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# IMPROVED BOUNDS FOR SMALL-SAMPLE ESTIMATION\*

SERGE GRATTON<sup>†</sup> AND DAVID TITLEY-PELOQUIN<sup>‡</sup>

**Abstract.** We derive improved error bounds for small-sample statistical estimation of the matrix Frobenius norm. The bounds rigorously establish that small-sample estimators provide reliable order-of-magnitude estimates of norms and condition numbers, for matrices of arbitrary rank, even when very few random samples are used.

**Key words.** statistical estimation, small-sample estimation, norm estimation, condition number estimation

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**1. Introduction.** The Frobenius norm of a matrix  $B \in \mathbb{R}^{m \times n}$  is in principle straightforward to compute. In many applications, however, one is interested in the Frobenius norm of a matrix whose entries are either too expensive to compute explicitly or not available at all. For example,  $B$  might be the inverse of a known matrix  $A$  of large dimensions, and explicitly computing a factorization of  $A$  that would reveal  $A^{-1}$  might be too expensive. Another example is condition number estimation, in which the matrix  $B$  is the (unknown) matrix representation of the Fréchet derivative of a given matrix function; see, e.g., [14, 15, 16, 3, 11, 2, 7, 8], to cite only a few examples. For a more thorough discussion of other applications, we refer to [1] and the references therein.

In this paper we investigate some properties of two randomized estimators of the Frobenius norm of a matrix  $B \in \mathbb{R}^{m \times n}$ . The estimators only require  $B$  through the action of a matrix-vector product:  $u \leftarrow Bv$ . We are interested in “small-sample” estimation as defined by Gudmundsson, Kenney, and Laub [12, 13]. Specifically, we wish to prove that, with high probability, a realization of the estimator is close in magnitude to  $\|B\|_F$  even when very few random samples are used. In other words,

$$(1.1) \quad \text{Prob} \left\{ \frac{\|B\|_F}{\tau} \leq \text{estimator}_k(B) \leq \tau \|B\|_F \right\} \geq 1 - \delta(k, \tau),$$

where  $\delta(k, \tau) \rightarrow 0$  as the number of samples  $k$  and/or the tolerance  $\tau > 1$  increases, and  $\delta(k, \tau)$  is close to 0 even for small  $k$  and for  $\tau$  not too large. We present error bounds that do not deteriorate as the rank of  $B$  increases, thereby settling a conjecture from [12]. Our results also lead to an improvement of probabilistic relative error bounds from [1] and [19].

**2. The Gaussian and GKL estimators.** First we recall the Gaussian estimator, as well as the small-sample statistical estimator of Gudmundsson, Kenney, and Laub [12, 13], which we abbreviate as the GKL estimator.

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DEFINITION 2.1. Let  $Z$  be an  $n \times k$  matrix with  $k \leq n$  whose entries are mutually independent standard normal random variables, and let  $Q$  be the  $n \times k$  “thin”  $Q$  factor in the QR decomposition of  $Z$ . The Gaussian estimator of  $\|B\|_F$  is defined as

$$(2.1) \quad \psi_k(B) = \frac{1}{\sqrt{k}} \|BZ\|_F,$$

while the GKL estimator is defined as

$$(2.2) \quad \eta_k(B) = \frac{\sqrt{n}}{\sqrt{k}} \|BQ\|_F.$$

The GKL estimator has been widely used for norm and condition number estimation. It is shown in [12] that if  $B$  has rank  $r$ ,

$$(2.3) \quad \text{Prob} \left\{ \frac{\|B\|_F}{\tau} \leq \eta_k(B) \leq \tau \|B\|_F \right\} \geq 1 - r \left( 1 - \mathcal{I}\left(\frac{k\tau^2}{n}\right) + \mathcal{I}\left(\frac{k}{n\tau^2}\right) \right),$$

where  $\mathcal{I}(\alpha) = 1$  if  $\alpha \geq 1$  and

$$\mathcal{I}(\alpha) = \frac{\int_0^\alpha t^{(k-2)/2} (1-t)^{(n-k-2)/2} dt}{\int_0^1 t^{(k-2)/2} (1-t)^{(n-k-2)/2} dt}$$

is a regularized Beta function if  $0 < \alpha < 1$ . When the rank of  $B$  is close to 1, the right-hand side of (2.3) increases fast toward 1 as  $k$  and/or  $\tau$  increase. On the other hand, when  $r$  is large, the bound becomes very pessimistic. Furthermore, because  $r$  is not generally known a priori, for prediction purposes the best one can do is use (2.3) with  $r = \min\{m, n\}$ , leading to a very pessimistic bound. It is conjectured in [12] that the bound (2.3) holds without the factor  $r$ . It is this conjecture which motivated the present study.

