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Estimation of the bilinear form $y^* f(A)x$ for Hermitian matrices

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For a Hermitian matrix $A \in \mathbb{C}^{p\times p}$, given vectors $x, y \in \mathbb{C}^p$ and for suitable functions f, the bilinear form $y^* f(A)x$ is estimated by extending the extrapolation method proposed by C. Brezinski in 1999. Families of one term and two term estimates $e_{f,\nu}$, $\nu \in \mathbb{C}$ and $\hat{e}_{f,n,k}$, $n, k \in \mathbb{Z}$, respectively, are derived by extrapolation of the moments of the matrix A. For the positive definite case, bounds for the optimal value of ν, which leads to an efficient one term estimate in only one matrix vector product, are derived. For $f(A) = A^{-1}$, a formula approximating this optimal value of ν is specified. Numerical results for several matrix functions and comparisons are provided to demonstrate the effectiveness of the extrapolation method.

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1. Preliminaries and motivation for the problem

Let A be a complex Hermitian matrix of dimension p, x, y complex vectors of length p and f a suitable smooth function defined on the spectrum of the matrix A. The subject of this work is to estimate the bilinear form $y^* f(A)x$ by developing an approach based on the extrapolation of the moment $(x, f(A)y)$ of the matrix A.

The computation of $y^* f(A)x$ arises in network analysis [13], in machine learning, in statistics, in many linear algebra problems and other disciplines. In particular, estimates for the following problems can be derived.

– *Elements of a matrix $f(A)$.* For $x = \delta_i$ and $y = \delta_j$, where the vector δ_i denotes the ith column of the identity matrix of dimension p, we get estimates for the elements of the matrix $f(A)$. In network analysis, for an adjacency matrix A, the ith diagonal element of $exp(A)$ leads to the notion of the "subgraph centrality" of the ith node, whereas the ij element represents the "subgraph communicability" between the ith and the jth node, which measures how easy it is to send a message from node i to node j in a graph [11]. For $f(A) = A^k$, $k \in \mathbb{N}$, $(A^k)_{ii}$ is the number of closed walks of length k based at node i, whereas $(A^k)_{ij}$ is the number of walks of length k that connects nodes i and j. Estimates for the whole diagonal of the matrix $f(A)$ can be derived as well. Extracting diagonal entries of a matrix inverse is important in uncertainty quantification [3,23].

– *Trace of a matrix $f(A)$.* For appropriately selected vectors $x = y$ and using a result of Hutchinson [12], estimates for the trace of the matrix $f(A)$ $(\mathrm{Tr}(f(A)))$ can be found. The computation of the trace of a matrix function arises in physics, in quantum chemistry for the estimation of density of states [26]. In network analysis, for an adjacency matrix A, the "Estrada index" is defined as the $\mathrm{Tr}(exp(A))$ [11]. For $f(A) = A^{-1}$, another approach was recently developed in [31].

– *Determinant of a matrix A.* The evaluation of the determinant of a matrix A appears in lattice quantum chromodynamics and other areas. Estimates for the determinant of a matrix $(det(A))$ are obtained by estimating the $\mathrm{Tr}(log(A))$ [17,22].

– *Partial eigenvalue sum.* In solid state physics the computation of the total energy of an electronic structure requires the evaluation of partial eigenvalue summations. For an appropriate selection of a function f, the estimation of the $\mathrm{Tr}(f(A))$ leads to the estimation of the partial sum of the eigenvalues of a matrix A [2].

– *Machine Learning.* The optimization problem that occurs in the training of a Gaussian process requires the evaluation of the $\mathrm{Tr}(T^{-1}S)$, for appropriate matrices T, S [5].

– *Square of the error norm.* Let y be an approximation of the direct solution u of the linear system $Au = x$, obtained either by a direct or by an iterative method. Let $r = Au - Ay$ be the residual. For $f(A) = A^{-2}$, the quantity $r^T f(A)r$ gives the square of the error norm $\|u - y\|^2$ of the linear system. Estimates for this quantity have been developed in [6].

– *Bilinear form* $y^*A^{-1}x$. The evaluation of $y^*A^{-1}x$ is needed in signal processing, nuclear physics, quantum mechanics, computational fluid dynamics [18,27,28], in solid state physics and in optimization [16,19,18]. In numerical linear algebra, the computation of this bilinear form is needed for the determination of the A-norm [19,25], and for the computation of particular elements of the solution of a linear system. Furthermore, the estimation of the scalar value y^*u, where u solves the linear system $Au = x$, is needed in computing error bounds for iterative methods and in solving inverse problems, least and total least squares problems [17].

In this paper, for a Hermitian matrix $A \in \mathbb{C}^{p\times p}$ and vectors $x, y \in \mathbb{C}^p$, estimates for the bilinear form $y^*f(A)x$ are obtained by extrapolation of the moments of the matrix A. The derived family of the one term estimates $e_{f,\nu}$ depends on a parameter $\nu \in \mathbb{C}$ and requires only few floating point operations of order $\mathcal{O}(p^2)$, reduced to $\mathcal{O}(dp)$ for a banded matrix of bandwidth d. In fact, the appropriate selection of an optimal value of ν which provides exact estimates is not yet specified. However, for the positive definite case, this value is bounded and a satisfactory statistical approximation is developed. Furthermore, for $f(A) = A^{-1}$ a concrete approximation of this optimal value is specified. Two term estimates $\hat{e}_{f,n,k}$, for $n, k \in \mathbb{Z}$, are also developed and tested throughout the numerical results attaining a satisfactory relative error.

The outline of the paper is as follows. The theoretical approach and the estimates for the bilinear form $y^*f(A)x$ are introduced in Section 2. Specifically, the case for $x = y$ is developed in Subsection 2.1. In Subsection 2.2 bounds and approximations leading to more accurate one term estimates are presented, whereas in Subsection 2.3, the case for $x \neq y$ is discussed. Numerical experiments are reported in Section 3 and concluding remarks end the paper.

Throughout the paper $\|x\|$ denotes the Euclidean norm of a vector x, $\|A\|$ is the spectral norm of a matrix A, $(\cdot,\cdot)$ denotes the inner product, $\bar{\alpha}$ denotes the complex conjugate of a value $\alpha \in \mathbb{C}$, the superscript $*$ denotes the conjugate transpose and the symbol $\simeq$ means "approximately equal to". The maximum and the minimum eigenvalues of a matrix are denoted by λ_1 and λ_p, respectively.

2. Families of estimates via an extrapolation procedure

Claude Brezinski in 1999 introduced an extrapolation approach for estimating the norm of the error when solving a linear system [6]. This approach was extended in [8] to the estimation of the trace of the inverse of a linear operator on a Hilbert space and in [7] to the estimation of the trace of the power of positive self-adjoint linear operators. In [14] families of estimates for the bilinear form $x^TA^{-1}y$ based on extrapolation of the moments of the matrix $A \in \mathbb{R}^{p\times p}$ at the point -1 were derived. In this work, the extrapolation procedure is generalized for the derivation of estimates for the bilinear form $y^*f(A)x$, for a Hermitian matrix $A \in \mathbb{C}^{p\times p}$ and given vectors $x, y \in \mathbb{C}^p$.

2.1. Estimates for the quadratic form $x^* f(A)x$

Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian matrix. The spectral decomposition of this matrix is

$$A = V\Lambda V^* = \sum_{k=1}^{p} \lambda_k v_k v_k^*,$$

where $V = [v_1, \dots, v_p]$ is an orthonormal matrix, whose columns v_k are the normalized eigenvectors of the matrix A and Λ is a diagonal matrix, whose diagonal elements are the eigenvalues $\lambda_k \in \mathbb{R}$ of the matrix A [21].

