Norm and trace estimation with random rank-one vectors

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Abstract

A few matrix-vector multiplications with random vectors are often sufficient to obtain reasonably good estimates for the norm of a general matrix or the trace of a symmetric positive semi-definite matrix. Several such probabilistic estimators have been proposed and analyzed for standard Gaussian and Rademacher random vectors. In this work, we consider the use of rank-one random vectors, that is, Kronecker products of (smaller) Gaussian or Rademacher vectors. It is not only cheaper to sample such vectors but it can sometimes also be much cheaper to multiply a matrix with a rank-one vector instead of a general vector. In this work, theoretical and numerical evidence is given that the use of rank-one instead of unstructured random vectors still leads to good estimates. In particular, it is shown that our rank-one estimators multiplied with a modest constant constitute, with high probability, upper bounds of the quantity of interest. Partial results are provided for the case of lower bounds. The application of our techniques to condition number estimation for matrix functions is illustrated.

1 Introduction

This work is concerned with estimating the norm of a matrix $A \in \mathbb{R}^{m \times n}$ or the trace of a symmetric positive semi-definite matrix $B \in \mathbb{R}^{n \times n}$, which are given implicitly via matrix-vector products. Given an integer factorization $n = \hat{n} \cdot \tilde{n}$, we say that $x \in \mathbb{R}^n$ has rank one if it takes the form $x = \hat{x} \otimes \tilde{x}$, where $\hat{x} \in \mathbb{R}^{\hat{n}}$, $\tilde{x} \in \mathbb{R}^{\tilde{n}}$ are nonzero and $\otimes$ denotes the Kronecker product. Equivalently, the $\hat{n} \times \tilde{n}$ matrix obtained from reshaping $x$ has rank one. In this work, we specifically target a setting where it is (much) cheaper to multiply with a rank-one vector than with a general vector. Short sums of Kronecker products have this property and such matrices arise in a variety of applications; see, e.g., [10, 26]. More intricately, condition number estimation for matrix equations and matrix functions involves linear operators that can often be cheaply applied to rank-one vectors; see Section 4 for details. Another situation involving such operators arises in the context of error estimates for low-rank tensor approximation [22].

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**Existing work.** Norm estimation is a classical topic in matrix analysis; see Chapter 15 in the book by Higham \[15\] for a comprehensive overview. A single matrix-vector product $Ax$ with a random vector $x$ chosen from a suitable distribution can already give a good first estimate of the norm of $A$. A classical result by Dixon \[8\] shows that the spectral norm $\|A\|_2$ is bounded by $\theta \|Ax\|_2$ with probability at least $1 - 0.8 \sqrt{n} \theta^{-1/2}$ if $x$ is distributed uniformly on the unit sphere in $\mathbb{R}^n$. The normalization of $x$ implies that $\|Ax\|_2$ is always a lower bound but it also leads to the unfavorable appearance of $\sqrt{n}$ in the tail probability. The latter can be avoided when choosing $x$ from $\mathcal{N}(0, I_n)$. This choice of $x$ is called standard Gaussian (or normal) random vector. In this case, Lemma 4.1 in \[14\] states that

$$\|A\|_2 \leq \theta \|Ax\|_2 \quad \text{holds with probability at least } 1 - \sqrt{2\pi \theta^{-1}}.$$  

(1.1)

This upper bound is not ideal because the expected value of $\|Ax\|_2^2$ is not $\|A\|_2^2$ but $\|A\|_F^2$, where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix. In turn, one expects that $\|Ax\|_2$ tends to overestimate $\|A\|_2$ by a factor $\|A\|_F/\|A\|_2$, which can be between 1 and $\sqrt{n}$ depending on the singular value distribution of $A$.

There are numerous approaches to go beyond the simple estimate $\|Ax\|_2$ and construct estimators that improve upon (1.1). A straightforward modification suggested, e.g., in \[14\] is to choose $k \geq 2$ independent Gaussian vectors $x_1, \ldots, x_k$ and return the maximum estimator $\max\{\|Ax_1\|_2, \ldots, \|Ax_k\|_2\}$. On the one hand, this increases the success probability in (1.1) to $1 - (\sqrt{2\pi \theta^{-1}})^k$, but, on the other hand, this also increases the risk of overestimation.

A second approach starts with the observation that $\|A\|_F^2 = \text{trace}(B)$, where $B = A^T A$, which suggests the use of the stochastic trace estimator

$$\text{Est}_k = \frac{1}{k} \sum_{i=1}^k x_i^T B x_i,$$

going back to Hutchinson \[19\] Because $\text{Est}_k$ is a sub-exponential random variable with mean $\text{trace}(B)$, one can apply Chernoff bounds to obtain concentration inequalities that yield relative upper and lower bounds \[11, 11, 29\]. For example, the proof of Corollary 3.3 in \[11\] establishes

$$\text{trace}(B) \leq \frac{\text{Est}_k}{1 - \varepsilon} \quad \text{holds with probability at least } 1 - \exp(-k\rho\varepsilon^2/4) \text{ for all } 0 < \varepsilon < 1,$$

(1.2)

$$\text{trace}(B) \geq \frac{\text{Est}_k}{1 + \varepsilon} \quad \text{holds with probability at least } 1 - \exp(-k\rho\varepsilon^2/2) \text{ for all } 0 < \varepsilon,$$

(1.3)

with the stable rank $\rho = \|B\|_F^2/\|B\|_2^2$. One disadvantage of (1.2) compared to (1.1) is that the bound on the failure probability for fixed $k$ does not converge to 0 when loosening the upper bound (that is, when letting $\varepsilon \to 1$). For example, for $\rho = 1$, the success probability cannot be larger than $1 - \exp(-k/4) \approx 1 - 0.78^k$. This issue is addressed in \[11\] by a combination with the techniques from \[13\].

The entries of a Rademacher vector are independent random variables that are either 1 or $-1$, both with probability $1/2$. As shown in \[29\], bounds of the type (1.2) and (1.3) also hold (with different constants) when $x_1, \ldots, x_k$ are independent Rademacher vectors.
A third approach to improve (1.1) is to apply a few steps of the power or Lanczos method to \( B \) with a standard Gaussian starting vector; see, e.g., [8, 17, 24]. We will not consider such an approach in this work because repeated application of \( B \) to the same vector makes it difficult to benefit from rank-one structure of the starting vector.

**New results.** In this work, we develop and analyze estimators that operate with vectors \( \tilde{x} \otimes \hat{x} \), where \( \tilde{x} \) and \( \hat{x} \) are independent random vectors. A simple calculation shows that \( \|A(\tilde{x} \otimes \hat{x})\|_2^2 \) retains the property of being an unbiased estimator of \( \|A\|_F^2 \) for common choices of distributions for the entries of \( \tilde{x}, \hat{x} \); see Lemma 2.1. For the specific case that both \( \tilde{x}, \hat{x} \) are standard Gaussian vectors, Theorem 2.2, one of our main results, shows that

\[
\|A\|_2 \leq \theta \|A(\tilde{x} \otimes \hat{x})\|_2 \quad \text{holds with probability at least} \quad 1 - 2\pi^{-1}(2 + \ln(1 + 2\theta))\theta^{-1}. \tag{1.4}
\]

Compared to (1.1), the success probability only becomes slightly worse. Using the maximum estimator mentioned above, this probability can be easily improved, while the risk of overestimation can be quantified with the lower bounds from Theorems 2.3 and 2.4. We also explain why it is not possible to have a result of the form (1.4) when \( \tilde{x}, \hat{x} \) are Rademacher vectors. In contrast, an upper bound of the form (1.2) holds for rank-one standard Gaussian and Rademacher vectors, see Theorem 3.1 while we have a lower bound of the form (1.3) only in the Rademacher case, see Theorem 3.2.

We would like to stress that the rank-one structure significantly complicates the theory because the techniques used in existing work on norm and trace estimation do not carry over. For example, when \( x, \tilde{x}, \hat{x} \) are standard Gaussian vectors the distribution of \( x \) is invariant under orthogonal transformations but the distribution of \( \tilde{x} \otimes \hat{x} \) is not. The random variable \( \|Ax\|_2^2 \) is subexponential but this property, which is frequently assumed in concentration inequalities, is not enjoyed by \( \|A(\tilde{x} \otimes \hat{x})\|_2^2 \).

Although random rank-one vectors/measurements have been used and analyzed in compressed sensing, particularly in the context of matrix recovery [5, 6, 20, 25] and phase retrieval [32], we are not aware of existing work that addresses the questions discussed in this paper.

## 2 Small-sample estimation

Hutchinson [19] has shown that \( \|Ax\|_2^2 \) is an unbiased estimator of \( \|A\|_F^2 \) if \( x \) contains independent random variables with mean zero and variance one, which includes standard normal and Rademacher random variables. The following lemma extends this result to rank-one vectors.

**Lemma 2.1.** Let \( A \in \mathbb{R}^{m \times n} \), \( n = \tilde{n} \cdot \hat{n} \), and let \( \tilde{x}, \hat{x} \) be random vectors that contain \( \tilde{n} + \hat{n} \) independent random variables with mean zero and variance one. Then \( \mathbb{E}[\|A(\tilde{x} \otimes \hat{x})\|_2^2] = \|A\|_F^2 \).