Next we turn to the Gaussian estimator in (2.1). It is straightforward to verify that  $\psi_k^2(B)$  is a linear combination of independent chi-squared variables with  $k$  degrees of freedom, denoted  $\chi_i^2(k)$  below:

$$(2.4) \quad \psi_k^2(B) = \frac{1}{k} \sum_{i=1}^r \sigma_i^2 \chi_i^2(k),$$

where  $\sigma_1 \geq \dots \geq \sigma_r > 0$  are the nonzero singular values of  $B$ . From this we have

$$\mathbb{E}\{\psi_k^2(B)\} = \|B\|_F^2, \quad \text{Var}\{\psi_k^2(B)\} = \frac{2}{k} \sum_{i=1}^r \sigma_i^4 \leq \frac{2}{k} \|B\|_F^4.$$

Recall that for small-sample estimation, we are restricted to  $k \ll n$  and we are interested in order-of-magnitude estimation. The following proposition establishes that in this setting the two estimators  $\eta_k(B)$  and  $\psi_k(B)$  are essentially equivalent.

PROPOSITION 2.2. For any matrix  $B \in \mathbb{R}^{m \times n}$  and any  $\tau > 0$ , the estimators  $\psi_k(B)$  and  $\eta_k(B)$  defined in (2.1) and (2.2) satisfy

$$\text{Prob} \left\{ 1 - \frac{\sqrt{k} + \tau}{\sqrt{n}} \leq \frac{\psi_k(B)}{\eta_k(B)} \leq 1 + \frac{\sqrt{k} + \tau}{\sqrt{n}} \right\} \geq 1 - 2 \exp \left( -\frac{\tau^2}{2} \right).$$

*Proof.* Because  $Z = QR$  with  $Q^T Q = I_k$ ,

$$\psi_k(B) = \frac{\sqrt{n}}{\sqrt{k}} \frac{\|BQR\|_F}{\sqrt{n}} \leq \frac{\sqrt{n}}{\sqrt{k}} \frac{\|BQ\|_F \|R\|_2}{\sqrt{n}} = \eta_k(B) \frac{\|R\|_2}{\sqrt{n}} = \eta_k(B) \frac{\|Z\|_2}{\sqrt{n}}.$$

On the other hand,

$$\eta_k(B) = \frac{\sqrt{n}}{\sqrt{k}} \|BQRR^{-1}\|_F \leq \frac{\sqrt{n}}{\sqrt{k}} \|BZ\|_F \|R^{-1}\|_2 = \psi_k(B) \frac{\sqrt{n}}{\sigma_{\min}(Z)},$$

where  $\sigma_{\min}(\cdot)$  denotes the smallest singular value. It follows that

$$\frac{\sigma_{\min}(Z)}{\sqrt{n}} \leq \frac{\psi_k(B)}{\eta_k(B)} \leq \frac{\|Z\|_2}{\sqrt{n}}.$$

To complete the proof we use a result of Gordon [9, 10] popularized by Davidson and Szarek [6]: for any  $\tau > 0$ ,

$$\sqrt{n} - \sqrt{k} - \tau \leq \sigma_{\min}(Z) \leq \|Z\|_2 \leq \sqrt{n} + \sqrt{k} + \tau$$

holds with probability at least  $1 - 2\exp(-\tau^2/2)$ .  $\square$

Proposition 2.2 is not very surprising: the fact that Gaussian and random orthonormal matrices behave the same way is well known and dates at least as far back as [17].

In the following section we present new bounds of the form (1.1) for  $\psi_k(B)$ . By Proposition 2.2, these bounds also essentially apply for  $\eta_k(B)$  when  $k \ll n$ . Our bounds are stated in terms of the stable rank of  $B$ ,

$$(2.5) \quad \rho(B) = \frac{\|B\|_F^2}{\|B\|_2^2}.$$

The concept of stable rank dates at least as far back as [4, 5]; see, for example, [20, 21] for many examples of its use in linear algebra. In contrast to (2.3), our bounds are useful even when the matrix  $B$  has a large rank: they do not deteriorate with increasing  $r$  but improve with increasing  $\rho$ .