Let us consider a function f, defined on the spectrum of the matrix A. Then, it holds that $f(A) = Vf(\Lambda)V^*$ [20]. In order the matrix $f(A)$ to be also Hermitian, it is necessary to assume that the spectrum of this matrix takes only real values i.e. $f(\Lambda) \in \mathbb{R}^{p\times p}$. Thus, in the case of functions such as the logarithm or the square root, we must assume that the matrix $A \in \mathbb{C}^{p\times p}$ should have no eigenvalues on the closed negative real axis.

For a complex vector $x \in \mathbb{C}^p$ it holds that $Ax = \sum_{k=1}^{p} \lambda_k (x, v_k)v_k$ and $f(A)x = \sum_{k=1}^{p} f(\lambda_k)(x, v_k)v_k$. The moments of the matrix A are the quantities [7]

$$c_r(x) = (x, A^r x), \quad r \in \mathbb{R}. \tag{1}$$

Using the spectral decomposition of the matrix A, the moments $c_r(x)$ can be expressed as sums

$$c_r(x) = x^* A^r x = \sum_{k=1}^{p} \lambda_k^r (x, v_k)(v_k, x) = \sum_{k=1}^{p} \lambda_k^r (x, v_k)\overline{(x, v_k)} = \sum_{k=1}^{p} \lambda_k^r \alpha_k \bar{\alpha}_k, \tag{2}$$

where $\alpha_k = (x, v_k)$. The function moment is defined $c_f(x) = (x, f(A)x)$ and can be expressed as the following sum,

$$(x, f(A)x) = \sum_{k=1}^{p} f(\lambda_k)(x, v_k)\overline{(x, v_k)} = \sum_{k=1}^{p} f(\lambda_k) a_k \bar{\alpha}_k. \tag{3}$$

We consider as interpolation conditions one or two terms of the summation of relation (2) for some moments $c_n(x)$ with a nonnegative integer index n. Then, the moments $c_f(x)$ can be estimated by extrapolating these interpolation conditions to the formula (3).

In what follows, the moments $c_r(x)$ and $c_f(x)$ will be denoted as c_r and c_f, respectively, and all the denominators of the estimates are assumed to be different from zero.

One-term estimate

Approximations of c_f can be obtained by keeping only one term in the summation (3), that is,

$$(x, f(A)x) \simeq f(l)a\bar{a} = f(l)|a|^2,$$

where the unknowns l and $|a|^2$ are determined by imposing the following interpolation conditions

$$c_0 = (x,x) = x^*x = x^*\sum_k (x,v_k)v_k = \sum_k (x,v_k)(v_k,x) \simeq |a|^2,$$
$$c_1 = (x,Ax) = x^*Ax = \sum_k \lambda_k (x,v_k)(v_k,x) \simeq l|a|^2,$$
$$c_2 = (x,A^2x) = x^*A^2x = \sum_k \lambda_k^2 (x,v_k)(v_k,x) \simeq l^2|a|^2.$$

From this nonlinear system we obtain $l = c_0^{j-1}c_1^{1-2j}c_2^{j}$, $j = 0, \frac{1}{2}, 1$. The range of values of l can be extended to any complex number $\nu = \eta + i\zeta$ because $c_0^{\eta+i\zeta-1}c_1^{1-2(\eta+i\zeta)}c_2^{\eta+i\zeta} = (|a|^2)^{\eta+i\zeta-1}(l|a|^2)^{1-2(\eta+i\zeta)}(l^2|a|^2)^{\eta+i\zeta} = l$. In the following Proposition, we obtain the family of the one term estimates $e_{f,\nu}$ for the moment c_f.

Proposition 1. *Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian matrix. Then the family of the one term estimates $e_{f,\nu}$ for the moment c_f is*

$$e_{f,\nu} = f(c_0^{\nu-1}c_1^{1-2\nu}c_2^{\nu})c_0, \quad \nu \in \mathbb{C}. \tag{4}$$

Proof. By substituting the aforementioned values of l for any $\nu \in \mathbb{C}$ in $c_f \simeq f(l)c_0$, it follows directly that $c_f \simeq f(c_0^{\nu-1}c_1^{1-2\nu}c_2^{\nu})c_0 = e_{f,\nu}$. □

Remark 1. Following a similar procedure with the one adopted in [14], it can be proved that $e_{f,0}$ coincides with the approximation of c_f, obtained using the one-node complex Gauss quadrature rule, and one Lanczos iteration. This estimate is a lower or upper bound, if the derivative of order 2 of the function f has a constant sign on the spectrum of the matrix A [24,17]. For $\nu = 0$ and $f(A) = A^r$ we get $e_{f,0} = \frac{c_1^r}{c_0^{r-1}}$, which is the one term estimate given in [7]. For $r = -1$ we get $e_{f,0} = \frac{c_0^2}{c_1}$, which is the one term estimate given in [8].

Proposition 2. *The family of estimates (4) satisfy the relation*

$$e_{f,\nu} = f\left(\rho^{\nu}\ \frac{c_1}{c_0}\right)c_0, \quad \textit{where } \rho = c_0c_2/c_1^2 \geq 1, \quad \nu \in \mathbb{C}.$$

For an increasing function f and for real values of ν, $e_{f,\nu}$ is also an increasing function of ν for $c_1 > 0$ and decreasing for $c_1 < 0$, whereas for a decreasing function f, $e_{f,\nu}$ is an increasing function of ν for $c_1 < 0$ and decreasing for $c_1 > 0$.

Proof. It holds $l = c_0^{\nu-1}c_1^{1-2\nu}c_2^{\nu} = \left(\frac{c_0c_2}{c_1^2}\right)^{\nu}\frac{c_1}{c_0} = \rho^{\nu}\ \frac{c_1}{c_0}$, where $\rho = c_0c_2/c_1^2$. Thus $e_{f,\nu} = f\left(\rho^{\nu}\ \frac{c_1}{c_0}\right)c_0$. The Cauchy–Schwarz inequality [21] $|(x,Ax)|^2 \leq (x,x)(Ax,Ax)$ implies

$c_1^2 \leq c_0\ c_2$ and thus $\rho = c_0 c_2/c_1^2 \geq 1$. The formula $l = \rho^\nu\ \frac{c_1}{c_0}$ is an increasing function of $\nu \in \mathbb{R}$ for $c_1 > 0$ and decreasing for $c_1 < 0$. Then the monotony of the function f determines the monotony of $e_{f,\nu}$. $\square$

For real matrices, a family of estimates for c_{-1} is also given in [14]. For symmetric positive definite matrices, another family of estimates for the moment c_{-1}^2 is given in [10].

Lemma 1. *If $\rho = 1$ then $e_{f,\nu} = c_f$, $\forall\ \nu \in \mathbb{C}$.*

Proof. If $\rho = 1$ then $c_1^2 = c_0 c_2$, thus the Cauchy–Schwarz inequality holds as equality i.e. Ax and x are linearly dependent. In this case, there exists a nonzero $\lambda \in \mathbb{R}$ such that $Ax = \lambda x$, which also implies $f(A)x = f(\lambda)x$. Therefore, we have $c_1 = (x, Ax) = (x, \lambda x) = \lambda c_0$ and similarly $c_f = f(\lambda)c_0$. Thus $c_f = f(c_1/c_0)c_0$, which is equal to $e_{f,\nu}$ for $\rho = 1$. $\square$

Lemma 2. *Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian matrix and f an invertible function. There exists a value $\nu_o \in \mathbb{C}$ given by*

$$\nu_o = \frac{log(f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1})}{log(\rho)}, \quad \rho = c_0 c_2/c_1^2 \neq 1 \tag{5}$$

such that e_{f,ν_o} gives the exact value of c_f.