**Proof.** We let \( a_i \in \mathbb{R}^{\tilde{n} \hat{n}} \) denote the \( i \)th column of \( A^T \) and reshape \( a_i \) into the \( \hat{n} \times \tilde{n} \) matrix \( A_i \), that is, \( \text{vec}(A_i) = a_i \). By standard properties of the Kronecker product [9],

\[
\|A(\tilde{x} \otimes \hat{x})\|_2^2 = \sum_{i=1}^{m} ((\tilde{x} \otimes \hat{x})^T a_i)^2 = \sum_{i=1}^{m} (\tilde{x}^T A_i \hat{x})^2. \tag{2.1}
\]
Because of the assumptions on $\hat{x}$ we have $E[\hat{x}\hat{x}^T] = I_{\hat{n}}$ and, therefore,

$$\mathbb{E}[(\hat{x}^T A_1 \hat{x})^2] = \mathbb{E} [\hat{x}^T A_1^2 \hat{x}^T A_1 \hat{x}] = \mathbb{E}_x [\mathbb{E}_x [\hat{x}^T A_1^2 \hat{x}^T A_1 \hat{x} | \hat{x}]]$$

$$= \mathbb{E}_x [\hat{x}^T A_1^2 \hat{x}] = \mathbb{E}_x [\|A_1 \hat{x}\|^2_2] = \|A_1\|^2_F.$$

Inserted into (2.1), we obtain $E[\|A(\hat{x} \otimes \hat{x})\|^2_2] = \sum \|A_i\|^2_F = \sum \|a_i\|^2_2 = \|A\|^2_F. \quad \Box$

2.1 One-sample estimation: Upper bound for rank-one Gaussian vectors

We proceed with our first main result, which bounds the risk of underestimating the spectral norm when using a single Kronecker product of standard Gaussian random vectors. Note that the derivation of our result relies on an anti-concentration inequality that exploits specific properties of the distribution.

**Theorem 2.2.** Let $A \in \mathbb{R}^{m \times n}$ and $n = \hat{n} \cdot \tilde{n}$. Suppose that $\hat{x} \sim \mathcal{N}(0, I_{\hat{n}})$ and $\tilde{x} \sim \mathcal{N}(0, I_{\tilde{n}})$, and let $\theta > 1$. Then the inequality

$$\|A\|_2 \leq \theta \|A(\hat{x} \otimes \tilde{x})\|_2 \quad (2.2)$$

holds with probability at least $1 - \frac{2}{\pi} (2 + \ln(1 + 2\theta)) \theta^{-1}$.

**Proof.** Let $x = \hat{x} \otimes \tilde{x}$. We will bound the probability that (2.2) fails:

$$\mathbb{P}\{\|A\|_2 > \theta \|Ax\|_2\} = \mathbb{P}\{\|A\|^2_2 > \theta^2 \|Ax\|^2_2\} = \mathbb{P}\{\|A^T A\|_2 > \theta^2 x^T A^T A x\}.$$

Consider the spectral decomposition $A^T A = U \Lambda U^T = \lambda_1 u_1 u_1^T + \cdots + \lambda_n u_n u_n^T$, $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$, and note that

$$\theta^2 x^T A^T A x = \theta^2 \sum_{j=1}^n \lambda_j (x^T u_j)^2 \geq \theta^2 \lambda_1 (x^T u_1)^2.$$

Therefore, if $\|A^T A\|_2 > \theta^2 x^T A^T A x$, then $\|A^T A\|_2 > \theta^2 \lambda_1 (x^T u_1)^2$, and, since $\|A^T A\|_2 = \lambda_1$, we have

$$\mathbb{P}\{\|A^T A\|_2 > \theta^2 x^T A^T A x\} \leq \mathbb{P}\{\lambda_1 > \theta^2 \lambda_1 (x^T u_1)^2\} = \mathbb{P}\{(x^T u_1)^2 < \frac{1}{\theta^2}\}. \quad (2.3)$$

To bound the last probability, we need to control the random variable $X := x^T u_1$. For this purpose, reshape the vector $u_1 \in \mathbb{R}^{\hat{n}}$ as a matrix: $u_1 = \text{vec}(U_1)$ with $U_1 \in \mathbb{R}^{\hat{n} \times \tilde{n}}$, and consider its singular value decomposition

$$U_1 = \hat{V} \Sigma \hat{V}^T, \quad \hat{V} = [\hat{v}_1, \ldots, \hat{v}_r] \in \mathbb{R}^{\hat{n} \times r}, \quad \hat{V} = [\tilde{v}_1, \ldots, \tilde{v}_r] \in \mathbb{R}^{\tilde{n} \times r}, \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_r) \in \mathbb{R}^{r \times r},$$

with $r = \min\{\hat{n}, \tilde{n}\}$ and $\sum_{i=1}^r \sigma_i^2 = \|U_1\|^2_F = \|u_1\|^2_2 = 1$. Using $x = \hat{x} \otimes \tilde{x} = \text{vec}(\hat{x} \tilde{x}^T)$, we obtain

$$x^T u_1 = \text{vec}(\hat{x} \tilde{x}^T) \text{vec}(U_1) = \text{trace}(\hat{x} \tilde{x}^T U_1) = \hat{x}^T U_1 \tilde{x} = \sum_{i=1}^r \sigma_i \hat{x}_i \tilde{x}_i,$$

where $\hat{x}_i := \hat{v}_i^T \hat{x}$ and $\tilde{x}_i := \tilde{v}_i^T \tilde{x}$ are independent standard normal random variables, because $\hat{V}^T \hat{x} \sim \mathcal{N}(0, I_r)$ and $\tilde{V}^T \tilde{x} \sim \mathcal{N}(0, I_r)$ follow from the orthogonality of $\hat{V}$ and $\tilde{V}$. For a random
variable $Z$, let $F_Z$ denote its cumulative distribution function, and let $\varphi_Z(t)$ denote its characteristic function. The characteristic function for the product of two standard normal random variables is given by $1/\sqrt{1 + t^2}$ and hence

$$\varphi_{\sigma_i \hat{x}_i \tilde{x}_i}(t) = \frac{1}{\sqrt{1 + \sigma_i^2 t^2}}.$$ 

Since $X = \sum_{i=1}^r \sigma_i \hat{x}_i \tilde{x}_i$ is a sum of independent random variables, its characteristic function is given by

$$\varphi_X(t) = \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}}.$$ 

We now apply Lévy’s theorem, see, e.g., [30, Corollary 2], to reformulate (2.3) in terms of characteristic functions:

$$\mathbb{P}\left\{(x^T u_1)^2 < \frac{1}{\theta^2}\right\} = \mathbb{P}\left\{-\frac{1}{\theta} < x^T u_1 < \frac{1}{\theta}\right\} = F_X\left(\frac{1}{\theta}\right) - F_X\left(-\frac{1}{\theta}\right) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin(t/\theta)}{t} \varphi_X(t) \, dt = \frac{2}{\pi} \int_0^{\infty} \frac{\sin(t/\theta)}{t} \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} \, dt. \quad (2.4)$$

To bound this oscillatory integral, we use $\sin(t/\theta) \leq t/\theta$ for $t \in [0, \theta]$ and $\sin(t/\theta) \leq 1$ elsewhere. Also, using $\sum_{i=1}^r \sigma_i^2 = 1$, note that

$$\prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} = \frac{1}{\sqrt{1 + \sum_{i=1}^r \sigma_i^2 t^2 + \text{positive terms}}} \leq \frac{1}{\sqrt{1 + t^2}}.$$ 

This gives

$$\int_0^{\infty} \frac{\sin(t/\theta)}{t} \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} \, dt \leq \int_0^{\theta} \frac{\sin(t/\theta)}{t} \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} \, dt + \int_0^{\infty} \frac{\sin(t/\theta)}{t} \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} \, dt \leq \int_0^{\theta} \frac{\sin(t/\theta)}{t} \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} \, dt + \int_{\theta}^{\infty} \frac{1}{t} \prod_{i=1}^r \frac{1}{\sqrt{1 + \sigma_i^2 t^2}} \, dt \leq \int_0^{\theta} \frac{1}{t} \sqrt{1 + t^2} \, dt + \int_0^{\infty} \frac{1}{t} \sqrt{1 + t^2} \, dt = \theta^{-1} \ln(\theta + \sqrt{1 + \theta^2}) + \ln (\theta^{-1} + \sqrt{1 + \theta^{-2}}) \leq \theta^{-1} \ln(1 + 2\theta) + \ln (1 + 2\theta^{-1}) \leq \theta^{-1} \ln(1 + 2\theta) + 2\theta^{-1} = \theta^{-1} (2 + \ln(1 + 2\theta)),$$

which, when inserted into (2.4), implies the claim of the theorem.
Comparing the bounds (2.2) and (1.1), the use of rank-one Gaussian vectors instead of Gaussian vectors comes with a slight penalty. The following table shows the bounds for the failure probability $\mathcal{P} := \mathbb{P} \{ \| A \|_2 > \theta \| A x \|_2 \}$ for different values of $\theta$:

| $\theta$ | Gaussian vectors: $\mathcal{P} \leq \sqrt{\frac{2}{\pi}} \cdot \frac{1}{\theta}$ | Rank-one Gaussian vectors: $\mathcal{P} \leq 2 \cdot \frac{1}{\theta} \cdot (2 + \ln(1 + 2\theta))$ |
|-----------|------------------------------------------------|-------------------------------------------------|
| 5         | 0.159577                                         | 0.55957                                         |
| 10        | 0.079788                                         | 0.321144                                        |
| 20        | 0.039894                                         | 0.181869                                        |
| 50        | 0.015957                                         | 0.084226                                        |
| 100       | 0.007978                                         | 0.046494                                        |

Quite trivially, Theorem 2.2 can also be applied to the Frobenius norm $\| A \|_F$. Multiplying both sides of (2.2) by $\sqrt{\rho} = \| A \|_F / \| A \|_2$, it follows that

$$\mathbb{P} \{ \| A \|_F \leq \theta \sqrt{\rho} \cdot (\varrho \otimes \hat{x}) \|_2 \} \geq 1 - \frac{2}{\pi} (2 + \ln(1 + 2\theta)) \theta^{-1}. \quad (2.5)$$

Given that $1 \leq \rho \leq n$, this bound suggests that, as the stable rank of $A$ increases, $\| A (\varrho \otimes \hat{x}) \|_2$ needs to be multiplied with a larger constant in order to remain a reliable upper bound for $\| A \|_F$. However, this seems to be entirely an artifact of our derivation of the bound. The numerical experiments in Section 2.5 below demonstrate that (2.5) tends to be tight when the stable rank is small but is overly pessimistic when the stable rank is large.