### 3. Improved convergence bounds.

**3.1. Chernoff bounds.** The Gaussian estimator  $\psi_k(B)$  is one of several randomized estimators surveyed in [1] and [19]. In our notation, [1, Theorem 5.2] shows that for  $\epsilon < 0.1$ ,

$$(3.1) \quad \text{Prob}\left\{|\psi_k^2(B) - \|B\|_F^2| \leq \epsilon \|B\|_F^2\right\} \geq 1 - 2\exp\left(-\frac{k}{20}\epsilon^2\right).$$

Thus, for any  $\epsilon \in (0, 0.1)$  and  $\delta \in (0, 1)$ , at least  $k = 20\epsilon^{-2} \ln(2/\delta)$  samples are required to ensure that

$$\text{Prob}\left\{|\psi_k^2(B) - \|B\|_F^2| \leq \epsilon \|B\|_F^2\right\} \geq 1 - \delta.$$

In [19, Theorem 3], this result is improved to

$$(3.2) \quad k = 8\rho^{-1}\epsilon^{-2} \ln(2/\delta).$$

The value of  $k$  in (3.2) can be very large when  $\epsilon$  is small because of the  $\epsilon^{-2}$  factor. Recall, however, that in the setting of small-sample estimation one does not require  $\|B\|_F$  with a great deal of accuracy and one is limited to using a small value of  $k$ . The following theorem applies in this setting.

**THEOREM 3.1.** *Let  $B \in \mathbb{R}^{m \times n}$  be a matrix of rank  $r$  and stable rank  $\rho$  whose Frobenius norm is to be estimated, and let  $\psi_k(B)$  be defined by (2.1). For any  $\tau > 1$  and  $k \leq n$ ,*

$$(3.3) \quad \text{Prob}\{\psi_k(B) \geq \tau \|B\|_F\} \leq \exp\left(-\frac{k\rho}{2}(\tau-1)^2\right),$$

$$(3.4) \quad \text{Prob}\left\{\psi_k(B) \leq \frac{\|B\|_F}{\tau}\right\} \leq \exp\left(-\frac{k\rho}{4} \frac{(\tau^2-1)^2}{\tau^4}\right),$$

and

$$(3.5) \quad \begin{aligned} & \text{Prob}\left\{\frac{\|B\|_F}{\tau} < \psi_k(B) < \tau \|B\|_F\right\} \\ & \geq 1 - \exp\left(-\frac{k\rho}{2}(\tau-1)^2\right) - \exp\left(-\frac{k\rho}{4} \frac{(\tau^2-1)^2}{\tau^4}\right). \end{aligned}$$

*Proof.* We use the same idea as in [1] and [19]. Namely, we use the fact that

$$(3.6) \quad \begin{aligned} & \text{Prob}\left\{\frac{\|B\|_F}{\tau} < \psi_k(B) < \tau \|B\|_F\right\} \\ & = 1 - \text{Prob}\{\psi_k(B) \geq \tau \|B\|_F\} - \text{Prob}\{\psi_k(B) \leq \|B\|_F/\tau\} \end{aligned}$$

and bound each probability in the right-hand side separately by using a Chernoff approach. For any  $t > 0$ , by Markov's inequality we have

$$(3.7) \quad \begin{aligned} \text{Prob}\{\psi_k(B) \geq \tau \|B\|_F\} &= \text{Prob}\{\exp(tk\psi_k^2(B)) \geq \exp(tk\tau^2\|B\|_F^2)\} \\ &\leq \frac{\mathbb{E}\{\exp(tk\psi_k^2(B))\}}{\exp(tk\tau^2\|B\|_F^2)}. \end{aligned}$$

In the above, the numerator is the moment generating function (MGF) of the random variable  $k\psi_k^2(B)$ . Recall from (2.4) that this is a linear combination of independent chi-squared variables with  $k$  degrees of freedom. It is known (see, e.g., [18, section 3.2]) that its MGF is defined for  $|t| < \frac{1}{2\sigma_1^2}$  and satisfies

$$\begin{aligned} \mathbb{E}\{\exp(tk\psi_k^2(B))\} &= \prod_{i=1}^r (1 - 2\sigma_i^2 t)^{-k/2} \\ &= \exp\left(-\frac{k}{2} \sum_{i=1}^r \ln(1 - 2\sigma_i^2 t)\right) = \exp\left(\frac{k}{2} \sum_{i=1}^r \sum_{j=1}^{\infty} \frac{(2\sigma_i^2 t)^j}{j}\right), \end{aligned}$$

where  $\sigma_1 \geq \dots \geq \sigma_r > 0$  are the nonzero singular values of  $B$ . Pick  $t = \frac{\mu}{2\sigma_1^2}$  for some  $\mu \in (0, 1)$ . Then from (3.7),