Proof. It holds $c_f \in \mathbb{C}$, $\rho \in \mathbb{R}$, $\rho > 1$ and $c_1 \in \mathbb{R}$ positive or negative. Let us denote the complex number $f^{-1}(\frac{c_f}{c_0}) = r_e e^{i\theta_e}$ and let $c_1 > 0$. We have $log(f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1}) = log(r_e c_0/c_1) + i\theta_e$ and thus $\nu_o = \frac{log(f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1})}{log(\rho)} = \frac{log(r_e c_0/c_1)}{log(\rho)} + i\frac{\theta_e}{log(\rho)} = \zeta + \xi i$. Therefore $e_{f,\nu_o} = f(\rho^{\zeta+\xi i} c_1/c_0)c_0 = f(\rho^\zeta e^{(\xi log(\rho^2))i/2} c_1/c_0)c_0 = f(\rho^\zeta e^{i\theta_e} c_1/c_0)c_0$, since $\xi log(\rho^2)/2 = \theta_e$. It holds $e_{f,\nu_o} = f(\rho^\zeta e^{i\theta_e} c_1/c_0)c_0 = c_f$, since the real and the imaginary part of $\rho^\zeta e^{i\theta_e} c_1/c_0$ equals the real and the imaginary part, respectively, of $f^{-1}(\frac{c_f}{c_0}) = r_e e^{i\theta_e}$. In case that $c_1 < 0$, then $log(f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1}) = log(r_e c_0/|c_1|) + i(\theta_e - \pi)$ and $\nu_o = \frac{log(f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1})}{log(\rho)} = \frac{log(r_e c_0/|c_1|)}{log(\rho)} + i\frac{(\theta_e - \pi)}{log(\rho)} = \zeta + \xi i$. Therefore $e_{f,\nu_o} = f(\rho^{\zeta+\xi i} c_1/c_0)c_0 = f(\rho^\zeta e^{(\xi log(\rho^2))i/2} c_1/c_0)c_0 = f(\rho^\zeta e^{i(\theta_e-\pi)} c_1/c_0)c_0$, since $\xi log(\rho^2)/2 = \theta_e - \pi$. It holds $e_{f,\nu_o} = c_f$, since the real and the imaginary part of $\rho^\zeta e^{i\theta_e - \pi} c_1/c_0$ equals the real and the imaginary part, respectively, of $f^{-1}(\frac{c_f}{c_0}) = r_e e^{i\theta_e}$. $\square$

Remark 2. For the non-invertible function $f(A) = A^r$, r even, the numerator of ν_o in relation (5) can be replaced by $log(\left(\frac{c_f}{c_0}\right)^{1/r} \frac{c_0}{c_1})$. Indeed, since $r \cdot \nu_o = log(\frac{c_f c_0^{r-1}}{c_1})/log(\rho)$ we notice that the equality $\rho^{r\cdot\nu_o} = \frac{c_f c_0^{r-1}}{c_1}$ holds, which implies that $e_{f,\nu_o} = c_f$.

In what follows, the value ν_o of (5) will be referred as the optimal value of ν_o.

Two-term estimate

Similarly, by keeping two terms in the summation (3), c_f is approximated by

$$c_f \simeq f(l_1)|a_1|^2 + f(l_2)|a_2|^2.$$

The unknowns l_i and $|a_i|^2$, $i = 1, 2$, are determined by imposing the interpolation conditions

$$c_n(x) = (x, A^n x) \simeq l_1^n |a_1|^2 + l_2^n |a_2|^2, \; n \in \mathbb{Z}.$$

The preceding interpolation conditions mean, in fact, that the moments $c_n(x)$ satisfy the difference equation $c_{n+1} - rc_n + qc_{n-1} = 0$, where $r = l_1 + l_2$ and $q = l_1 l_2$.

Solving the system of $c_{n+1} - rc_n + qc_{n-1} = 0$ and $c_{n+2+k} - rc_{n+1+k} + qc_{n+k} = 0$, for $k, n \in \mathbb{Z}$, we get the following expressions.

$$r = \frac{c_{n-1}c_{n+2+k} - c_{n+1}c_{n+k}}{c_{n-1}c_{n+1+k} - c_n c_{n+k}}, \quad q = \frac{c_n c_{n+2+k} - c_{n+1}c_{n+1+k}}{c_{n-1}c_{n+1+k} - c_n c_{n+k}},$$
$$l_{1,2} = (r \pm \sqrt{r^2 - 4q})/2, \quad |a_1|^2 = \frac{c_0 l_2 - c_1}{l_2 - l_1}, \quad |a_2|^2 = \frac{c_1 - c_0 l_1}{l_2 - l_1}. \tag{6}$$

Therefore, we obtain the family of the two term estimates $\hat{e}_{f,n,k}$ for the moment c_f, given by the following Proposition.

Proposition 3. *Let $A \in \mathbb{C}^{p \times p}$ be a Hermitian matrix. Then the family of the two term estimates $\hat{e}_{f,n,k}$ for the moment c_f is*

$$\hat{e}_{f,n,k} = f(l_1)|a_1|^2 + f(l_2)|a_2|^2, \quad n, k \in \mathbb{Z} \tag{7}$$

where l_1, l_2, $|a_1|^2$, $|a_2|^2$ are given by the formulae (6).

Proof. It follows directly by keeping two terms in the summation (3), where l_1, l_2, $|a_1|^2$, $|a_2|^2$ are given by the formulae (6). □

Remark 3. Following a similar procedure with the one adopted in [14], it can be proved that $\hat{e}_{f,1,0}$ coincides with the approximation of c_f obtained using the two-nodes complex Gauss quadrature rule, and two Lanczos iterations and thus it can be also considered as a lower or upper bound for it, depending on the sign of the derivative of order 4 of the function f [24,17]. Setting $n = 1$, $k = 0$ and $f(A) = A^r$, the estimate $\hat{e}_{f,1,0}$ is the two term estimate given in [7] which leads to the estimation of the trace of powers of a matrix. For $r = -1$ we obtain the two term estimate given in [8].

2.2. Bounds and approximation of the optimal value ν_o for positive definite matrices

The one term estimate $e_{f,\nu}$ for $\nu = \nu_o$ gives the exact value of the function moment c_f in only one matrix-vector product. Indeed, the computation of ν_o from formula (5) cannot be obtained in practice, since it requires the a priori knowledge of the exact moment c_f. However, for Hermitian positive definite matrices, bounds for ν_o can be produced. In this case, the function moment c_f and the optimal value ν_o are taking only real values.

Lemma 3. *Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian positive definite matrix and f a monotonic function. Then the optimal value ν_o is real.*

Proof. Let us consider an increasing function f. The inequality $\lambda_p \leq \frac{x^*Ax}{x^*x} \leq \lambda_1$ [21, p. 176] can be applied for the matrix $f(A)$, that is $f(\lambda_p) \leq \frac{x^*f(A)x}{x^*x} \leq f(\lambda_1)$, since $\lambda_{min}(f(A)) = f(\lambda_p)$ and $\lambda_{max}(f(A)) = f(\lambda_1)$. The matrix A is positive definite so $\lambda_p > 0$ and thus $f(0) < f(\lambda_p) < \frac{c_f}{c_0}$. Since f^{-1} is also increasing, it holds $0 < f^{-1}(\frac{c_f}{c_0})$. Then $f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1} > 0$ and thus $\nu_o = \frac{log(f^{-1}(\frac{c_f}{c_0})\frac{c_0}{c_1})}{log(\rho)} \in \mathbb{R}$. The case for a decreasing function f can be proved similarly. □

Corollary 1. *Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian positive definite matrix and $x \in \mathbb{C}^p$. For any monotonic function f, the optimal value ν_o is bounded as*

$$\frac{log(\lambda_p c_0/c_1)}{log(\rho)} \leq \nu_o \leq \frac{log(\lambda_1 c_0/c_1)}{log(\rho)}.$$

Proof. For an increasing function f it holds $f(\lambda_p) \leq \frac{c_f}{c_0} \leq f(\lambda_1)$, which implies $\lambda_p \leq f^{-1}(\frac{c_f}{c_0}) \leq \lambda_1$, since f^{-1} has the same monotony, and thus the result. The case for a decreasing function f can be proved in a similar way. □

Depending on the convexity of the function f^{-1}, further bounds for ν_o can be derived.