### 2.2 One-sample estimation: Lower bounds for rank-one Gaussian vectors

As discussed in the introduction, the result of Lemma 2.1 indicates that $\| A (\varrho \otimes \hat{x}) \|_2$ tends to overestimate $\| A \|_2$. The following result guarantees that an overestimation by a factor much larger than $\sqrt{n}$ is unlikely.

**Theorem 2.3.** Let $A \in \mathbb{R}^{m \times n}$, and $n = \hat{n} \cdot \tilde{n}$ with $\tilde{n} \leq \hat{n}$. Suppose that $\hat{x} \sim \mathcal{N}(0, I_{\hat{n}})$ and $\tilde{x} \sim \mathcal{N}(0, I_{\tilde{n}})$, and let $\theta > 1$. The inequality

$$\| A \|_2 \geq n^{-1/2} \theta^{-1} \| A (\tilde{x} \otimes \hat{x}) \|_2 \quad (2.6)$$

holds with probability at least $1 - 2e^{-\tilde{n}(\theta-1-\ln\theta-1)/2}$.

**Proof.** Proceeding with the spectral decomposition of $A^T A$ as in the proof of Theorem 2.2 it follows that the probability of (2.6) failing for $x = \tilde{x} \otimes \hat{x}$ is

$$\mathbb{P} \{ \| A x \|_2 > \sqrt{n} \theta \| A \|_2 \} = \mathbb{P} \left\{ \sum_{j=1}^{n} \lambda_j (x^T u_j)^2 > \lambda_1 n \theta^2 \right\} \leq \mathbb{P} \{ \| x \|_2^2 > n \theta^2 \} \quad (2.7)$$

where the last inequality uses $\sum_{j=1}^{n} \lambda_j (x^T u_j)^2 \leq \lambda_1 \sum_{j=1}^{n} (x^T u_j)^2 = \lambda_1 \| x \|_2^2$. Because $\| x \|_2 = \| \tilde{x} \|_2 \| \hat{x} \|_2$ and $n = \hat{n} \cdot \tilde{n}$, it follows that $\| x \|_2^2 > n \theta^2$ is only possible if $\| \tilde{x} \|_2^2 > \hat{n} \theta$ or $\| \hat{x} \|_2^2 > \tilde{n} \theta$. Thus,

$$\mathbb{P} \{ \| \tilde{x} \|_2^2 > n \theta^2 \} \leq \mathbb{P} \{ \| \tilde{x} \|_2^2 > \hat{n} \theta \} \leq 2 \cdot \mathbb{P} \{ \| \tilde{x} \|_2^2 > \tilde{n} \theta \}. \quad (2.8)$$

6
Now, $\|\tilde{x}\|_2^2$ is a chi-square random variable with $\tilde{n}$ and its properties (see Lemma A.1 in the Appendix) imply

$$
P\{\|\tilde{x}\|_2^2 > \tilde{n}\theta\} \leq (\theta e^{1-\theta})^{\tilde{n}/2},$$

which concludes the proof.

As already discussed for the upper bound, one directly obtains a corresponding result for the Frobenius norm by multiplying (2.6) with $\sqrt{\rho}$:

$$
P\left\{ \|A\|_F \geq \sqrt{m}^{1/2} \|A(\tilde{x} \otimes \hat{x})\|_2 \right\} \geq 1 - 2e^{-\tilde{n}(\theta - \ln(\theta - 1))/2}.
\quad (2.8)$$

Another bound for the Frobenius norm estimates is obtained by using a different approach.

**Theorem 2.4.** Let $A \in \mathbb{R}^{m \times n}$ and $n = \tilde{n} \cdot \hat{n}$. Suppose that $\tilde{x} \sim \mathcal{N}(0, I_{\tilde{n}})$ and $\hat{x} \sim \mathcal{N}(0, I_{\hat{n}})$, and let $\theta > 2$. The inequality

$$\|A\|_F \geq \theta^{-1} \|A(\tilde{x} \otimes \hat{x})\|_2$$

holds with probability at least $1 - \sqrt{2\theta} e^{-\theta + 2}$.

**Proof.** Using, once again, the spectral decomposition of $A^T A$ as in the proof of Theorem 2.2 and denoting $x = \tilde{x} \otimes \hat{x}$, the failure probability equals

$$
P\{\|Ax\|_2 > \theta \|A\|_F\} = P\left\{x^T A^T A x > \theta^2 \cdot \text{trace}(A^T A)\right\} = P\left\{\sum_{i=1}^{n} \lambda_i (x^T u_i)^2 > \theta^2 \sum_{i=1}^{n} \lambda_i\right\}
= P\left\{\sum_{i=1}^{n} \mu_i (x^T u_i)^2 > \theta^2\right\},$$

where $\mu_i := \frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j} \in [0, 1]$, which satisfy $\sum_{i=1}^{n} \mu_i = 1$. Exploiting that the function $f(\xi) = e^{\sqrt{1+\xi}}$ is convex on $[0, +\infty)$, Jensen’s inequality gives

$$f\left(\sum_{i=1}^{n} \mu_i \cdot t^2(x^T u_i)^2\right) \leq \sum_{i=1}^{n} \mu_i f\left(t^2(x^T u_i)^2\right) = \sum_{i=1}^{n} \mu_i e^{\sqrt{1+t^2(x^T u_i)^2}} \leq \sum_{i=1}^{n} \mu_i e^{1+t|x^T u_i|} = e \sum_{i=1}^{n} \mu_i e^{t|x^T u_i|}$$

for all $t > 0$. Combined with the monotonicity of $f$ as well as Markov’s inequality, we obtain

$$P\left\{\sum_{i=1}^{n} \mu_i (x^T u_i)^2 > \theta^2\right\} \leq P\left\{f\left(\sum_{i=1}^{n} \mu_i \cdot t^2(x^T u_i)^2\right) > f(t^2\theta^2)\right\} \leq P\left\{e \sum_{i=1}^{n} \mu_i e^{t|x^T u_i|} > e^{\sqrt{1+t^2\theta^2}}\right\} \leq E \left[ \sum_{i=1}^{n} \mu_i e^{t|x^T u_i|} \right] e^{1-\sqrt{1+t^2\theta^2}} = \left(\sum_{i=1}^{n} \mu_i E[e^{t|x^T u_i|}]\right) e^{1-\sqrt{1+t^2\theta^2}}.
\quad (2.9)$$
Since $e^{\theta t} \leq e^a + e^{-a}$, we obtain for $0 < t < 1$ that

$$
E[e^{\theta (x^T u_i)}] \leq E[e^{\theta (x^T v_i)}] + E[e^{\theta (x^T (-u_i))}] \leq 2\frac{1}{\sqrt{1 - t^2}},
$$

where we used Corollary A.3 in the last step. Plugged into (2.9), it follows that

$$
P\left\{ \sum_{i=1}^{n} \mu_1 (x^T u_i)^2 > \theta^2 \right\} \leq 2e^{-\sqrt{1+t^2}\theta^2} \leq 2\theta e^{-\theta + 2},
$$

where the last inequality follows from setting $t = \sqrt{1-2/\theta}$.


\textbf{Example 2.5.} To illustrate the theoretical results presented above, we generate matrices with different singular value decompositions, and compare their norms with randomized estimates. More precisely, we consider the following seven $n \times n$ matrices:

- rank-one matrices $A_1 = U_1(e_1 e_1^T)$, $A_2 = U_2(e_1 e_1^T) V_2^T$, where $e_1 = [1, 0, \ldots, 0]^T$;
- matrices $A_3 = U_3 D$, $A_4 = U_4 D V_4^T$, where $D$ is diagonal with $D_{ii} = i^2$;
- matrices $A_5 = U_5 D$, $A_6 = U_6 D V_6^T$, where $D$ is diagonal with $D_{ii} = e^{-i/2}$;
- the matrix $A_7$ is a random Gaussian matrix.

Here, $U_i$ and $V_i$ are chosen randomly from the uniform distribution on orthogonal matrices.

For each of these matrices, we sample 100,000 vectors $x = \hat{x} \otimes \hat{x}$ for $\hat{x}, \hat{x} \sim \mathcal{N}(0, I)$ in order to estimate the probability that one of the inequalities $\|A_i\| \leq \tau \|A_i x\|_2$ or $\|A_i\| \geq \tau^{-1} \|A_i x\|_2$ fails, with $\tau \in [1, 100]$. The obtained results are shown in Figure 1. We have chosen $n = 16$ and $n = 196$ for $\|\cdot\| \equiv \|\cdot\|_2$ and $\|\cdot\| \equiv \|\cdot\|_F$, respectively.

Figure 1(a) displays failure probabilities for the upper bound $\|A_i\|_2 \leq \tau \|A_i x\|_2$ as well as the corresponding bound by Theorem 2.2 with $\tau = \theta$. The bound happens to be quite tight for the rank-one matrices $A_1$ and $A_2$. Although the bound is significantly less tight for the other matrices, for which the spectral and Frobenius norms are different, this demonstrates that the result of Theorem 2.3 cannot be improved significantly without taking additional properties of the matrix into account.

Figure 1(b) displays failure probabilities for the lower bound $\|A_i\|_2 \geq \tau^{-1} \|A_i x\|_2$ as well as the corresponding bound by Theorem 2.3 with $\tau = \sqrt{n} \theta$. Clearly, the bound is not sharp but it correctly captures the exponential decay of the probabilities with respect to $\theta$.