$$\begin{aligned} \text{Prob}\{\psi_k(B) \geq \tau \|B\|_F\} &\leq \exp\left(\frac{k}{2} \sum_{i=1}^r \sum_{j=1}^{\infty} \frac{\mu^j \sigma_i^{2j}}{j \sigma_1^{2j}}\right) \exp\left(\frac{-\mu k \rho \tau^2}{2}\right) \\ &= \exp\left(-\frac{k\rho}{2} \mu (\tau^2 - 1) + \frac{k}{2} \sum_{i=1}^r \sum_{j=2}^{\infty} \frac{\mu^j \sigma_i^{2j}}{j \sigma_1^{2j}}\right). \end{aligned}$$

In the above,

$$\sum_{i=1}^r \sum_{j=2}^{\infty} \frac{\mu^j \sigma_i^{2j}}{j \sigma_1^{2j}} \leq \sum_{i=1}^r \sum_{j=2}^{\infty} \frac{\mu^j \sigma_i^{2j}}{\sigma_1^{2j}} = \sum_{i=1}^r \frac{\mu^2 \sigma_i^4 / \sigma_1^4}{1 - \mu \sigma_i^2 / \sigma_1^2} \leq \frac{\mu^2 \rho}{1 - \mu},$$

which gives

$$\text{Prob}\{\psi_k(B) \geq \tau \|B\|_F\} \leq \exp\left(-\frac{k\rho}{2} \left(\mu(\tau^2 - 1) - \frac{\mu^2}{1 - \mu}\right)\right).$$

It is straightforward to verify that over all  $\mu \in (0, 1)$ , the smallest bound is achieved when  $\mu = 1 - \tau^{-1}$ , leading to (3.3).

Similarly, for any  $t \in (0, 1/(2\sigma_1^2))$  we have

$$\begin{aligned} \text{Prob}\{\psi_k(B) \leq \|B\|_F / \tau\} &= \text{Prob}\{\exp(-tk\psi_k^2(B)) \geq \exp(-tk\|B\|_F^2 / \tau^2)\} \\ &\leq \mathbb{E}\{\exp(-tk\psi_k^2(B))\} \exp(tk\|B\|_F^2 / \tau^2) \\ &= \exp\left(\frac{k}{2} \sum_{i=1}^r \sum_{j=1}^{\infty} \frac{(-1)^j (2\sigma_i^2 t)^j}{j} + \frac{tk\|B\|_F^2}{\tau^2}\right). \end{aligned}$$

Picking  $t = \frac{\mu}{2\sigma_1^2}$  for some  $\mu \in (0, 1)$ , we obtain

$$\text{Prob}\{\psi_k(B) \leq \|B\|_F / \tau\} \leq \exp\left(-\frac{k\rho}{2} \mu(1 - \tau^{-2}) + \frac{k}{2} \sum_{i=1}^r \sum_{j=2}^{\infty} \frac{(-1)^j \mu^j \sigma_i^{2j}}{j \sigma_1^{2j}}\right).$$

In the above,

$$\left| \sum_{i=1}^r \sum_{j=2}^{\infty} \frac{(-1)^j \mu^j \sigma_i^{2j}}{j \sigma_1^{2j}} \right| \leq \sum_{i=1}^r \frac{\mu^2 \sigma_i^4}{2\sigma_1^4} \leq \frac{\mu^2 \rho}{2},$$

leading to

$$\text{Prob}\{\psi_k(B) \leq \|B\|_F / \tau\} \leq \exp\left(-\frac{k\rho}{2} \left(\mu(1 - \tau^{-2}) - \frac{\mu^2}{2}\right)\right).$$

It is straightforward to verify that  $\mu = 1 - \tau^{-2}$  gives the optimal bound (3.4). Substituting (3.3) and (3.4) into (3.6) completes the proof.  $\square$

We can use Theorem 3.1 to determine the number of samples  $k$  required to estimate  $\|B\|_F$  to within a given factor  $\tau$  with probability at least  $1 - \delta$ .