Lemma 4. *Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian positive definite matrix. For the estimation of the moment c_f it holds $\nu_o \geq 0$, if f^{-1} is concave and $\nu_o \leq 0$, if f^{-1} is convex.*

Proof. Let us suppose that f^{-1} is a concave function. Considering the Jensen's inequality [21] for the matrix $f(A)$ and the function f^{-1} we have $f^{-1}(c_f/c_0) \geq c_1/c_0$ which implies $\nu_o \geq \frac{log(1)}{log(\rho)} = 0$. Similarly it is proved that it holds $\nu_o \leq 0$, for a convex function f^{-1}. □

Corollary 2. *From Lemma 4, for the matrix functions $exp(A)$ and A^r, $r > 1$ it holds $\nu_o \geq 0$, whereas for the matrix functions $log(A)$ and A^r, $r < 1$ it holds $\nu_o \leq 0$.*

Corollary 3. *Let $A \in \mathbb{R}^{p\times p}$ be a Hermitian positive definite matrix and f a monotonic function. For the estimation of the moment c_f, the optimal value ν_o can be lower or* *upper bounded by the quantity* $\frac{log\left(f^{-1}\left(\frac{\hat{e}_{f,1,0}}{c_0}\right)\frac{c_0}{c_1}\right)}{log(\rho)}$*, depending on the sign of the derivative of order 4 of the function* f*.*

Proof. From Remark 3 the two term estimate $\hat{e}_{f,1,0}$ coincides with the lower or upper bound for c_f obtained using Gauss quadrature rule and two Lanczos iterations. In case that $\hat{e}_{f,1,0}$ is a lower bound for c_f and f is an increasing function, then the inequality $\hat{e}_{f,1,0} \leq c_f$ implies $f^{-1}\left(\frac{\hat{e}_{f,1,0}}{c_0}\right)\frac{c_0}{c_1} \leq f^{-1}\left(\frac{c_f}{c_0}\right)\frac{c_0}{c_1}$, since f^{-1} is also increasing, and thus $\frac{log\left(f^{-1}\left(\frac{\hat{e}_{f,1,0}}{c_0}\right)\frac{c_0}{c_1}\right)}{log(\rho)} \leq \nu_o$. Similarly, for a decreasing function f, then the inequality $\hat{e}_{f,1,0} \leq c_f$ results to $\frac{log\left(f^{-1}\left(\frac{\hat{e}_{f,1,0}}{c_0}\right)\frac{c_0}{c_1}\right)}{log(\rho)} \geq \nu_o$. If $\hat{e}_{f,1,0} \geq c_f$ and f is an increasing function, it holds $\frac{log\left(f^{-1}\left(\frac{\hat{e}_{f,1,0}}{c_0}\right)\frac{c_0}{c_1}\right)}{log(\rho)} \geq \nu_o$, whereas for a decreasing function f, we get $\frac{log\left(f^{-1}\left(\frac{\hat{e}_{f,1,0}}{c_0}\right)\frac{c_0}{c_1}\right)}{log(\rho)} \leq \nu_o$. $\square$

From the lower and upper bounds for ν_o specified in Corollaries 1–3, we get an interval into which the optimal value ν_o lies. This indicates a range of values for an appropriate selection of $\nu \in \mathbb{R}$.

For $f(A) = A^{-1}$, a direct approximation of ν_o, leading to an efficient one term estimate for the moment c_{-1}, can be specified as follows.

Corollary 4. *Let* $A \in \mathbb{C}^{p\times p}$ *be a Hermitian positive definite matrix. In case that the extreme eigenvalues of the matrix* A *are close enough and are larger than unity, then for the estimation of the moment* c_{-1}*, the optimal value* ν_o *can be approximated by the quantity*

$$\frac{log(\frac{c_1^2}{c_0c_2})}{log(\frac{c_1c_3}{c_2^2})} = \tilde{\nu}_o. \tag{8}$$

Proof. It holds that $\lambda_p \leq \frac{c_1}{c_0} \leq \lambda_1$ [21]. It can be also proved that $\lambda_p \leq \frac{(x,Ay)}{(x,y)} \leq \lambda_1$. By considering the last inequality for $y = A^i x$, it is derived that $\lambda_p \leq \frac{c_{i+1}}{c_i} \leq \lambda_1$. Therefore, the sequence of moments $\frac{c_{i+1}}{c_i} \in [\lambda_p, \lambda_1]$ and increases as i increases [9], i.e. $\frac{c_i}{c_{i-1}} \leq \frac{c_{i+1}}{c_i}$, $\forall\ i \in \mathbb{R}$ $(1')$. In addition, $|\frac{c_{i+1}}{c_i} - \frac{c_{i+2}}{c_{i+1}}| \leq \lambda_1 - \lambda_p$. Similarly, the sequence of moments $\frac{c_i}{c_{i+1}} \in [\frac{1}{\lambda_1}, \frac{1}{\lambda_p}]$ decreases as i increases, i.e. $\frac{c_i}{c_{i+1}} \geq \frac{c_{i+1}}{c_i+2}$, $\forall\ i \in \mathbb{R}$ $(2')$, and $|\frac{c_i}{c_{i+1}} - \frac{c_{i+1}}{c_{i+2}}| \leq \frac{1}{\lambda_p} - \frac{1}{\lambda_1}$. We notice that, the terms of the aforementioned sequences of moments are close enough, since the extreme eigenvalues of the matrix A are close enough from the assumption.