Figure 1(c) displays failure probabilities for the upper bound $\|A_i\|_F \leq \tau \|A_i x\|_2$ as well as the corresponding bound from (2.5), with $\tau = \sqrt{n} \theta$. As the bound depends on the stable rank, the dashed lines shown in the figure differ for matrices with different stable rank. Solid and dashed lines of the same color and mark belong to the same matrix $A_i$. Again, the bounds are quite tight for low (stable) rank but becomes increasingly loose as the stable rank increases. In fact, the bound increases with larger stable rank while estimated failure probabilities actually decrease.

Figure 1(d) displays failure probabilities for the upper bound $\|A_i\|_F \leq \tau^{-1} \|A_i x\|_2$ as well as the corresponding bound (2.8), with $\tau = \sqrt{n/\rho} \theta$. Again, this bound depends on the stable rank.
Although far off for matrices of low (stable) rank, it correctly captures the observation that the exponential decay becomes faster as the stable rank $\rho$ increases. In contrast, the bound from Theorem (2.8) does not depend on $\rho$ and is clearly preferable when $\rho$ is small or no estimate of $\rho$ is available.

### 2.3 Small-sample estimation: Rank-one Gaussian vectors

As discussed in the introduction, a simple way to reduce the failure probability of upper bounds is to use a maximum estimator. In our setting, this translates into

$$\text{Max}_k := \max_{j=1,\ldots,k} \|A(\tilde{x}_j \otimes \hat{x}_j)\|_2$$

with independent standard Gaussian vectors $\tilde{x}_j, \hat{x}_j$ for $j = 1, \ldots, k$.

Using Theorem 2.2 one obtains

$$\mathbb{P}\{\|A\|_2 \leq \theta \cdot \text{Max}_k\} \geq 1 - \left(\frac{2}{\pi} (2 + \ln(1 + 2\theta)) \theta^{-1}\right)^k.$$ (2.10)

For example, for $\theta = 10$, choosing $k = 7$ is sufficient to guarantee a success probability of more than 99.9%.

Of course, taking the maximum for several samples increases the risk of overestimation. But this increase can be easily mitigated by accepting a slight increase of the overestimation factor. By Theorem 2.4, the probability that $\|A(\tilde{x} \otimes \hat{x})\|_2$ overestimates $\|A\|_F$ by more than a factor 10 is less than 0.15%. For the maximum estimator one has (again by Theorem 2.4) that

$$\mathbb{P}\{\|A\|_F \geq \theta^{-1} \cdot \text{Max}_k\} \geq \left(1 - \sqrt{2\theta} e^{-\theta + 2}\right)^k.$$ 

For $k = 7$, the probability that $\text{Max}_k$ overestimates $\|A\|_F$ by more than a factor 12.1 is again less than 0.15%.

### 2.4 One-sample estimation: Rank-one Rademacher vectors

In this section, we discuss whether the results from Sections 2.1 and 2.2 can be extended when we choose $\tilde{x}$ and $\hat{x}$ to be Rademacher instead of standard Gaussian vectors in the rank-one vector $x = \tilde{x} \otimes \hat{x}$.

It turns out that it is not possible to have an upper bound of the form presented in Theorem 2.2 for Rademacher vectors. To see this, consider the matrix $A = uu^T \in \mathbb{R}^{n \times n}$ with $u = e/\sqrt{n}$, where $e$ denotes the vector of all ones. Then $A^TA = A$ and

$$\mathbb{P}\{\|A\|_2 > \theta\|Ax\|_2\} = \mathbb{P}\{\|ATA\|_2 > \theta^2 (x^Tu)^2 \} = \mathbb{P}\{x^Tu < \theta^{-2}\} = \mathbb{P}\{-\theta^{-1} < x^Tu < \theta^{-1}\}.$$ 

Now $x^Tu = (\tilde{x} \otimes \hat{x})^Tu = n^{-1/2}(\hat{x}^Te)(\tilde{x}^Te)$, which implies

$$\mathbb{P}\{x^Tu = 0\} = \mathbb{P}\{(\hat{x}^Te)(\tilde{x}^Te) = 0\} \geq \mathbb{P}\{\hat{x}^Te = 0\}.$$
(a) Theorem 2.2 (dashed line) vs. estimated failure probabilities for $\|A_i\|_2 > \tau \|Ax\|_2$ (solid line).

(b) Theorem 2.3 (dashed line) vs. estimated failure probabilities for $\|A_i\|_2 < \tau^{-1} \|Ax\|_2$ (solid line).

(c) Bound (2.5) (dashed lines) vs. estimated failure probabilities for $\|A_i\|_F > \tau \|Ax\|_2$ (solid lines).

(d) Theorem 2.4 (dashed black line) versus estimated failure probabilities for $\|A_i\|_F < \tau^{-1} \|Ax\|_2$. Upper bounds (2.8) are also shown (dashed colored lines).

Figure 1: Theoretical bounds on failure probabilities versus estimates; see Example 2.5 for details.
For even \( \hat{n} \), the sum \( \hat{x}^T e = \hat{x}_1 + \cdots + \hat{x}_{\hat{n}} \) equals zero when exactly \( \hat{n}/2 \) of the entries are equal to 1. As this happens with probability \( \left( \frac{\hat{n}}{\hat{n}/2} \right)^{\hat{n}/2} \), we obtain the lower bound

\[
P\{ \|A\|_2 > \theta \|Ax\|_2 \} \geq P\{ x^T u = 0 \} \geq 2^{-\hat{n}} \left( \frac{\hat{n}}{\hat{n}/2} \right) \approx \frac{1}{\sqrt{n\pi/2}},
\]

for any \( \theta > 1 \). In particular, and in contrast to the result of Theorem 2.2, the failure probability does not converge to zero as \( \theta \) increases. Let us stress that this is not an artifact of using rank-one vectors; an analogous negative result can be obtained when using an (unstructured) Rademacher vector \( x \).

On the other hand, because Rademacher vectors are bounded, the risk of overestimation becomes zero beyond a certain threshold. More specifically, it always holds that \( \|\hat{x}\|_2 = \sqrt{n} \), \( \|\tilde{x}\|_2 = \sqrt{\tilde{n}} \), and hence, for all matrices \( A \), by equation (2.7) we have

\[
P\{ \|Ax\|_2 > \sqrt{n} \|A\|_2 \} \leq P\{ \|x\|_2 > \sqrt{n} \} = P\{ \|\hat{x}\|_2 \cdot \|\tilde{x}\|_2 > \sqrt{n} \} = 0.
\]

This is in contrast to the result of Theorem 2.3, which yields a small but nonzero risk for Gaussian vectors.

3 Large-sample estimation of the trace

In this section, we analyze the use of random rank-one vectors in stochastic trace estimators for estimating \( \text{trace}(B) = \|A\|_F^2 \) with \( B = A^T A \):

\[
\hat{\text{Est}}_k = \frac{1}{k} \sum_{i=1}^{k} (\tilde{x}_i \otimes \hat{x}_i)^T B(\tilde{x}_i \otimes \hat{x}_i).
\]  

(3.1)

By Lemma 2.1 we have \( E[\hat{\text{Est}}_k] = \text{trace}(B) \). The following theorem shows that \( \hat{\text{Est}}_k \) times a modest factor is an upper bound of \( \text{trace}(B) \) with high probability for larger \( k \).

**Theorem 3.1.** Let \( 0 < \varepsilon < 1 \) and consider the trace estimator \( \hat{\text{Est}}_k \) defined in (3.1), where \( \tilde{x}_i, \hat{x}_i \) are either independent standard Gaussian or independent Rademacher random vectors. Then the bound

\[
\text{trace}(B) \leq \frac{1}{1 - \varepsilon} \hat{\text{Est}}_k
\]

holds with probability at least \( 1 - \exp(-k\varepsilon^2/18) \).

**Proof.** The proof is divided into two parts. First, we follow the arguments from [29] and use a Chernoff bound. We then arrive at the problem of bounding the moment generating function of decoupled Gaussian / Rademacher chaos, which will be discussed in the second part.

Consider the spectral decomposition \( B = U\Lambda U^T \) with \( U \) orthogonal and \( \Lambda \) diagonal containing the eigenvalues \( \lambda_1 \geq \cdots \geq \lambda_n \geq 0 \) on the diagonal. Letting \( u_j \) denote the \( j \)th column of \( U \) and \( x_i = \tilde{x}_i \otimes \hat{x}_i \), we obtain

\[
\hat{\text{Est}}_k = \frac{1}{k} \sum_{i=1}^{k} x_i^T U\Lambda U^T x_i = \frac{1}{k} \sum_{i=1}^{k} \sum_{j=1}^{n} \lambda_j (x_i^T q_j)^2 = \frac{1}{k} \sum_{j=1}^{n} \lambda_j \sum_{i=1}^{k} z_{ij}^2,
\]

where \( z_{ij} = x_i^T q_j \).
where we set \( z_{ij} := x_i^T q_j \). The statement of the theorem is equivalent to showing that \( \exp(-k\varepsilon^2/18) \) is an upper bound for

\[
P := \Pr\{ \text{Est}_k < (1 - \varepsilon) \text{trace}(B) \} = \Pr\left\{ \sum_{j=1}^{n} \frac{\lambda_j}{\text{trace}(B)} \sum_{i=1}^{k} z_{ij}^2 < k(1 - \varepsilon) \right\}.
\]

By the Chernoff bound, it holds for arbitrary \( t > 0 \) that

\[
P \leq \exp(tk(1 - \varepsilon)) \mathbb{E}\left[ \exp\left( -\sum_{j=1}^{n} \frac{\lambda_j}{\text{trace}(B)} \sum_{i=1}^{k} t z_{ij}^2 \right) \right]
\]

\[
\leq \exp(tk(1 - \varepsilon)) \sum_{j=1}^{n} \frac{\lambda_j}{\text{trace}(B)} \mathbb{E}\left[ \exp\left( -\sum_{i=1}^{k} t z_{ij}^2 \right) \right]
\]

\[
= \exp(tk(1 - \varepsilon)) \sum_{j=1}^{n} \frac{\lambda_j}{\text{trace}(B)} \prod_{i=1}^{k} \mathbb{E}\left[ \exp\left( -t z_{ij}^2 \right) \right],
\]

where we used Jensen’s inequality and the convexity of the exponential in the second inequality, and the independence of \( z_{ij} \) for different \( i \) in the equality.