**COROLLARY 3.2.** *In the notation of Theorem 3.1, for any  $\tau \geq 2$  and  $\delta \in (0, 1)$ , at least*

$$k = 4\rho^{-1} \frac{\tau^4}{(\tau^2 - 1)^2} \ln\left(\frac{2}{\delta}\right)$$

*samples are required to ensure that*

$$\text{Prob}\left\{\frac{\|B\|_F}{\tau} < \psi_k(B) < \tau \|B\|_F\right\} \geq 1 - \delta.$$

*Proof.* If  $\tau \geq 2$ , then  $(\tau - 1)^2 \geq \frac{(\tau^2 - 1)^2}{2\tau^4}$ . Thus from (3.5)

$$\text{Prob}\left\{\frac{\|B\|_F}{\tau} < \psi_k(B) < \tau\|B\|_F\right\} \geq 1 - 2 \exp\left(-\frac{k\rho}{4} \frac{(\tau^2 - 1)^2}{\tau^4}\right).$$

The result follows by setting the above equal to  $1 - \delta$  and solving for  $k$ .  $\square$

Theorem 3.1 can also be used to improve the constant factor in known relative error bounds.

**COROLLARY 3.3.** *In the notation of Theorem 3.1, for any  $\epsilon \in (0, \frac{1}{2})$ ,*

$$\text{Prob}\left\{|\psi_k(B) - \|B\|_F| \leq \epsilon\|B\|_F\right\} \geq 1 - 2 \exp\left(-\frac{k\rho}{2}\epsilon^2\right).$$

*Therefore, for any  $\epsilon \in (0, \frac{1}{2})$  and  $\delta \in (0, 1)$ , at least*

$$(3.8) \quad k = 2\rho^{-1}\epsilon^{-2} \ln\left(\frac{2}{\delta}\right)$$

*samples are required to ensure that*

$$\text{Prob}\left\{|\psi_k(B) - \|B\|_F| \leq \epsilon\|B\|_F\right\} \geq 1 - \delta.$$

*Proof.* Note that

$$|\psi_k(B) - \|B\|_F| \leq \epsilon\|B\|_F \iff (1 - \epsilon)\|B\|_F \leq \psi_k(B) \leq (1 + \epsilon)\|B\|_F.$$

Taking  $\tau = 1 + \epsilon$  in (3.3) and  $\tau = 1/(1 - \epsilon)$  in (3.4) we obtain

$$\begin{aligned} & \text{Prob}\left\{|\psi_k(B) - \|B\|_F| \leq \epsilon\|B\|_F\right\} \\ & \geq 1 - \exp\left(-\frac{k\rho}{2}\epsilon^2\right) - \exp\left(-\frac{k\rho}{2}\epsilon^2 \frac{(2 - \epsilon)^2}{2}\right) \\ & \geq 1 - 2 \exp\left(-\frac{k\rho}{2}\epsilon^2\right). \end{aligned}$$

The result follows by setting the above equal to  $1 - \delta$  and solving for  $k$ .  $\square$

As with (3.2), the bound (3.8) on the number of samples inevitably depends on  $\epsilon^{-2}$ . However, the factor 8 in (3.2) is reduced to a factor 2. In other words, four times fewer samples than predicted by (3.2) are in fact required.

**3.2. A combined bound.** We now return to the result given in Theorem 3.1. For fixed  $k$  and  $\tau$ , the bound (3.5) increases very fast toward 1 as the stable rank  $\rho$  increases. For example, suppose that  $B \in \mathbb{R}^{m \times n}$  with  $n = r = 1000$  and  $\|B\|_F = 10\|B\|_2$ . Even with small values of  $k = \tau = 2$ , the bound states that

$$\text{Prob}\left\{\frac{\|B\|_F}{2} < \psi_2(B) < 2\|B\|_F\right\} \geq 1 - 10^{-12}.$$

This is much closer to 1 than the lower bound (2.3), even if, as conjectured in [12], (2.3) holds without the factor  $r$ . (In this example, the lower bound (2.3) is negative, while ignoring the factor  $r$  in (2.3) gives 0.7610 to four digits.)

On the other hand, when  $\rho$  is close to 1, the two exponential terms (3.3) and (3.4) exhibit different behavior. The bound (3.3) on the probability of overestimation remains quite small, even for small values of  $k$  and  $\tau$ . For example, in the extreme case  $\|B\|_F = \|B\|_2$ , with  $k = \tau = 3$ , we have



$$\exp\left(-\frac{k\rho}{2}(\tau-1)^2\right) = \exp(-6) \leq 0.0025.$$

Clearly this term further decreases with increasing  $k$  and  $\tau$ .