From Lemma 2, for $f(A) = A^{-1}$, the value of ν_o equals to $log\left(\frac{c_0^2}{c_{-1}c_1}\right)/log\left(\frac{c_0c_2}{c_1^2}\right)$. From relations $(1')$ and $(2')$ for $i = 0$ we have $\frac{c_0}{c_{-1}} \leq \frac{c_1}{c_0}$ and $\frac{c_1}{c_2} \leq \frac{c_0}{c_1}$. Thus, in the quantity $\frac{c_0^2}{c_{-1}c_1}$ we can replace the quotient $\frac{c_0}{c_{-1}}$ by its upper bound $\frac{c_1}{c_0}$ and the quotient $\frac{c_0}{c_1}$ by its lower bound $\frac{c_1}{c_2}$ getting the approximation $\frac{c_0^2}{c_1c_{-1}} \simeq \frac{c_1^2}{c_2c_0}$. This approximation is expected to be satisfactory since the quantities $\frac{c_0}{c_{-1}}$ and $\frac{c_0}{c_1}$ are actually replaced by the next terms of the sequences $\frac{c_{i+1}}{c_i}$ and $\frac{c_i}{c_{i+1}}$, respectively, and are expected to be close enough to them from our assumption. This results to $\left|log\left(\frac{c_0^2}{c_1 c_{-1}}\right) - log\left(\frac{c_1^2}{c_2 c_0}\right)\right| = \left|log\left(\frac{c_0^2/(c_1 c_{-1})}{c_1^2/(c_2 c_0)}\right)\right| \simeq log(1) = 0$, since $\frac{c_0^2/(c_1 c_{-1})}{c_1^2/(c_2 c_0)} \simeq 1$, and therefore $log\left(\frac{c_0^2}{c_1 c_{-1}}\right) \simeq log\left(\frac{c_1^2}{c_2 c_0}\right)$. In a similar way, since $\frac{c_2}{c_1} \leq \frac{c_3}{c_2}$ and $\frac{c_1}{c_2} \leq \frac{c_0}{c_1}$, in the quantity $\frac{c_0 c_2}{c_1^2}$ we can replace the quotient $\frac{c_0}{c_1}$ by its lower bound $\frac{c_1}{c_2}$ and the quotient $\frac{c_2}{c_1}$ by its upper bound $\frac{c_3}{c_2}$ getting the approximation $\frac{c_0 c_2}{c_1^2} \simeq \frac{c_1 c_3}{c_2^2}$. This results to $log\left(\frac{c_0 c_2}{c_1^2}\right) \simeq log\left(\frac{c_1 c_3}{c_2^2}\right)$. We set $\tilde{\nu}_o = log(\frac{c_1^2}{c_0 c_2})/log(\frac{c_1 c_3}{c_2^2})$ and since the numerator and the denominator of ν_o are approximated by the numerator and the denominator of $\tilde{\nu}_o$, respectively, we can consider that ν_o is approximated by $\tilde{\nu}_o$. $\square$

2.3. Estimates for the bilinear form $y^* f(A)x$

For $x \neq y$, the bilinear moments of the matrix A are the quantities

$$c_r(x, y) = (x, A^r y), \; r \in \mathbb{R}. \tag{9}$$

The bilinear function moments $c_f(x, y) = (x, f(A)y)$ can be estimated by adopting the following procedures.

(i) From the polarization identity,

$$c_f(x, y) = (x, f(A)y) = \frac{1}{4}((s, f(A)s) - (t, f(A)t) + i(w, f(A)w) - i(z, f(A)z)),$$

where $s = x + y$, $t = x - y$, $w = x + iy$ and $z = x - iy$, as introduced in [17,1,14]. The moment $c_f(x, y)$ is approximated by estimating the quadratic moments of the right hand side of the identity, by using the one term estimates $e_{f,\nu}$ or the two term estimates $\hat{e}_{f,n,k}$.

(ii) From the spectral decomposition of the matrix A,

$$c_f(x, y) = y^* f(A)x = \sum_{k=1}^{p} f(\lambda_k)(x, v_k)(v_k, y) = \sum_{k=1}^{p} f(\lambda_k)\alpha_k \beta_k, \tag{10}$$

where $\alpha_k = (x, v_k)$ and $\beta_k = (v_k, y)$. Keeping only one term in the summation (10) and following the procedure described in Section 2.1, a family of one term estimates for the moment $c_f(x, y)$ is given by

$$e_{f,\nu} = f(c_0(x, y)^{\nu-1} c_1(x, y)^{1-2\nu} c_2(x, y)^{\nu})c_0 = f(\rho^{\nu}\frac{c_1}{c_0})c_0, \quad \nu \in \mathbb{C},$$

where $\rho = c_0(x, y)c_2(x, y)/c_1^2(x, y)$. In case that the vectors x, y are orthogonal, then the above family of estimates $e_{f,\nu}$ cannot be used, since $c_0(x, y) = 0$.

Lemma 5. *Let $A \in \mathbb{C}^{p\times p}$ be a Hermitian matrix and f an invertible function. There exists a value $\nu_o \in \mathbb{C}$ given by*

$$\nu_o = \frac{log\left(f^{-1}\left(\frac{c_f(x,y)}{c_0(x,y)}\right)\frac{c_0(x,y)}{c_1(x,y)}\right)}{log(\rho)}, \quad \rho \neq 1,$$

such that e_{f,ν_o} gives the exact value of c_f.

Proof. Let $c_1(x,y) = r_1 e^{i\theta_1}$, $c_0(x,y) = r_0 e^{i\theta_0}$, $\rho = r_\rho e^{i\theta_\rho}$, $c_f(x,y) \in \mathbb{C}$. Let us denote $f^{-1}(\frac{c_f(x,y)}{c_0(x,y)}) = r_f e^{i\theta_f}$. Then $log(f^{-1}(\frac{c_f(x,y)}{c_0(x,y)})\frac{c_0(x,y)}{c_1(x,y)}) = log(r_f r_0/r_1) + i(\theta_f + \theta_0 - \theta_1)$ and

$$\begin{aligned}\nu_o &= \frac{log(f^{-1}(\frac{c_f(x,y)}{c_0(x,y)})\frac{c_0(x,y)}{c_1(x,y)})}{log(\rho)}\\ &= \frac{(log(\frac{r_f r_0}{r_1})log(r_\rho) + (\theta_f+\theta_0-\theta_1)\theta_\rho) + i(log(r_\rho)(\theta_f+\theta_0-\theta_1) - log(\frac{r_f r_0}{r_1})\theta_\rho)}{log^2(r_\rho)+\theta_\rho^2}\\ &= \zeta + \xi i.\end{aligned}$$

Therefore $e_{f,\nu_o} = f(\rho^{\zeta+\xi i}c_1/c_0)c_0 = f(r_\rho^\zeta r_1 e^{-\xi\theta_\rho}e^{i\theta_f}/r_0)c_0$ which equals $c_f(x,y)$, since $r_\rho^\zeta r_1 e^{-\xi\theta_\rho}e^{i\theta_f}/r_0 = r_f e^{i\theta_f}$. □

Remark 4. Keeping two terms in the summation (10), along the same lines as in Section 2.1 and using the moments $c_i(x,y)$ instead of the moments c_i, a family of two term estimates similar with the estimates $\hat{e}_{f,n,k}$ of Section 2.1 is obtained.

In the case that A is a real symmetric positive definite matrix, $x, y \in \mathbb{R}^p$ and for $f(A) = A^r$, some further bounds for the bilinear form $y^T A^r x$ can be given.

Proposition 4. *Let $A \in \mathbb{R}^{p\times p}$ be a symmetric positive definite matrix and $x \in \mathbb{R}^p$. Then,*

$$\frac{1}{4}\left(\frac{c_1^r(s)}{c_0^{r-1}(s)} - m\frac{c_1^r(t)}{c_0^{r-1}(t)}\right) \leq y^T A^r x \leq \frac{1}{4}\left(m\frac{c_1^r(s)}{c_0^{r-1}(s)} - \frac{c_1^r(t)}{c_0^{r-1}(t)}\right),$$

where $r \in \mathbb{Z}$, $s = x+y$, $t = x-y$, $m = (\frac{(1+\kappa(A))^2}{4\kappa(A)})^{2^d-1}$, $d = \begin{cases} r-1, & r>1\\ |r|, & r<0,\ r=1.\end{cases}$

Proof. From [7] it holds $\frac{c_1^r(x)}{c_0^{r-1}(x)} \leq x^T A^r x \leq m\frac{c_1^r(x)}{c_0^{r-1}(x)}$, where $c_1^r(x)/c_0^{r-1}(x)$ is the one term estimate $e_{f,0}$ for the moment $c_r(x)$. Since A is a symmetric positive definite matrix, from the polarization identity it holds $(x, A^r y) = ((s, A^r s) - (t, A^r t))/4$, where $s = x+y$ and $t = x-y$. As a result,

$$\frac{c_1^r(s)}{c_0^{r-1}(s)} \leq s^T A^r s \leq m\frac{c_1^r(s)}{c_0^{r-1}(s)} \quad \text{and} \quad -m\frac{c_1^r(t)}{c_0^{r-1}(t)} \leq -t^T A^r t \leq -\frac{c_1^r(t)}{c_0^{r-1}(t)},$$

which implies $\frac{c_1^r(s)}{c_0^{r-1}(s)} - m\frac{c_1^r(t)}{c_0^{r-1}(t)} \leq s^T A^r s - t^T A^r t \leq m\frac{c_1^r(s)}{c_0^{r-1}(s)} - \frac{c_1^r(t)}{c_0^{r-1}(t)}$. □

Table 1
Computational complexity of the estimates.