It remains to bound the moment generating function \( \mathbb{E}\left[ \exp\left( -t z_{ij}^2 \right) \right] \). To simplify the notation we let \( Q \in \mathbb{R}^{n \times \tilde{n}} \) denote the matrix such that \( \text{vec}(Q) = u_j \) and drop indices. Then \( z = \hat{x}^T Q \tilde{x} \), a random variable that is sometimes called decoupled (order-2) chaos. Using that \( \exp(-t\alpha^2) \leq 1 - t\alpha^2 + \frac{1}{2}t^2\alpha^4 \) holds for any fixed \( \alpha \in \mathbb{R} \), we obtain

\[
\mathbb{E}\left[ \exp\left( -t z^2 \right) \right] \leq 1 - t\mathbb{E}[z^2] + \frac{1}{2}t^2 \mathbb{E}[z^4].
\]

For both, Rademacher and Gaussian random vectors \( \hat{x} \) and \( \tilde{x} \), we have that

\[
\mathbb{E}[z^2] = \|Q\|^2_F, \quad \mathbb{E}[z^4] \leq 9\|Q\|^4_F.
\]

For the Rademacher case, this follows from Khintchine inequalities; see, e.g., [28 Section 6.8]. For the Gaussian case, see Lemma [A.2] in the appendix. Because of \( \|q_j\|_2 = 1 \), the matrix \( U \) has Frobenius norm 1 and we thus arrive at

\[
P \leq \exp(tk(1 - \varepsilon)) \left( 1 - t + \frac{9}{2}t^2 \right)^k.
\]

Taking the logarithm and applying Taylor expansion, we obtain

\[
\frac{1}{k} \log P \leq t(1 - \varepsilon) + \log \left( 1 - t + \frac{9}{2}t^2 \right) \leq t(1 - \varepsilon) + \left( -t + \frac{9}{2}t^2 \right).
\]

For \( t = \varepsilon/9 \), the right-hand side equals \(-\varepsilon^2/18\), which concludes the proof.

Deriving a lower bound estimate for \( \text{Est}_k \) turns out to be more difficult. The following theorem only consider the case of Rademacher vectors; it is shown that \( n^{-1} \cdot \text{Est}_k \) times a modest factor is a lower bound of \( \text{trace}(B) \) with high probability.
Theorem 3.2. Let $\varepsilon > 0$ and consider the trace estimator $\text{Est}_k$ defined in (3.1) for independent Rademacher random vectors $\tilde{x}_i, \hat{x}_i$. Then the bound

$$\text{trace}(B) \geq \frac{1}{(n-1)\varepsilon + 1} \text{Est}_k$$

holds with probability at least $1 - \exp(-k\varepsilon)$, provided that $(n-1)^2 \geq 48 \cdot \varepsilon^{-1}$.

Proof. Along the lines of the first part of the proof of Theorem 3.1, it can be shown that the statement of the theorem is equivalent to showing that $\exp(-k\varepsilon)$ is an upper bound on

$$\mathbb{P}\left\{ \sum_{j=1}^{n} \frac{\lambda_j}{\text{trace}(B)} \sum_{i=1}^{k} z_{ij}^2 > k((n-1)\varepsilon + 1) \right\} = \mathbb{P}\left\{ \sum_{i=1}^{k} X_i > k(n-1)\varepsilon \right\}.$$

Here,

$$X_i = \sum_{j=1}^{n} \frac{\lambda_j}{\text{trace}(B)} z_{ij}^2 - 1.$$

are zero-mean independent random variables that are bounded; using $|z_{ij}| \leq |\tilde{x}_i|^T |U_j| |\tilde{x}_i| \leq \sqrt{n}$ with $\text{vec}(U_j) = u_j$ one obtains $|X_i| \leq n - 1$. Using that $\mathbb{E}[z_{ij}^2] = 1$ and $\mathbb{E}[z_{ij}^4] = 9$, it can be shown that $\mathbb{E}[X_i^2] \leq 8$. Plugging these bounds into Bernstein’s inequality completes the proof:

$$\mathbb{P}\left\{ \sum_{i=1}^{k} X_i > k(n-1)\varepsilon \right\} \leq \exp\left[ -\frac{(n-1)^2 k^2 \varepsilon^2 / 2}{8k + (n-1)^2 k \varepsilon / 3} \right] \leq \exp(-k\varepsilon),$$

where we used the imposed condition on $k$ in the second inequality.

It is not clear whether a bound of the type presented in Theorem 3.2 extends to the Gaussian case. A major obstacle one faces in deriving such a bound is that $z_{ij}^2$ is not subexponential and therefore Chernoff-type bounds do not apply. This failure of being subexponential is reflected in the strong growth of the moment bounds (which are tight for rank-one matrices) from Lemma A.2 of the Appendix.

4 Numerical Experiments

4.1 Performance of standard and rank-one estimators

The purpose of this section is to numerically assess the impact of using rank-one random vectors instead of unstructured random vectors on the performance of the trace estimator $\text{Est}_k$; see (3.1). For this purpose, the following 8 examples have been chosen to illustrate different aspects of the estimators.

**Ones**, matrix of all ones; $n = 2500$, $\tilde{n} = \hat{n} = 50$, estimation of $\text{trace}(A) = 2500$.

**Rank-one**, matrix $vv^T$ where $v = \text{vec}(I_{\tilde{n}})$ with the identity matrix $I_{\tilde{n}}$; $n = 2500$, $\tilde{n} = \hat{n} = 50$, estimation of $\text{trace}(A) = 50$. 

13
ACTIVSg2000, from the SuiteSparse Matrix Collection [7] originating from a synthetic electric grid model [3]; $n = 4000$, $\tilde{n} = 80$, $\hat{n} = 50$, estimation of $\|A^{-1}\|_F^2 = \text{trace}(A^{-T}A^{-1}) \approx 1.5 \times 10^4$.

ACTIVSg10K, same source as ACTIVSg2000 but now $n = 20000$, $\tilde{n} = 200$, $\hat{n} = 100$, estimation of $\|A^{-1}\|_F^2 \approx 1.3 \times 10^5$.

CFD, from the SuiteSparse Matrix Collection [7] (matrix Rothberg/cfd1) and originating from the discretization of a fluid dynamics problem; $n = 70656$, $\tilde{n} = 276$, $\hat{n} = 256$, estimation of $\text{trace}(A) = 70656$.

CFDinv, identical with CFD but estimation of $\text{trace}(A^{-1}) \approx 6.0 \times 10^5$ instead.

Laplace, matrix from second-order finite difference discretization of Poisson equation on unit square; $n = 2500$, $\tilde{n} = \hat{n} = 50$, estimation of $\text{trace}(A^{-1}) \approx 0.61$.

Convdiff, matrix from finite difference discretization of convection-diffusion equation on unit square (matrix from [23] Sec. 7.2 with $c_s = 1$); $n = 2500$, $\tilde{n} = \hat{n} = 50$, estimation of $\|A^{-1}\|_F^2 \approx 0.0042$.

In all examples for which the trace is estimated the involved matrix is symmetric positive semi-definite. The matrices Ones and Rank-one both have rank one but the stable rank of their (only) singular vector reshaped as a matrix is very different. The discussion in Section 2.4 has singled out Ones as a bad example when estimating with Rademacher vectors. CFD is an example used in [1]. For both, Laplace and Convdiff, the matrix $A$ can be represented in the form $C_1 \otimes I_{\tilde{n}} + I_{\hat{n}} \times C_2$ for smaller, sparse matrices $C_1, C_2$. Such matrices are of particular interest for our new rank-one estimators because the application of $A^{-1}$ (or $A^{-T}$) corresponds to the solution of a matrix Sylvester equation and such an equation can be solved much more efficiently when the right-hand side has low rank [31].