The bound (3.4) on the probability of underestimation may be quite large for small  $k$  when  $\rho$  is small. Once again in the extreme case  $\|B\|_F = \|B\|_2$ , with  $k = \tau = 3$ , we have

$$\exp\left(-\frac{k}{2} \frac{\|B\|_F^2}{\|B\|_2^2} \frac{(\tau^2 - 1)^2}{2\tau^4}\right) = \exp\left(-\frac{16}{27}\right) \approx 0.5529.$$

Furthermore, although this term is a decreasing function of  $k$  and of  $\tau$ , it does not tend to 0 with increasing  $\tau$ . Consequently, if  $\rho$  is close to 1, the bound (3.5) may be quite pessimistic when  $k$  is not very large and  $\tau$  is very large, i.e., if we are interested in a very rough estimate of  $\|B\|_F$  using very few samples. The following theorem extends Theorem 3.1 by providing a bound that is useful when  $\rho$  is close to 1 and/or  $\tau$  is very large.

**THEOREM 3.4.** *In the notation of Theorem 3.1,*

$$(3.9) \quad \begin{aligned} & \text{Prob}\left\{\frac{\|B\|_F}{\tau} < \psi_k(B) < \tau\|B\|_F\right\} \\ & \geq 1 - \exp\left(-\frac{k\rho}{2}(\tau-1)^2\right) - \omega(B, k, \tau), \end{aligned}$$

where

$$\omega(B, k, \tau) = \min\left\{\exp\left(-\frac{k\rho(\tau^2-1)^2}{4\tau^4}\right), \mathcal{P}\left(\frac{k\rho}{\tau^2}\right)\right\}$$

and

$$(3.10) \quad \mathcal{P}(\alpha) = \frac{\int_0^{\alpha/2} t^{(k-2)/2} \exp(-t) dt}{\int_0^\infty t^{(k-2)/2} \exp(-t) dt}$$

is a regularized gamma function.

*Proof.* We only modify the bound (3.4) on underestimation from Theorem 3.1. Recall from (2.4) that

$$k\psi_k^2(B) = \sum_{i=1}^r \sigma_i^2 \chi_i^2(k),$$

where the random variables  $\chi_i^2(k)$  are mutually independent. Therefore,

$$(3.11) \quad \begin{aligned} \text{Prob}\left\{\psi_k(B) \leq \frac{\|B\|_F}{\tau}\right\} &= \text{Prob}\left\{\sum_{i=1}^r \sigma_i^2 \chi_i^2(k) \leq \frac{k\|B\|_F^2}{\tau^2}\right\} \\ &\leq \text{Prob}\left\{\bigcap_{i=1}^r \left(\sigma_i^2 \chi_i^2(k) \leq \frac{k\|B\|_F^2}{\tau^2}\right)\right\} \\ &= \prod_{i=1}^r \text{Prob}\left\{\chi_i^2(k) \leq \frac{k\|B\|_F^2}{\tau^2 \sigma_i^2}\right\} \\ &= \prod_{i=1}^r \mathcal{P}\left(\frac{k\|B\|_F^2}{\tau^2 \sigma_i^2}\right) \\ &\leq \mathcal{P}\left(\frac{k\rho}{\tau^2}\right). \end{aligned}$$

The rest of the proof is as in Theorem 3.1. Since we have two upper bounds (3.4) and (3.11) for the probability of underestimation, the minimum of the two is also a valid bound.  $\square$

In contrast to (3.4), the bound (3.11) decreases toward 0 as  $\tau$  increases, and is an increasing function of  $\rho$ . Thus, (3.4) is more suitable when  $\rho$  is large, while (3.11) is preferable when  $\rho$  is close to 1 or  $\tau$  is very large.

**4. Numerical experiments.** We give some numerical experiments to illustrate the behavior of our bounds as a function of  $k$ ,  $\tau$ , and  $\rho$ .

First we test whether our bound in Theorem 3.4 is descriptive by comparing it to empirical probabilities. For each value of  $k$  and  $\tau$  tested, we compute  $10^5$  realizations of  $\psi_k(B)$  and count the number of times that

$$(4.1) \quad \frac{\|B\|_F}{\tau} \leq \psi_k(B) \leq \tau \|B\|_F$$

holds, divided by  $10^5$ . Without loss of generality we test matrices  $B$  that are square, diagonal, and of size  $n = 100$ . The diagonal elements  $\sigma_i$  of  $B$  are chosen to obtain different values of the stable rank  $\rho$ , as follows:

- (a)  $\rho = 1$  :  $\sigma_1 = 1$  and  $\sigma_i = 0$  for  $i > 1$ .
- (b)  $\rho \approx 1.2$  :  $\sigma_1 = 10\pi/\sqrt{126}$  and  $\sigma_i = 1/(i-1)$  for  $i > 1$ .
- (c)  $\rho \approx 4$  :  $\sigma_i = \max\{10^{-10}, (\sqrt{3}/2)^{i-1}\}$
- (d)  $\rho = 25$  :  $\sigma_1 = 1$  and  $\sigma_i = \sqrt{24/(n-1)}$  for  $i > 1$ .

