(2\bar{\kappa}_{\rm all}^2 \land 8d\right)\right\} \le \alpha/2. \end{cases}$$

This system is equivalent to

$$\bar{\kappa}_{\text{all}} \ge 8\left(2\log\frac{4n^2}{\alpha}\right)^{1/2} \quad \text{and} \quad \bar{\kappa}_{\text{all}} \ge 4\left(\frac{d}{2}\log\frac{4n^2}{\alpha}\right)^{1/4}.$$

Therefore, if the $\bar{\kappa}_{all}$ ratio satisfies

$$\bar{\kappa}_{\text{all}} \ge 4\left(\left(d\log(4n^2/\alpha)\right)^{1/4} \vee \left(8\log(4n^2/\alpha)\right)^{1/2}\right),$$

we have $\mathbf{P}(\Omega_0) \geq 1 - \alpha$. \Box

Estimation of the number of inliers k^* 4

In this section, we assume that the noise magnitudes $\sigma, \sigma^{\#}$ are known, while no information about k^* is available. Throughout this section, it will become clear that it is not necessary to know individual noise magnitudes σ and $\sigma^{\#}$. On the downside, we need to know $\sigma_0^2 = \sigma^2 + \sigma^{\#2}$. The estimator for unknown parameter k^* is defined as follows:

 $\widehat{k} = 1 + \max\left\{k \in \{0, \dots, n-1\} : \widehat{\Phi}(k+1) - \widehat{\Phi}(k) < \sigma_0^2 \log(d + \lambda_{n,d,\alpha}^2/4)\right\}$

with $\lambda_{n,d,\alpha}$ as in (2). Notice that in this matching size estimation procedure, the quantity σ_0^2 exposes, and some additional care is necessary to deal with the case of unknown σ_0^2 . For this reason, and for simplicity of presentation, we assume that σ_0^2 is known. We are now ready to formulate our second main result.

Theorem 2 Let $\alpha \in (0, 1)$. If $\bar{\kappa}_{all} > \lambda_{n,d,\alpha}$, then

$$\mathbf{P}(\widehat{k} = k^* \text{ and } \widehat{\pi}_{\widehat{k}} = \pi^*) \ge 1 - \alpha.$$

In other words, Theorem 2 states that $\lambda_{n,d,\alpha}$ is an upper bound on the separation distance in the case of unknown k^* . We begin with two auxiliary lemmas. Let us define the minimum possible error as $\widehat{L}(k) = \min_{\pi \in \mathcal{P}_k} L^{\text{LSL}}(\pi)$.

Lemma 3 On event $\Omega_0 = \{8\zeta_1 \leq \bar{\kappa}_{all}; 4\sqrt{d} \zeta_2 \leq \bar{\kappa}_{all}^2\}, we have$

$$\widehat{L}(k^*+1) - \widehat{L}(k^*) \ge \log\left(1 + \frac{\bar{\kappa}_{\text{all}}^2}{4d + \bar{\kappa}_{\text{all}}^2}\right) + \log\left(d + \frac{\bar{\kappa}_{\text{all}}^2}{2}\right).$$

Proof. We have already seen in the proof of Theorem 1 that $\hat{\pi}_{k^*} = \pi^*$ on Ω_0 . Therefore,

$$\widehat{L}(k^*+1) - \widehat{L}(k^*) = L^{\text{LSL}}(\widehat{\pi}_{k^*+1}) - L^{\text{LSL}}(\pi^*).$$

Applying the proof of Lemma 1 to $\pi = \hat{\pi}_{k^*+1}, \pi_0 = \pi^*$, we have

$$\begin{split} \widehat{L}(k^* + 1) - \widehat{L}(k^*) &= L^{\text{LSL}}(\widehat{\pi}_{k^* + 1}) - L^{\text{LSL}}(\pi^*) \\ &\geq \log\left(1 + \frac{\bar{\kappa}_{\text{all}}^2}{4d + \bar{\kappa}_{\text{all}}^2}\right) + (|S_{\widehat{\pi}_{k^* + 1}}| - |S_0|) \log\left(d + \frac{\bar{\kappa}_{\text{all}}^2}{2}\right) \\ &= \log\left(1 + \frac{\bar{\kappa}_{\text{all}}^2}{4d + \bar{\kappa}_{\text{all}}^2}\right) + \log\left(d + \frac{\bar{\kappa}_{\text{all}}^2}{2}\right), \end{split}$$

which concludes the proof. \Box

Lemma 4 On the event $\Omega_0 = \{8\zeta_1 \leq \bar{\kappa}_{all}; 4\sqrt{d}\zeta_2 \leq \bar{\kappa}_{all}^2\}$, for every $k < k^*$, we have $\widehat{L}(k+1) - \widehat{L}(k) \le \log(d + \sqrt{d}\zeta_2).$