When the trace of $A$ itself is estimated, we used its exact trace as reference value Exact. When the trace or Frobenius norm of $A^{-1}$ are estimated, we used $\text{Est}_{1000}$ with standard Gaussian random vectors as reference value Exact. For each matrix and each type of random vector, we repeated 10 000 times the computation of $\text{Est}_k$ with $k$ ranging from 1 to up to 50 and computed the minimum of $-\text{Exact}/\text{Est}_k$ and the maximum of $\text{Est}_k/\text{Exact}$ across all 10 000 runs for each $k$. The lower and upper curves in each plot of Figure 2 display the minima/maxima vs. $k$ for four different types of random vectors: standard Gaussian, rank-one Gaussian, Rademacher, and rank-one Rademacher vectors. For example, for the matrix Ones and $k = 20$, it can be seen that all curves stay between $-20$ and $10$, which implies that for all 10 000 samples of $\text{Est}_k$, the bounds $\text{Est}_k/10 \leq \text{Exact} \leq 20 \cdot \text{Est}_k$ were satisfied. For nearly all configurations, using rank-one random vectors instead of unstructured random vectors only has a modest impact on these worst-case under- and overestimation factors. Additional data is given in Appendix B, which shows that the inequalities

$$\text{Est}_{10}/30 \leq \text{Exact} \leq 30 \cdot \text{Est}_{10}$$

are nearly always satisfied across all matrices and all types of random vectors.
Figure 2: Performance of trace estimators for 8 different matrices. See Section 4.1 for details.
4.2 Fréchet derivative norm estimation

In this section we describe an application in which random vectors of the form $\tilde{x} \otimes \tilde{x}$ are exploited to significantly speed up computation. Given a matrix function $f$ and a matrix $A \in \mathbb{R}^{n \times n}$, our goal is to estimate the operator norm of the Fréchet derivative, which is a linear map $Df\{A\} : \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$ uniquely defined by the property $f(A + X) = f(A) + Df\{A\}(X) + \mathcal{O}(\|X\|_F^2)$. It is well-known \cite{16} that under certain conditions on the smoothness of $f$,

$$
Df\left(\begin{bmatrix} A & X \\ 0 & A \end{bmatrix}\right) = \begin{bmatrix} f(A) & Df\{A\}(X) \\ 0 & f(A) \end{bmatrix}.
$$

(4.1)

By vectorizing the matrices in its domain and range, the action of $Df\{A\}$ can be represented by an $n^2 \times n^2$ matrix $K_A$ such that $\text{vec}(Df\{A\}(X)) = K_A x$, where $x = \text{vec}(X)$. This yields

$$
\|Df\{A\}\| = \|K_A\|_2 = \sup_{\|x\|_2 = 1} \|K_A x\|_2 = \sqrt{\lambda_{\text{max}}(K_A^T K_A)}.
$$

Therefore, to compute $\|Df\{A\}\|$, one may apply the power method to the matrix $K_A^T K_A$ to compute its largest eigenvalue. The power method requires evaluating $K_A x$ and $K_A^T x$ for several vectors $x$, i.e., evaluating $Df\{A\} X$ and $Df\{A^T\} X$ for several matrices $X$, where $\text{vec}(X) = x$. This is executed via (4.1): the matrix function $f$ is evaluated at a $2n \times 2n$ matrix, and the top right block is read from the resulting matrix. For larger $n$, such computation may be very demanding.

If we are only interested in an upper bound for $\|Df\{A\}\|$ instead of its exact value, we can apply techniques discussed in Section 2.3 to $x_j = \tilde{x}_j \otimes \tilde{x}_j$, where $\tilde{x}_j$ and $\tilde{x}_j$ are standard Gaussian vectors of length $n$, for $j = 1, \ldots, k$. Using the maximum estimator

$$
\text{Max}_k = \max_{j=1,\ldots,k} \|K_A (\tilde{x}_j \otimes \tilde{x}_j)\|_2 = \max_{j=1,\ldots,k} \|Df\{A\}(\tilde{x}_j \tilde{x}_j^T)\|_F
$$

and applying (2.10) then guaranties the following:

$$
\mathbb{P}\{\|Df\{A\}\| \leq \theta \cdot \text{Max}_k\} \geq 1 - \left(\frac{2}{\pi} (2 + \ln(1 + 2\theta)) \theta^{-1}\right)^k.
$$

Computing the matrix-vector products in (4.2) reduces to evaluating $Df\{A\}(X_j)$ for rank-one matrices $X_j = \tilde{x}_j \tilde{x}_j^T$. This can be done far more efficiently than evaluating $Df\{A\}(X)$ for general matrices $X$, by using Algorithm\cite{1} slightly adapted from \cite{21}. Algorithm\cite{1} also needs to evaluate the function $f$, but for matrices of sizes at most $2\ell \times 2\ell$, where the final dimension $\ell$ of the Krylov subspace is significantly smaller than $n$. This is the source of the significant speedup when compared to the power method. Also note that only the first iteration of the power method can benefit from Algorithm\cite{1} as the later iterates are generally not matrices of rank one.

To illustrate this difference, we ran both the power method and the 99.9% confidence maximum estimator ($\theta = 10$, $k = 7$) to estimate $\|Df\{A\}\|$, where $f$ is the matrix exponential, and $A = -0.01(I_n \otimes T_n + T_n \otimes I_n)$. Here $T_n$ is the tridiagonal matrix with $2/(n - 1)^2$ on the main diagonal and $-1/(n - 1)^2$ on the first upper and lower subdiagonal, i.e., the 1D discrete Laplacian on $[0,1]$. Running in Matlab R2019b on an Intel i5 4690K processor, we obtain the following results:
Algorithm 1: Arnoldi method for approximating $Df\{A\}(cd^T)$

1. for $\ell = 1, 2, \ldots$ do

2. Perform one step of the Arnoldi method to obtain an orthonormal basis $U_\ell$ of the Krylov subspace $K_\ell(A, c)$ and $G_\ell = U_\ell^T A U_\ell$, $\tilde{c} = U_\ell^T c$.

3. Perform one step of the Arnoldi method to obtain an orthonormal basis $V_\ell$ of the Krylov subspace $K_\ell(A^T, d)$ and $H_\ell = V_\ell^T A^T V_\ell$, $\tilde{d} = V_\ell^T d$.

4. Compute $F_\ell = f \left( \begin{bmatrix} G_\ell & \tilde{c} \tilde{d}^T \\ 0 & H_\ell^T \end{bmatrix} \right)$ and set $X_\ell = F_\ell(1:\ell, \ell+1:2\ell)$.

5. if converged then

6. Stop the loop.

7. Return $U_\ell X_\ell V_\ell^T$.

| $n$ | time(power method) | $\|Df\{A\}\|$ | time($\text{Max}_k$) | $\theta \cdot \text{Max}_k$ | maximum $\ell$ |
|-----|-------------------|----------------|----------------|----------------|------------|
| 10  | 0.12              | 0.86           | 0.05           | 147.10         | 20         |
| 20  | 1.81              | 0.85           | 0.10           | 151.00         | 30         |
| 30  | 16.49             | 0.78           | 0.38           | 115.44         | 45         |
| 40  | 74.06             | 0.80           | 1.18           | 102.13         | 55         |
| 50  | 275.52            | 0.82           | 2.95           | 93.38          | 70         |

Note that $A$ is an $n^2 \times n^2$ matrix. We ran 7 iterations of the power method; the third column shows the approximation of $\|Df\{A\}\|$ it reported. The fifth column shows the 99.9% confidence upper bound for $\|Df\{A\}\|$ as reported by the maximum estimator. In the last column is the maximum dimension $\ell$ of all Krylov subspaces needed for the computation of $\text{Max}_k$. We stop the Arnoldi iteration once $\|F_\ell - \begin{bmatrix} F_{\ell-1} & 0 \\ 0 & 0 \end{bmatrix}\| < 10^{-8}$, as suggested in [2, Section 2.3]. All times are given in seconds. While the upper bounds provided by the maximum estimators are, in this case, about 100 times larger than the actual norm of the Fréchet derivative, this may be sufficient as a rough estimate. Such an estimate can be rapidly computed by using random vectors studied in this paper.

5 Conclusions

In this work we have provided theoretical and experimental evidence that rank-one random vectors are suited for norm and trace estimation. While their performance is consistently worse compared to unstructured vectors, this can be easily mitigated by, e.g., increasing the constants or increasing the number of samples in the stochastic trace estimator.

It is tempting to ask whether the results of this paper have a meaningful extension to higher-order tensors. As one of the simplest examples, one could imagine estimating the Euclidean norm $\|z\|_2$ of a vector $z \in \mathbb{R}^{n^d}$, representing the vectorization of an order-$d$ tensor $Z$, via inner products $\langle x^T z \rangle$ with $x = x_d \otimes x_{d-1} \cdots x_1$ for independent random vectors $x_1, \ldots, x_d$ of length $n$. Existing work in quantum physics [12] indicates that such an attempt is futile for larger $d$; the probability
to get a meaningful estimate of $\|z\|_2$ is exponentially small in $d$ for nearly every tensor $Z$. In the techniques used in this work, this curse of dimensionality raises its ugly head, e.g., in the Khinchine inequalities \[27\] and, more generally, the moments of order-$d$ chaos. For example, an extension of Lemma A.2 to arbitrary $d$ would feature bounds that grow exponentially with $d$ and become tight for rank-one tensors.

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The following lemma provides a Chernoff bound for chi-square distributions. This result is certainly well known; we include it for completeness.

**Lemma A.1.** Let $X$ be a random variable having a chi-square distribution with $k$ degrees of freedom. For $\theta > 1$, it holds that

$$
P \{ X > k \theta \} \leq \left( \theta e^{1-\theta} \right)^{k/2}.
$$

**Proof.** For $t > 0$, we let $M_X(t) = (1 - 2t)^{-k/2}$ denote the moment generating function of $X$. By the Markov inequality,

$$
P \{ X > k \theta \} = P \{ tX/k > t \theta \} = P \{ e^{tX/k} > e^{t\theta} \}
\leq E[e^{tX/k}] \cdot e^{-t\theta} = M_X(t/k) e^{-t\theta} = (1 - 2t/k)^{-k/2} e^{-t\theta},
$$

which holds for $t/k < 1/2$. Choosing $t = k/2 - k/2\theta$ implies

$$
P \{ X > k \theta \} \leq \theta^{k/2} e^{k/2(1-\theta)} = \left( \theta e^{1-\theta} \right)^{k/2}.
$$

The following two results on the moments and the moment generating function of decoupled second-order Gaussian chaos are closely related to existing results by Latala [27]; see also the monograph [4]. We include these results for the convenience of the reader.
Lemma A.2. Let $Q \in \mathbb{R}^{n \times n}$, and let $\hat{x} \sim \mathcal{N}(0, I_n)$, $\tilde{x} \sim \mathcal{N}(0, I_n)$. For $Z = \hat{x}^T Q \tilde{x}$ it holds that

$$E[Z^2] = \|Q\|_F^2, \quad E[Z^4] = 3(2\|Q\|_{(4)}^4 + \|Q\|_F^4) \leq 9\|Q\|_F^4,$$

where $\| \cdot \|_{(4)}$ denotes the Schatten-$4$ norm [18, Sec. 7.4] of a matrix. For any even $k$, we have

$$E[Z^k] \leq ((k - 1)!!)^2 \|Q\|_F^k, \quad (A.1)$$

where $(k - 1)!! = (k - 1)(k - 3) \cdots 3 \cdot 1$ denotes the double factorial. For odd $k$, $E[Z^k] = 0$.