Results are given in Table 4.1, rounded to four digits. We write 1, as opposed to 1.0000, when the empirical probability is exactly 1, i.e., when all  $10^5$  realizations of  $\psi_k(B)$  satisfy (4.1). We observe that if  $\rho$  is close to 1, the lower bound (3.9) can be pessimistic when  $k < 3$  and/or  $\tau < 3$ . However, when  $k \geq 3$  and  $\tau \geq 3$ , the bound gives a good indication of the actual probability. In case (a) the empirical probability is sometimes slightly lower than the lower bound. This is merely the effect of sampling error.

**5. Conclusion.** The purpose of the present paper is to derive a bound of the form (1.1) for small-sample estimation. Our main result is the combined bound in Theorem 3.4. We derived this bound for the Gaussian estimator  $\psi_k(B)$ , but by Proposition 2.2 it also essentially holds for the GKL estimator  $\eta_k(B)$  when  $k \ll n$ , which is typically how the estimators are used in practice.

Unlike the original small-sample bounds from [12], but similarly to those in [1, 19], our bounds hold independently of the rank of  $B$ . Instead, they depend on  $\rho$ , the stable rank of  $B$ . Uniform bounds that hold for all  $B$  are readily obtained by replacing  $\rho$  by its lower bound 1 (or its upper bound  $\min\{m, n\}$  in (3.11)).

Even when  $\rho$  is very close to 1, our bounds behave similarly to the bounds for the case  $\text{rank}(B) = 1$  in (2.3), on which the small-sample estimation theory is based. Similarly to [19, Theorem 3], our bounds increase very quickly toward 1 as the stable rank of  $B$  increases. If  $\|B\|_F$  is significantly larger than  $\|B\|_2$ , say,  $\|B\|_F \geq 5\|B\|_2$ , then the probability of obtaining a good order-of-magnitude estimate is overwhelmingly close to 1. Thus, small-sample estimation works generally for matrices  $B$  not only of rank 1 but of any rank.

TABLE 4.1  
 Empirical probability of (4.1) (top) and bound in (3.9) (bottom).

(a) Case  $\rho = 1$

$\tau \backslash k$	1	2	3	4	5
2	0.5717 0.0105	0.7608 0.4109	0.8551 0.6383	0.9071 0.7745	0.9393 0.8579
3	0.7357 0.6035	0.8948 0.8765	0.9546 0.9512	0.9784 0.9783	0.9894 0.9899
5	0.8410 0.8411	0.9600 0.9608	0.9893 0.9893	0.9970 0.9970	0.9988 0.9991
10	0.9209 0.9203	0.9900 0.9900	0.9986 0.9986	0.9998 0.9998	0.9999 1.0000

(b) Case  $\rho \approx 1.2$

$\tau \backslash k$	1	2	3	4	5
2	0.72360 0.03609	0.8849 0.4406	0.9455 0.6607	0.9729 0.7875	0.9869 0.8631
3	0.9214 0.6249	0.9877 0.8664	0.9976 0.9389	0.9995 0.9697	0.9999 0.9845
5	0.9955 0.8259	1 0.9528	1 0.9859	1 0.9956	1 0.9986
10	1 0.9125	1 0.988	1 0.9982	1 0.9997	1 1.0000

(c) Case  $\rho \approx 4$

$\tau \backslash k$	1	2	3	4	5
2	0.9878 0.2949	0.9995 0.6570	1 0.8125	1 0.8943	1 0.9399
3	0.9998 0.5459	1 0.7941	1 0.9066	1 0.9576	1 0.9808
5	1 0.6892	1 0.8521	1 0.9370	1 0.9749	1 0.9900
10	1 0.8415	1 0.9608	1 0.9893	1 0.9970	1 0.9991

(d) Case  $\rho = 25$

$\tau \backslash k$	1	2	3	4	5
2	1 0.9703	1 0.9991	1 1.0000	1 1.0000	1 1.0000
3	1 0.9928	1 0.9999	1 1.0000	1 1.0000	1 1.0000
5	1 0.9968	1 1.0000	1 1.0000	1 1.0000	1 1.0000
10	1 0.9978	1 1.0000	1 1.0000	1 1.0000	1 1.0000