Proof. Let $\hat{\pi}_k$ be a matching map from \mathcal{P}_k minimizing $L(\cdot)$, i.e., such that $L(\hat{\pi}_k) = \hat{L}(k)$. According to Lemma 1, we have $\hat{\pi}_k(i) = \pi^*(i)$ for every $i \in \hat{S}_k \triangleq S_{\hat{\pi}_k}$. One easily checks that there exists a set $\hat{S}_{k+1} \subset S^*$ of cardinality k+1 such that $\hat{S}_k \subset \hat{S}_{k+1}$ and $\hat{L}(k+1) = L(\hat{\pi}_{k+1})$, where $\hat{\pi}_{k+1}$ is the restriction of π^* to \hat{S}_{k+1} . Indeed, if π is any element of \mathcal{P}_{k+1} minimizing $L(\cdot)$, it is defined as a restriction of π^* on some set S of cardinality k+1. If we replace arbitrary k elements of S by those of \hat{S}_k and modify π accordingly, we will get a new mapping from \mathcal{P}_{k+1} for which the value of $L(\cdot)$ is less than or equal to $L(\pi)$. Therefore, we have found a matching map that minimizes $L(\cdot)$ over \mathcal{P}_{k+1} and has a support that is obtained by adding one point to \hat{S}_k . This implies that

$$\begin{aligned} \widehat{L}(k+1) - \widehat{L}(k) &= L(\widehat{\pi}_{k+1}) - L(\widehat{\pi}_k) \\ &= \sum_{i \in \widehat{S}_{k+1}} \log \|\eta_{i,\pi^*(i)}\|_2^2 - \sum_{i \in \widehat{S}_k} \log \|\eta_{i,\pi^*(i)}\|_2^2 \\ &= \sum_{i \in \widehat{S}_{k+1} \setminus \widehat{S}_k} \log \|\eta_{i,\pi^*(i)}\|_2^2 \le \log(d + \sqrt{d}\,\zeta_2). \end{aligned}$$

Now we will prove Theorem 2.

Proof of Theorem2 Lemma 2 implies that the event $\Omega_1 = \{8\zeta_1 \leq \lambda_{n,d,\alpha}; 4\sqrt{d}\zeta_2 \leq \lambda_{n,d,\alpha}^2\}$ has probability at least $1 - \alpha$. Since Ω_1 is included in Ω_0 , in view of Lemma 4, on Ω_1 , we have $\widehat{L}(k+1) - \widehat{L}(k) \leq \log(d + \lambda_{n,d,\alpha}^2/4)$ for any $k < k^*$. On the other hand, in view of Lemma 3, on the same event, we have

$$\begin{aligned} \widehat{L}(k^*+1) - \widehat{L}(k^*) &\geq \log\left(1 + \frac{\overline{\kappa}_{\text{all}}^2}{(\overline{\kappa}_{\text{all}}^2 + 4d)}\right) + \log\left(d + \frac{\overline{\kappa}_{\text{all}}^2}{2}\right) \\ &> \log\left(d + \lambda_{n,d,\alpha}^2/4\right). \end{aligned}$$

This implies $\hat{k} = k^*$, and, therefore, $\hat{\pi}_{\hat{k}} = \hat{\pi}_{k^*}$. Due to Theorem 1, on the same event Ω_1 , we have $\hat{\pi}_{k^*} = \pi^*$. \Box

5 Conclusion

In this work, we showed that the LSL estimator yields the minimax separation distance rate in the case when we allow outliers to be present in both datasets. It is worth noting that the minimax rate coincides with the one obtained in [4], and the statistical complexity of the problem is the same as in the case of outliers on one side or no outliers at all. The latter is proved in [3]. From the computational perspective, the complexity of computing $\hat{\pi}_k^{\text{LSL}}$ is the same as that of π_k^{LSS} . The problem reduces to the minimumcost-flow problem and can be solved efficiently. It would be interesting to investigate the case of anisotropic noise, i.e., considering general covariance Σ instead of $\sigma^2 \mathbf{I}_d$.

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