Proof. For the second moment, we obtain

$$E[Z^2] = E[\hat{x}^T Q \hat{x}] = E[\|Q \hat{x}\|_2^2] = \|Q\|_F^2,$$

where the second equality follows from the fact that for $y = Q^T \hat{x}$ with fixed $\hat{x}$, the random variable $y^T \hat{x}$ is normal with zero mean and variance $\|y\|_2^2$. Noting that the fourth moment of such a normal random variable is $3\|y\|_2^4$, an analogous argument shows $E[Z^4] = 3 \cdot E[\|Q^T \hat{x}\|_2^4]$. To proceed from here, we may assume – without loss of generality – that $\bar{n} \leq n$ and that $Q$ is a diagonal matrix with the singular values $\sigma_1 \geq \cdots \geq \sigma_{\bar{n}} \geq 0$ on the diagonal; see, e.g., the proof of Theorem 2.2. This gives

$$E[\|Q^T \hat{x}\|_2^4] = E[(\sigma_1 \hat{x}_1^2 + \cdots + \sigma_{\bar{n}} \hat{x}_{\bar{n}}^2)^2] = \sum_{i,j} \sigma_i^2 \sigma_j^2 E[\hat{x}_i \hat{x}_j^2]$$

$$= \sum_i \sigma_i^4 E[\hat{x}_i^4] + \sum_{i \neq j} \sigma_i^2 \sigma_j^2 E[\hat{x}_i^2] \cdot E[\hat{x}_j^2] = 3 \sum_i \sigma_i^4 + \sum_{i \neq j} \sigma_i^2 \sigma_j^2$$

$$= 2 \sum_i \sigma_i^4 + \sum_{i \neq j} \sigma_i^2 \sigma_j^2 = 2\|Q\|_{(4)}^4 + \|Q\|_F^4,$$

which establishes the claimed expression for $E[Z^4]$. The upper bound $9\|Q\|_{(4)}^4$ follows from $\|Q\|_{(4)} \leq \|Q\|_F$. For general even $k$, the statement and proof of (A.1) is contained in the proof of Lemma 7.1 in [5]. The proof that follows is slightly simpler. We first note that the $k$th moment of a centered normal random variable with variance $\sigma^2$ is given by $(k - 1)!! \sigma^k$. In turn, $E[Z^k] = (k - 1)!! \cdot E[\|Q^T \hat{x}\|_2^k]$. We proceed as above and obtain

$$E[\|Q^T \hat{x}\|_2^k] = \sum_{i_1, \ldots, i_k/2} \sigma_{i_1}^2 \cdots \sigma_{i_k/2}^2 E[\hat{x}_{i_1}^2 \cdots \hat{x}_{i_k/2}^2].$$

Using that $E[\hat{x}_i^{2p} \hat{x}_j^{2q}] = (2p - 1)!! \cdot (2q - 1)!! \leq (2(p + q) - 1)!! = E[\hat{x}_i^{2(p+q)}]$ for any $p, q \in \mathbb{N}$ and $i \neq j$, we obtain

$$E[\|Q^T \hat{x}\|_2^k] \leq (k - 1)!! \sum_{i_1, \ldots, i_k/2} \sigma_{i_1}^2 \cdots \sigma_{i_k/2}^2 = (k - 1)!! \cdot \|Q\|_F^k,$$

which concludes the proof of (A.1).

The statement on odd $k$ follows from the symmetry of the distribution: $Z$ and $-Z = \hat{x}^T Q(-\tilde{x})$ have the same distribution and hence $E[Z^k] = E[(-Z)^k] = E[-Z^k] = -E[Z^k]$. This shows $E[Z^k] = 0$. \qed
Corollary A.3. For $Z$ as in Lemma A.2 with $\|Q\|_F = 1$, the moment generating function exists and is bounded by

$$
\mathbb{E}[\exp(tZ)] \leq \frac{1}{\sqrt{1-t^2}}
$$

for $t < 1$.

Proof. Using the result of Lemma A.2, it follows that

$$
\mathbb{E}[\exp(tZ)] = \sum_{k=0}^{\infty} \frac{1}{k!} \mathbb{E}[Z^k] t^k = \sum_{k=0}^{\infty} \frac{1}{(2k)!} \mathbb{E}[Z^{2k}] t^{2k}
$$

$$
\leq \sum_{k=0}^{\infty} \frac{(k-1)!!}{(2k)!} t^{2k} = \sum_{k=0}^{\infty} \frac{1}{4^k} \binom{2k}{k} t^{2k} = \frac{1}{\sqrt{1-t^2}},
$$

where the last step follows from Taylor expansion. \[\square\]
## B Detailed data on performance of estimators

The following tables provide detailed data on the performance of trace/Frobenius norm estimation with the stochastic trace estimator using rank-one/unstructured Gaussian/Rademacher vectors.

Legend: \( G = \) Gaussian, \( G_1 = \) rank-one Gaussian, \( R = \) Rademacher, \( R_1 = \) rank-one Rademacher.

For each value of \( \theta \) and \( k \) the upper value shows the ratio of events that the estimator times \( \hat{\theta} \) does not provide an upper bound and the lower value shows the ratio of events that the estimator divided by \( \theta \) does not provide a lower bound. For example, when \( A \) is the matrix of all ones, the inequality \( \text{trace}(A) \leq 8 \cdot \text{Est}_5 \) fails for only 33 out of 10,000 events while the inequality \( \text{trace}(A) \geq 1/8 \cdot \text{Est}_5 \) fails for 1201 out of 10,000 events when using rank-one Gaussian vectors.

### Trace of matrix of all ones

| \( \theta = 1.2 \) | \( \theta = 2 \) | \( \theta = 4 \) | \( \theta = 8 \) | \( \theta = 30 \) |
|-------------------|----------------|----------------|----------------|----------------|
| \( k = 1 \) |
| \( G \) | 0.2758 | 0.1619 | 0.0467 | 0.0053 | 0.0000 |
| \( G_1 \) | 0.1814 | 0.1244 | 0.0637 | 0.0248 | 0.0016 |
| \( R \) | 0.2726 | 0.1587 | 0.0423 | 0.0058 | 0.0000 |
| \( R_1 \) | 0.1952 | 0.1332 | 0.0521 | 0.0210 | 0.0014 |

### Trace of \( vv^T \) with vectorized identity matrix \( v \)

| \( \theta = 1.2 \) | \( \theta = 2 \) | \( \theta = 4 \) | \( \theta = 8 \) | \( \theta = 30 \) |
|-------------------|----------------|----------------|----------------|----------------|
| \( k = 1 \) |
| \( G \) | 0.2810 | 0.1598 | 0.0455 | 0.0045 | 0.0000 |
| \( G_1 \) | 0.2729 | 0.1570 | 0.0490 | 0.0058 | 0.0000 |
| \( R \) | 0.3249 | 0.1244 | 0.0342 | 0.0040 | 0.0000 |
| \( R_1 \) | 0.3256 | 0.1196 | 0.0318 | 0.0020 | 0.0000 |

| \( k = 5 \) |
| \( G \) | 0.3063 | 0.0728 | 0.0011 | 0.0000 | 0.0000 |
| \( G_1 \) | 0.2594 | 0.1264 | 0.0303 | 0.0033 | 0.0000 |
| \( R \) | 0.3029 | 0.0742 | 0.0013 | 0.0000 | 0.0000 |
| \( R_1 \) | 0.2667 | 0.1294 | 0.0303 | 0.0039 | 0.0000 |

| \( k = 10 \) |
| \( G \) | 0.2912 | 0.0275 | 0.0000 | 0.0000 | 0.0000 |
| \( G_1 \) | 0.2807 | 0.1053 | 0.0155 | 0.0009 | 0.0000 |
| \( R \) | 0.2873 | 0.0298 | 0.0000 | 0.0000 | 0.0000 |
| \( R_1 \) | 0.2749 | 0.1024 | 0.0121 | 0.0008 | 0.0005 |

| \( \theta = 1.2 \) | \( \theta = 2 \) | \( \theta = 4 \) | \( \theta = 8 \) | \( \theta = 10 \) |
|-------------------|----------------|----------------|----------------|----------------|
| \( k = 1 \) |
| \( G \) | 0.6376 | 0.5187 | 0.3867 | 0.2796 | 0.1504 |
| \( G_1 \) | 0.7683 | 0.6959 | 0.5919 | 0.4937 | 0.3332 |
| \( R \) | 0.6282 | 0.5136 | 0.3791 | 0.2644 | 0.1361 |
| \( R_1 \) | 0.7401 | 0.6759 | 0.6100 | 0.4950 | 0.3406 |

| \( k = 5 \) |
| \( G \) | 0.4742 | 0.2248 | 0.0606 | 0.0143 | 0.0005 |
| \( G_1 \) | 0.6236 | 0.4493 | 0.2495 | 0.1201 | 0.0196 |
| \( R \) | 0.4733 | 0.2262 | 0.0605 | 0.0124 | 0.0006 |
| \( R_1 \) | 0.6114 | 0.4367 | 0.2357 | 0.1061 | 0.0193 |