## REFERENCES

- [1] H. AVRON AND S. TOLEDO, *Randomized algorithms for estimating the trace of an implicit symmetric positive semi-definite matrix*, J. ACM, 58 (2011), pp. 8:1–8:34.
- [2] M. BABOULIN, J. DONGARRA, AND R. LACROIX, *Computing least squares condition numbers on hybrid multicore/GPU systems*, Interdiscip. Topics Appl. Math. Model. Comput. Sci., 117 (2015), pp. 35–41.
- [3] M. BABOULIN, S. GRATTON, R. LACROIX, AND A. LAUB, *Statistical estimates for the conditioning of linear least squares problems*, in Proceedings of the 10th International Conference on Parallel Processing and Applied Mathematics, Lecture Notes in Comput. Sci. 8384, Springer-Verlag, New York, 2014, pp. 124–133.
- [4] J. BOURGAIN AND L. TZAFRIRI, *Invertibility of ‘large’ submatrices with applications to the geometry of Banach spaces and harmonic analysis*, Israel J. Math., 57 (1987), pp. 137–224.
- [5] J. BOURGAIN AND L. TZAFRIRI, *On a problem of Kadison and Singer*, J. Reine Angew. Math., 420 (1991), pp. 1–44.
- [6] K. R. DAVIDSON AND S. J. SZAREK, *Local operator theory, random matrices and Banach spaces*, in Handbook of the Geometry of Banach Spaces, W. B. Johnson and J. Lindenstrauss, eds., Elsevier Science, Amsterdam, 2001, pp. 317–366.
- [7] H. DIAO, Y. WEI, AND S. QIAO, *Structured condition numbers of structured Tikhonov regularization problem and their estimations*, J. Comput. Appl. Math., 308 (2016), pp. 276–300.
- [8] H. DIAO, Y. WEI, AND P. XIE, *Small sample statistical condition estimation for the total least squares problem*, Numer. Algorithms, 75 (2017), pp. 435–455.
- [9] Y. GORDON, *Some inequalities for Gaussian processes and applications*, Israel J. Math., 50 (1985), pp. 265–289.
- [10] Y. GORDON, *Gaussian processes and almost spherical sections of convex bodies*, Ann. Probab., 16 (1988), pp. 180–188.
- [11] S. GRATTON AND D. TITLEY-PELOQUIN, *Stochastic conditioning of matrix functions*, SIAM/ASA J. Uncertain Quantif., 2 (2014), pp. 763–783.
- [12] T. GUDMUNDSSON, C. KENNEY, AND A. LAUB, *Small-sample statistical estimates for matrix norms*, SIAM J. Matrix Anal. Appl., 16 (1995), pp. 776–792.
- [13] C. KENNEY AND A. LAUB, *Small-sample statistical condition estimates for general matrix functions*, SIAM J. Sci. Comput., 15 (1994), pp. 36–61, <https://doi.org/10.1137/0915003>.
- [14] A. J. LAUB AND J. XIA, *Applications of statistical condition estimation to the solution of linear systems*, Numer. Linear Algebra Appl., 15 (2008), pp. 489–513.
- [15] A. J. LAUB AND J. XIA, *Fast condition estimation for a class of structured eigenvalue problems*, SIAM J. Matrix Anal. Appl., 30 (2008), pp. 1658–1676.
- [16] A. J. LAUB AND J. XIA, *Statistical condition estimation for the roots of polynomials*, SIAM J. Sci. Comput., 31 (2008), pp. 624–643.
- [17] M. B. MARCUS AND G. PISIER, *Random Fourier Series with Applications to Harmonic Analysis*, Ann. Math. Stud., Princeton University Press, Princeton, NJ, 1981.
- [18] A. M. MATHAI AND S. B. PROVOST, *Quadratic Forms in Random Variables, Theory and Applications*, Stat. Textb. and Monogr. 126, CRC Press, BocaRaton, FL, 1992.
- [19] F. ROOSTA-KHORASANI AND U. ASCHER, *Improved bounds on sample size for implicit matrix trace estimators*, Foundations of Computational Mathematics, 15 (2015), pp. 1187–1212.
- [20] M. V. RUDELSON AND R. VERSHYNIN, *Sampling from large matrices: An approach through geometric functional analysis*, J. ACM, 54 (2007).
- [21] J. A. TROPP, *An introduction to matrix concentration inequalities*, Found. Trends Machine Learning, 8 (2015), pp. 1–230.