Matrix A	$x^* f(A)x$		$y^* f(A)x$			
			Polarization identity		Spectral decomposition	
	$e_{f,\nu}$	$\hat{e}_{f,n,k}$	$e_{f,\nu}$	$\hat{e}_{f,n,k}$	$e_{f,\nu}$	$\hat{e}_{f,n,k}$
dense	$\mathcal{O}(p^2)$	$\mathcal{O}(\lceil \frac{n+k+2}{2} \rceil p^2)$	$\mathcal{O}(4p^2)$	$\mathcal{O}(4\lceil \frac{n+k+2}{2} \rceil p^2)$	$\mathcal{O}(2p^2)$	$\mathcal{O}(2\lceil \frac{n+k+2}{2} \rceil p^2)$
banded	$\mathcal{O}(dp)$	$\mathcal{O}(\lceil \frac{n+k+2}{2} \rceil dp)$	$\mathcal{O}(4dp)$	$\mathcal{O}(4\lceil \frac{n+k+2}{2} \rceil dp)$	$\mathcal{O}(2dp)$	$\mathcal{O}(2\lceil \frac{n+k+2}{2} \rceil dp)$

Remark 5. The inequality of Proposition 4 shows that, if the matrix A is well conditioned, the quantity $(e_{f,0}(s) - e_{f,0}(t))/4$ is a fair estimate for the bilinear form $y^T A^r x$. Furthermore, this inequality can be used for determining lower and upper bounds for the optimal value ν_o.

3. Numerical examples

The one term estimates $e_{f,\nu}$ require the computation of only one matrix vector product for the estimation of the quadratic form $x^* f(A)x$, whereas the complexity of the two term estimates $\hat{e}_{f,n,k}$ depends on the integers n, k. Table 1 displays the number of arithmetic operations required for the approximation of $x^* f(A)x$ and of $y^* f(A)x$ by the polarization identity and by the spectral decomposition, as described in Subsection 2.3, using the estimates $e_{f,\nu}$ and $\hat{e}_{f,n,k}$, for dense matrices of dimension p and for banded matrices of bandwidth d. $\lceil x \rceil$ denotes the smallest integer not less than x. Depending on the matrix function, one evaluation of a function value will be added to the computational complexity.

Next, numerical experiments estimating several quantities are presented. All computations were performed in vectorized form in MATLAB (R2011b), 64-bit, on an Intel Core i7 computer, with 8 Gb RAM. Throughout the examples, the computed one term estimates were obtained by considering the mean value ν_m of some values of ν in the intervals of Corollaries 1–3. In case that $f(A) = A^{-1}$, from Corollary 4 the value of $\tilde{\nu}_o$ is assigned to ν_m. For the two term estimates $\hat{e}_{f,n,k}$, the values of $n = 1$, $k = 0, 2$ were selected. $\kappa(A)$ stands for the condition number of a matrix A.

Example 1 *(Estimating entries of a Hermitian positive definite matrix).* Firstly, we tested the *mhd1280b* matrix A of dimension 1280, obtained by the *University of Florida Sparse Matrix Collection* [15], which appears in electromagnetic problems. This matrix is Hermitian positive definite with $\kappa(A) = 4.74959e12$. In Tables 2, 3 and 4, estimates for the entries $f(A)_{i,i}$ are presented.

Example 2 *(Estimating bilinear moments of a Hermitian positive definite matrix).* A *random* Hermitian positive definite matrix A of dimension $p = 2000$, with $\kappa(A) = 4$ is considered, that is $[Q, R] = qr(rand(p) + i)$; $h = ceil(2 * rand(p, 1))$; $A = Q * diag(h) * Q'$; $A = A * A'$; in MATLAB notation. In Table 5, several bilinear forms of this matrix for x, y random normalized vectors are estimated.

Table 2
Relative error estimating $c_r(\delta_i)$, for the matrix A of dimension 1280.

$(A^r)_{ii}$	Relative error e_{f,ν_m}	Relative error $\hat{e}_{f,1,0}$
$(A^{-1})_{25,25}$	Exact ($\rho = 1$)	
$(A^{-1})_{900,900}$	1.4282e-2	3.7827e-2
$(A^{-1})_{1203,1203}$	1.0658e-2	3.7428e-2
$(A^{1/2})_{3,3}$	Exact ($\rho = 1$)	
$(A^{1/2})_{100,100}$	7.9706e-4	1.0036e-3
$(A^{1/2})_{565,565}$	2.9474e-3	9.0694e-3

Table 3
Relative error estimating $c_f(\delta_i)$, for the matrix A of dimension 1280.

$f(A)_{ii}$	Relative error e_{f,ν_m}	Relative error $\hat{e}_{f,1,0}$
$log(A)_{1,1}$	Exact ($\rho = 1$)	
$log(A)_{8,8}$	5.3330e-3	1.5656e-2
$log(A)_{900,900}$	3.8360e-4	1.7959e-3
$log(A)_{1203,1203}$	3.0935e-4	1.1446e-3

Table 4
Relative error estimating $c_f(\delta_i)$, for the matrix A of dimension 1280.

$f(A)_{ii}$	Relative error e_{f,ν_m}	Relative error $\hat{e}_{f,1,0}$
$exp(A)_{7,7}$	Exact ($\rho = 1$)	
$exp(A)_{500,500}$	1.0650e-6	1.5124e-13
$exp(A)_{1000,1000}$	2.3271e-8	2.8256e-11
$exp(A)_{1203,1203}$	6.0033e-7	1.1741e-14

Table 5
Relative error estimating $c_f(x, y)$, for the matrix A of dimension 2000.

Quantity	Relative error e_{f,ν_m}	Relative error $\hat{e}_{f,1,2}$
$c_{exp}(x, y) = 3.9415e1 + 2.6811e - 2i$	1.6264e-3	1.9844e-15
$c_{log}(x, y) = 9.9929e - 1 + 7.1643e - 4i$	3.0391e-4	3.4441e-15
$c_{1/2}(x, y) = 1.4631 + 5.1679e - 4i$	2.0450e-4	1.5179e-15
$c_{-1}(x, y) = 2.0166e - 1 - 3.8759e - 4i$	3.0931e-3	7.0210e-15

Example 3 *(Approximation of $x^T A^{-1} x$ for Covariance matrices).* We considered a symmetric positive definite matrix $A = [a_{ij}]$ of dimension 1000 with entries computed via a decaying positive definite covariance function, that is $a_{ii} = 1+i$ and $a_{ij} = \frac{1}{|i-j|}$ for $i \neq j$. This matrix A simulates a *Covariance* matrix since the decaying behavior away from the main diagonal simulates the decreasing correlation of high dimensional data samples in covariance matrix analysis (cf. [23,29,3] and the references therein). The matrix A is ill conditioned with $\kappa(A) = 7.2911e2$. In Table 6, the element $A^{-1}_{1,1} = 6.0584e - 1$ is approximated by the estimate $e_{f,\tilde{\nu}_o}$. Also, the estimates derived as lower bounds using Gauss quadrature with k Lanczos iterations [17] are reported. The optimal value of $\nu_o = -5.5771e-1$ and is approximated by $\tilde{\nu}_o = -5.4027e-1$ with relative error of order $\mathcal{O}(10^{-2})$.