| \( k = 10 \) |
| \( G \) | 0.3982 | 0.1079 | 0.0078 | 0.0001 | 0.0000 |
| \( G_1 \) | 0.5481 | 0.3153 | 0.1079 | 0.0271 | 0.0009 |
| \( R \) | 0.3930 | 0.1069 | 0.0117 | 0.0004 | 0.0000 |
| \( R_1 \) | 0.5507 | 0.3142 | 0.1085 | 0.0240 | 0.0005 |
| $\theta$ | $\theta = 1.2$ | $\theta = 2$ | $\theta = 4$ | $\theta = 8$ | $\theta = 30$ |
|---------|----------------|----------------|----------------|----------------|----------------|
| Frobenius norm of inverse of ACTIVSg2000 |
| $k = 1$ |
| G | 0.2619 | 0.1439 | 0.0396 | 0.0041 | 0.0000 |
| G1 | 0.6451 | 0.5144 | 0.3550 | 0.2284 | 0.0017 |
| G | 0.1977 | 0.1264 | 0.0554 | 0.0192 | 0.0008 |
| G1 | 0.7399 | 0.6385 | 0.4919 | 0.3303 | 0.0367 |
| R | 0.2687 | 0.1507 | 0.0390 | 0.0028 | 0.0000 |
| R1 | 0.6352 | 0.5044 | 0.3502 | 0.2189 | 0.0004 |
| k = 5 |
| G | 0.2978 | 0.0637 | 0.0006 | 0.0000 | 0.0000 |
| G1 | 0.4724 | 0.2079 | 0.0430 | 0.0039 | 0.0000 |
| G | 0.2521 | 0.1113 | 0.0210 | 0.0014 | 0.0000 |
| G1 | 0.6027 | 0.3786 | 0.1405 | 0.0309 | 0.0000 |
| R | 0.2949 | 0.0635 | 0.0005 | 0.0000 | 0.0000 |
| R1 | 0.4668 | 0.2064 | 0.0426 | 0.0036 | 0.0000 |
| k = 10 |
| G | 0.2702 | 0.0229 | 0.0000 | 0.0000 | 0.0000 |
| G1 | 0.4067 | 0.0991 | 0.0050 | 0.0002 | 0.0000 |
| G | 0.2694 | 0.0816 | 0.0074 | 0.0003 | 0.0000 |
| G1 | 0.5263 | 0.2398 | 0.0415 | 0.0018 | 0.0000 |
| R | 0.2702 | 0.0234 | 0.0000 | 0.0000 | 0.0000 |
| R1 | 0.4063 | 0.0946 | 0.0052 | 0.0001 | 0.0000 |
| Frobenius norm of inverse of ACTIVSg10K |
| $k = 1$ |
| G | 0.2717 | 0.1507 | 0.0394 | 0.0036 | 0.0000 |
| G1 | 0.6389 | 0.5135 | 0.3560 | 0.2129 | 0.0195 |
| G | 0.2108 | 0.1362 | 0.0583 | 0.0180 | 0.0003 |
| G1 | 0.7271 | 0.6289 | 0.4922 | 0.3469 | 0.1060 |
| R | 0.2750 | 0.1480 | 0.0360 | 0.0027 | 0.0000 |
| R1 | 0.6262 | 0.4961 | 0.3356 | 0.1929 | 0.0167 |
| k = 5 |
| G | 0.2848 | 0.0641 | 0.0006 | 0.0000 | 0.0000 |
| G1 | 0.4787 | 0.2116 | 0.0415 | 0.0038 | 0.0000 |
| G | 0.2678 | 0.1053 | 0.0171 | 0.0012 | 0.0000 |
| G1 | 0.5802 | 0.3629 | 0.1340 | 0.0313 | 0.0001 |
| R | 0.2869 | 0.0538 | 0.0002 | 0.0000 | 0.0000 |
| R1 | 0.4678 | 0.1963 | 0.0382 | 0.0036 | 0.0000 |
| k = 10 |
| G | 0.2532 | 0.0187 | 0.0000 | 0.0000 | 0.0000 |
| G1 | 0.4246 | 0.1004 | 0.0035 | 0.0001 | 0.0000 |
| G | 0.2680 | 0.0690 | 0.0047 | 0.0001 | 0.0000 |
| G1 | 0.5135 | 0.2339 | 0.0400 | 0.0027 | 0.0000 |
| R | 0.2514 | 0.0148 | 0.0000 | 0.0000 | 0.0000 |
| R1 | 0.4060 | 0.0867 | 0.0032 | 0.0001 | 0.0000 |
| R | 0.2502 | 0.0569 | 0.0037 | 0.0000 | 0.0000 |
| R1 | 0.5015 | 0.1669 | 0.0094 | 0.0001 | 0.0000 |
| Trace of CFD | Trace of inverse of CFD |
|-------------|-------------------------|
| $\theta = 1.2$ | $\theta = 1.2$ |
| $k = 1$ | $k = 1$ |
| $G$ | $G$ |
| 0.0000 | 0.0666 |
| 0.0000 | 0.0003 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $G1$ | $G1$ |
| 0.0602 | 0.1306 |
| 0.0826 | 0.0147 |
| 0.0000 | 0.0008 |
| 0.0000 | 0.0001 |
| $R$ | $R$ |
| 0.0000 | 0.0668 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R1$ | $R1$ |
| 0.0000 | 0.1109 |
| 0.0000 | 0.0126 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0007 |
| $\theta = 2$ | $\theta = 2$ |
| $k = 1$ | $k = 1$ |
| $G$ | $G$ |
| 0.0000 | 0.0040 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $G1$ | $G1$ |
| 0.0000 | 0.0732 |
| 0.0000 | 0.0007 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R$ | $R$ |
| 0.0000 | 0.0508 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R1$ | $R1$ |
| 0.0000 | 0.0049 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $\theta = 4$ | $\theta = 4$ |
| $k = 1$ | $k = 1$ |
| $G$ | $G$ |
| 0.0000 | 0.0002 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $G1$ | $G1$ |
| 0.0000 | 0.0344 |
| 0.0000 | 0.0001 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R$ | $R$ |
| 0.0000 | 0.0102 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R1$ | $R1$ |
| 0.0000 | 0.0001 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $\theta = 8$ | $\theta = 8$ |
| $k = 1$ | $k = 1$ |
| $G$ | $G$ |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $G1$ | $G1$ |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R$ | $R$ |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| $R1$ | $R1$ |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| Trace of inverse of Laplace | Frobenius norm of inverse of Convdiff |
|-----------------------------|----------------------------------------|
| $\theta = 1.2$ | $\theta = 1.2$ | $\theta = 2$ | $\theta = 4$ | $\theta = 8$ | $\theta = 30$ |
| $k = 1$ | $\theta = 1.2$ | $\theta = 2$ | $\theta = 4$ | $\theta = 8$ | $\theta = 30$ |
| $G$ | 0.0996 | 0.0006 | 0.0000 | 0.0000 | 0.0000 | 0.2679 | 0.1042 | 0.0144 | 0.0006 | 0.0000 | 0.5677 | 0.2909 | 0.0343 | 0.0002 | 0.0000 |
| $G1$ | 0.2521 | 0.0488 | 0.0030 | 0.0000 | 0.0000 | 0.2218 | 0.1232 | 0.0456 | 0.0121 | 0.0001 | 0.6945 | 0.5452 | 0.3344 | 0.1575 | 0.0093 |
| $R$ | 0.0975 | 0.0005 | 0.0000 | 0.0000 | 0.0000 | 0.2666 | 0.1034 | 0.0136 | 0.0004 | 0.0000 | 0.5697 | 0.2954 | 0.0390 | 0.0003 | 0.0000 |
| $R1$ | 0.2196 | 0.0346 | 0.0017 | 0.0001 | 0.0000 | 0.2165 | 0.1200 | 0.0443 | 0.0115 | 0.0004 | 0.6901 | 0.5364 | 0.3246 | 0.1453 | 0.0062 |
| $k = 5$ | $\theta = 1.2$ | $\theta = 2$ | $\theta = 4$ | $\theta = 8$ | $\theta = 30$ |
| $G$ | 0.0096 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2584 | 0.0188 | 0.0000 | 0.0000 | 0.0000 | 0.3684 | 0.0330 | 0.0000 | 0.0000 | 0.0000 |
| $G1$ | 0.1764 | 0.0042 | 0.0000 | 0.0000 | 0.0000 | 0.2665 | 0.0919 | 0.0125 | 0.0004 | 0.0000 | 0.5517 | 0.2783 | 0.0455 | 0.0017 | 0.0000 |
| $R$ | 0.0083 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2593 | 0.0182 | 0.0000 | 0.0000 | 0.0000 | 0.3731 | 0.0372 | 0.0000 | 0.0000 | 0.0000 |
| $R1$ | 0.1483 | 0.0021 | 0.0000 | 0.0000 | 0.0000 | 0.2728 | 0.0909 | 0.0120 | 0.0007 | 0.0000 | 0.5371 | 0.2570 | 0.0406 | 0.0010 | 0.0000 |
| $k = 10$ | $\theta = 1.2$ | $\theta = 2$ | $\theta = 4$ | $\theta = 8$ | $\theta = 30$ |
| $G$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2198 | 0.0031 | 0.0000 | 0.0000 | 0.0000 | 0.2696 | 0.0023 | 0.0000 | 0.0000 | 0.0000 |
| $G1$ | 0.1362 | 0.0003 | 0.0000 | 0.0000 | 0.0000 | 0.2763 | 0.0688 | 0.0039 | 0.0001 | 0.0000 | 0.4686 | 0.1431 | 0.0066 | 0.0000 | 0.0000 |
| $R$ | 0.0005 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2268 | 0.0033 | 0.0000 | 0.0000 | 0.0000 | 0.2641 | 0.0037 | 0.0000 | 0.0000 | 0.0000 |
| $R1$ | 0.0970 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2752 | 0.0634 | 0.0036 | 0.0000 | 0.0000 | 0.4618 | 0.1340 | 0.0033 | 0.0000 | 0.0000 |