In fact, the estimate $e_{f,\tilde{\nu}_o}$ attains a relative error of order $\mathcal{O}(10^{-3})$ in only one matrix vector product. However, a relative error of the same order can be obtained with Gauss quadrature in more than 15 iterations.

Table 6
Relative errors and estimates for the entry $A^{-1}_{1,1}$ of a *Covariance* like matrix A of dimension 1000.

	$e_{f,0}$ = Gauss $k = 1$	$e_{f,\tilde{\nu}_o}$	Gauss $k = 5$	Gauss $k = 15$	Gauss $k = 20$
Relative errors	1.7470e-1	5.9854e-3	6.1071e-2	1.2241e-2	5.0701e-3
Estimates	5.0000e-1	6.0222e-1	5.6884e-1	5.9843e-1	6.0277e-1

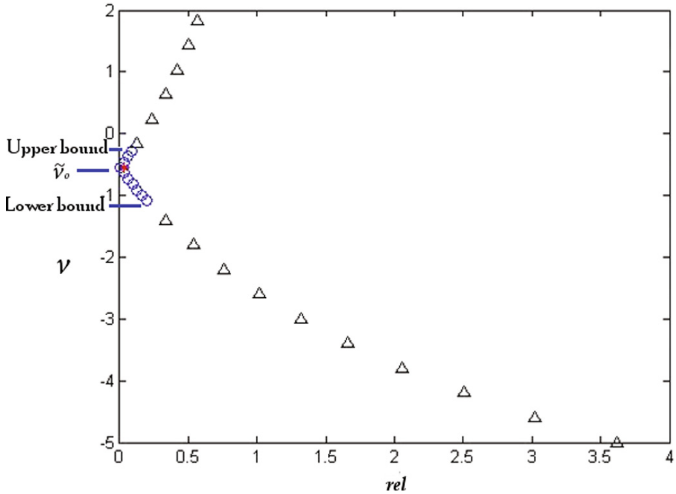

Fig. 1. The relative error of $e_{f,\nu}$ for various values of ν. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article.)

In Fig. 1 the relative error of $e_{f,\nu}$ for various values of ν is depicted. In this figure, the interval (lower and upper bound) for ν and the values ν_o and $\tilde{\nu}_o$ are determined. The black triangles represent the values of the relative error (x-axis) for ν outside the range which is specified by the Corollaries 1–3 (y-axis), whereas the blue circles represent the values of the relative error for ν in this range. The value of $\tilde{\nu}_o$ is indicated with a red mark. This value is actually very close to the optimal value ν_o which has relative error equal to zero (the blue mark which lies on the y-axis).

Example 4 *(Applications of Tr($f(A)$))*. For a Hermitian matrix A, the $\mathrm{Tr}(f(A))$ is connected with the moment c_f due to a result of Hutchinson [12]. According to this, it holds $E(c_f(x)) = \mathrm{Tr}(f(A))$, for $x \in X^p$ (the vector x has entries 1 and -1 with equal probability), where $E(\cdot)$ denotes the expected value. In our experiments, estimates for the $\mathrm{Tr}(f(A))$ are obtained by taking the mean value of the computed one or two term estimates for $c_f(x_i)$, for $N = 50$ vectors $x_i \in X^p$. In this way, we obtain the following families of one or two term estimates, $t_{f,\nu}$ or $\hat{t}_{f,n,k}$, respectively, for the $\mathrm{Tr}(f(A))$,

$$t_{f,\nu} = \frac{1}{N}\sum_{i=1}^{N} e_{f,\nu}(x_i),\ \nu \in \mathbb{C}, \quad \hat{t}_{f,n,k} = \frac{1}{N}\sum_{i=1}^{N} \hat{e}_{f,n,k}(x_i),\ n, k \in \mathbb{Z},$$

Table 7
Relative error estimating the partial sum of the eigenvalues ($c = 1$).

Matrix	μ	Relative error $\hat{t}_{f,1,0}$	Relative error $\hat{t}_{f,1,2}$
mhd1280	12	1.5502e-2	3.1870e-2
	20	3.2953e-2	6.4237e-3

Table 8
Relative error estimating the $\mathrm{Tr}(T^{-1}S)$.

p	Relative error t_{f,ν_m}	Relative error $\hat{t}_{f,1,0}$
500	4.0661e-3	4.6062e-3
1000	3.4904e-2	4.6803e-2
2000	2.3186e-2	3.4830e-2
4000	2.8217e-2	4.1651e-2

using the one term or the two term estimates, respectively. Next, two concrete applications requiring the computation of the $\mathrm{Tr}(f(A))$, are presented.

4.1 *(Partial eigenvalue sum).* In solid state physics the computation of the total energy of an electronic structure requires the evaluation of partial eigenvalue summations $\sum_{k=1}^{m} \lambda_k$, $m < p$. Let A be a Hermitian matrix of dimension p and $\lambda_1, \lambda_2, \ldots, \lambda_p \in \mathbb{R}$ its eigenvalues. Let μ be a real number such that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_m \leq \mu \leq \lambda_{m+1} \leq \ldots \leq \lambda_p$. It holds $\sum_{k=1}^{m} \lambda_k \simeq \mathrm{Tr}(f(A))$ for $f(z) = z/(1 + exp((z-\mu)/c))$, c being a constant [2]. In Table 7, the matrix *mhd1280* of Example 1 is tested.

4.2 *(Machine learning).* In machine learning the solution of the optimization problem that arises while training a Gaussian process requires the evaluation of $\mathrm{Tr}(T^{-1}S)$, for certain Toeplitz matrices T and S [5]. In Table 8, an example presented in [5] is tested.

Example 5 *(Estimation of the diagonal and the trace of $f(A)$).* In this example, the whole diagonal of a matrix $f(A)$ is estimated. The mean relative error of the diagonal entries of a matrix is defined as $(\sum_{i=1}^{p} |a_{ii} - e_{f,\nu_{dm}}(\delta_i)|/|a_{ii}|)/p$, where ν_{dm} is evaluated as the mean of the values ν_m along the diagonal. The summation of the estimates for all the diagonal elements of the matrix $f(A)$ gives an approximation of the $\mathrm{Tr}(f(A))$. In the next Examples, this method will be compared with the estimates $t_{f,\nu}$ and $\hat{t}_{f,n,k}$, described in Example 4.

5.1 *(Diagonal entries of the inverse of Covariance matrices).* In uncertainty quantification, the diagonal of the inverse of covariance matrices gives information about the quality of data [23]. We considered simulations of *Covariance* matrices $A = [a_{ij}]$, as described in Example 3, with elements $a_{ii} = 1 + i^{1/2}$ and $a_{ij} = \frac{1}{|i-j|^2}$ for $i \neq j$ [3]. The second column of Table 9 reports the mean relative error and the execution time in seconds for the estimation of the whole diagonal of the inverse of the matrices A of dimension $p = 100$, 1000 and 4000. In the last two columns of Table 9, the relative errors

Table 9
Estimating the whole diagonal and the trace of the matrix A^{-1}.

p	Mean relative error Diagonal of the matrix	Trace relative error Summation of the diagonal estimates	Trace relative error Hutchinson's method
100	4.3844e-3 (3.4110e-4 sec)	1.4594e-3	$t_{f,\tilde{\nu}_o}$ = 2.7608e-3, $\hat{t}_{f,1,0}$ = 4.2954e-2
1000	3.8349e-4 (3.7687e-3 sec)	1.5821e-3	$t_{f,\tilde{\nu}_o}$ = 2.3512e-2, $\hat{t}_{f,1,0}$ = 5.9944e-2
4000	1.0335e-4 (3.4380e-2 sec)	7.1217e-4	$t_{f,\tilde{\nu}_o}$ = 4.8938e-2, $\hat{t}_{f,1,0}$ = 8.7812e-2

Table 10
Relative error estimating $c_f(\delta_i)$, for the matrix C of dimension 3600.

$f(A)_{ii}$	Relative error e_{f,ν_m}	Relative error $\hat{e}_{f,1,0}$
$log(C)_{3,3}$	2.4334e-3	4.9577e-3
$log(C)_{900,900}$	2.2420e-3	5.0824e-3
$log(C)_{3000,3000}$	2.0183e-3	4.8145e-3

Table 11
Estimating the whole diagonal and the trace of the matrix $log(C)$.

Mean relative error Diagonal of the matrix	Trace relative error Summation of the diagonal estimates	Trace relative error Hutchinson's method
1.9717e-2 (2.1051e-2 sec)	8.4143e-4	t_{f,ν_m} = 8.7950e-2, $\hat{t}_{f,1,0}$ = 1.7756e-1

for the trace estimation based on the diagonal estimates and on the Hutchinson's result as described in Example 4, respectively, are added.

The same example, for matrices of dimension $p = 4000$, was tested in [14, Table 5.11] and in [23] for the estimation of $\mathrm{Tr}(A^{-1})$. In [14], the estimates were based on random values of ν and for the best reported value of ν, a relative error of order $\mathcal{O}(10^{-5})$ was attained. In the present work, an a priori value of ν was determined which directly resulted in a relative error of order $\mathcal{O}(10^{-4})$. In [23], the trace $Tr(A^{-1})$ was estimated with relative error of order $\mathcal{O}(10^{-3})$ and the mean relative error for the estimation of the whole diagonal of the inverse has order $\mathcal{O}(10^{-4})$ or $\mathcal{O}(10^{-5})$ for a large sample.

5.2 *(Diagonal entries of the $log(A)$).* We considered the ill conditioned matrix C = *bcsstk21* of dimension $p = 3600$, obtained by the *University of Florida Sparse Matrix Collection* [15]. In Table 10, the relative errors estimating few diagonal entries of the matrix $log(C)$, using the one and the two term estimates, are reported.

Table 11 presents the mean relative error and the execution time in seconds for the estimation of the whole diagonal and the trace. The relative errors of the trace estimation by the Hutchinson's method, using the one and the two term estimates, are reported as well.

Example 6 *(Networks).* In graph theory and network analysis for certain functions of adjacency matrices estimates for bilinear forms are needed [4,11]. Next, for adjacency matrices A, the relative errors estimating the quantities Estrada index = $\mathrm{Tr}(exp(A))$, sub-

Table 12
Relative error estimating the subgraph centrality and communicability of some nodes for the matrix *smallw* of dimension 2000.

$f(A)_{ii}$	Relative error $e_{f,1/2}$	Relative error $\hat{e}_{f,1,2}$
$exp(A)_{1,1}$	4.6587e-3	8.9605e-2
$exp(A)_{2,5}$	1.1205e-1	3.4187e-3
$exp(A)_{5,6}$	4.5246e-1	4.3746e-2
$exp(A)_{500,500}$	2.6364e-2	3.4245e-3
$exp(A)_{750,750}$	2.6188e-2	3.2438e-3
$exp(A)_{1850,1850}$	9.4466e-3	1.5136e-2

Table 13
Estimates and relative errors for the Estrada index for the matrix *smallw* of dimension 2000.

Exact	$t_{f,1/2}$	Relative error $t_{f,1/2}$	$\hat{t}_{f,1,2}$	Relative error $\hat{t}_{f,1,2}$
1.5871e4	1.5581e4	2.9848e-2	1.5576e4	1.7052e-2

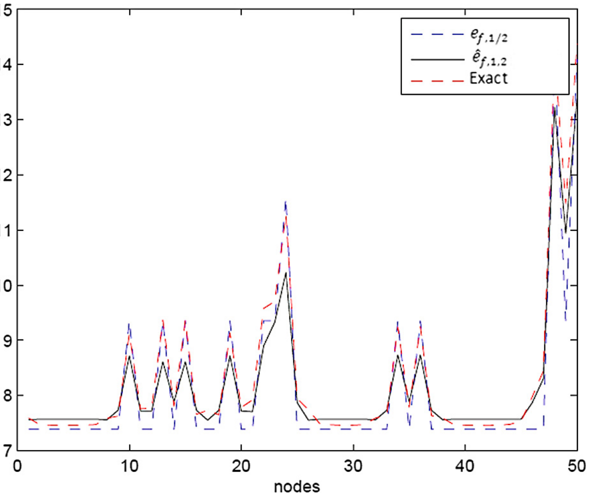

Fig. 2. Estimating the subgraph centrality of the matrix *smallw*.

graph centrality $= (exp(A))_{ii}$ and subgraph communicability $= (exp(A))_{ij}$ are presented. The adjacency matrices are sparse, symmetric with nonzero elements corresponding only to adjacency nodes, thus it often appears $c_1 = 0$. In this case the value of $\nu = 1/2$ is considered in formula (4).

In Tables 12 and 13, we tested the adjacency matrix *smallw* that represent connected simple graphs, taken from the toolbox CONTEST of MATLAB [30].

Fig. 2 shows the exact value and the behavior of $e_{f,1/2}$, $\hat{e}_{f,1,2}$, for estimating the subgraph centrality of the first 50 nodes of the matrix *smallw*.

4. Concluding remarks

In this paper, families of one term estimates $e_{f,\nu}$ and two term estimates $\hat{e}_{f,n,k}$ for the bilinear moment $c_f(x, y) = y^* f(A)x$, for any Hermitian matrix $A \in \mathbb{C}^{p \times p}$ and vectors

$x, y \in \mathbb{C}^p$, were derived based on the extrapolation of the bilinear function moments $(x, f(A)y)$ of the matrix A. The family of the one term estimates was expressed as a function of a variable $\nu \in \mathbb{C}$. For the positive definite case, an approximation of the optimal real value of ν, ν_o, was specified for the estimation of $x^* A^{-1} x$, whereas bounds for $\nu \in \mathbb{R}$ were determined for any monotonic function f. From these bounds, an a priori value of ν can be chosen, which directly leads to a satisfactory one term estimate in only $\mathcal{O}(p^2)$ arithmetic operations, improving in this way significantly the procedure proposed in [14]. Also, the two term estimates $\hat{e}_{f,n,k}$ for $n, k \in \mathbb{Z}$ give fair approximations, and are preferred in case that we cannot specify a satisfactory approximation of the optimal value ν_o, for the one term estimate. The presented numerical results showed that the estimates derived through extrapolation are efficient, they require low computational complexity and can be used in the approximation of useful quantities required in several linear algebra problems.

A major issue stemming from the estimation of $y^* f(A)x$ via extrapolation methods concerns whether these methods should be applied for this estimation. So far, it seems that for Hermitian positive definite matrices with rather close extreme eigenvalues which are larger than unity, the one term estimate $e_{f,\nu}$ corresponding to the a priori determined value of ν from Corollaries 1–3, should be a very good choice. Additionally, in case that $\rho \simeq 1$, the one term estimate approaches well the exact value. For Hermitian and non-Hermitian matrices, a thorough comparison of extrapolation methods with Gauss quadrature ones, for the single and for the block type case, is under consideration.

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