Extrapolation of operator moments, with applications to linear algebra problems

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MAIN TOPICS

- Motivation of the problem
- The mathematical landscape
- Extrapolation procedures and estimates
- Estimation of the
$$\begin{cases} \mathrm{Tr}(A^q),\ q \in Q \\ \text{error of the solution of the linear system } Ax = f \end{cases}$$
- Numerical results

Introduction

Let $\mathbf{A} \in \mathbf{R}^{\mathbf{p}\times\mathbf{p}}$ symmetric positive definite (spd) matrix.

We are interested in obtaining estimations of

- $\mathrm{\mathbf{Tr}}(\mathbf{A}^{\mathbf{q}}),\ \mathbf{q} \in \mathbf{Q}$
- $(\mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y})$, $\mathbf{x}$ is the exact solution of $\mathbf{A}\mathbf{x} = \mathbf{f}$,
  $\mathbf{y}$ is any approximation of $\mathbf{x}$,
  $\mathbf{e} = \|\mathbf{x}-\mathbf{y}\|$ is the **error**.

↪ These estimates will be obtained by

extrapolation of the moments of $\mathbf{A}$.

Motivation of the problem

Estimates for the **error** have applications in the

choice of the best parameter in Tikhonov regularization.

The computation of $\mathbf{Tr}(\mathbf{A}^{\mathbf{q}})$, have applications in

Statistics: specification of classical optimality criteria.

Matrix theory: computation of the characteristic polynomial.

Dynamical Systems: determination of their invariants.

Differential Equations: solution of Lyapunov matrix equation.

Crystals: for the selection of measurement directions in elastic strain determination of single crystals.

The singular value decomposition

The singular value decomposition of an spd matrix $\mathbf{A} \in \mathbf{R}^{\mathbf{p}\times\mathbf{p}}$ is

$$\mathbf{A} = \mathbf{U\Sigma U^T},$$

with $\mathbf{UU^T} = \mathbf{I_p}$, $\mathbf{\Sigma} = \mathbf{diag}(\sigma_\mathbf{1}, \ldots, \sigma_\mathbf{p})$ with $\sigma_1 \geq \cdots \geq \sigma_p > 0$.

$$\mathbf{A^q} = \mathbf{U\Sigma^q U^T}, \quad \mathbf{q} \in \mathbb{Q}.$$

Let x be an arbitrary nonzero vector in $\mathbb{R}^p$ and $U = [u_1, \ldots, u_p]$ It holds

$$\mathbf{A^q x} = \sum_{\mathbf{k=1}}^{\mathbf{p}} \sigma_\mathbf{k}^\mathbf{q} (\mathbf{u_k}, \mathbf{x}) \mathbf{u_k}.$$

The moments

The **moments** of A with respect to a vector z are defined by

$$\mathbf{c}_\nu(\mathbf{z}) = (\mathbf{z}, \mathbf{A}^\nu \mathbf{z}) = \sum_{\mathbf{k}} \sigma_{\mathbf{k}}^\nu \alpha_{\mathbf{k}}^{\mathbf{2}}(\mathbf{z}),$$

where $\alpha_{\mathbf{k}}(\mathbf{z}) = (\mathbf{z}, \mathbf{u}_{\mathbf{k}})$.

Extrapolation of moments was first introduced in

C. Brezinski, Error estimates for the solution of linear systems, **SIAM J. Sci. Comput.**, 21 **(1999)** 764–781.

Extrapolation procedures and estimates

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Using some moments with a **non–negative integer index**, we **estimate** the moments $c_q(z)$ for **any fixed index $\mathbf{q} \in \mathbf{Q}$**.

The estimates are based on the **integer moments** of A with $\nu = n \in N$.

For this purpose, we will **approximate** the moments $c_q(z)$

by interpolating or **extrapolating** the $\mathbf{c_n}(\mathbf{z})$'s, for different values of the non–negative integer index n, at the points $\mathbf{q}$, by a conveniently chosen function obtained by

keeping only one or two terms in the summations.

One–term estimates

Knowing $\mathbf{c_0(z)}$ and $\mathbf{c_1(z)}$, we will look for $\mathbf{s}$, and $\alpha\mathbf{(z)}$ satisfying the **interpolation conditions**

$$\begin{aligned} \mathbf{c_0(z)} &= \alpha^{\mathbf{2}}\mathbf{(z)} \\ \mathbf{c_1(z)} &= \mathbf{s}\alpha^{\mathbf{2}}\mathbf{(z)} \end{aligned}$$

and, then, $\mathbf{c_q(z)}$ will be **estimated** by

$$\mathbf{c_q(z)} \simeq \mathbf{e_q(z)} = \mathbf{s^q}\alpha^{\mathbf{2}}\mathbf{(z)}.$$

Proposition 1

$$\mathbf{c_q(z)} \simeq \mathbf{e_q(z)} = \frac{\mathbf{c_1^q(z)}}{\mathbf{c_0^{q-1}(z)}}.$$

- $\mathbf{e_q(z)} \in \mathbf{R}$, $q \in Q$, since $c_1(z) > 0$.

One–term estimates

Assume that $\mathbf{A}^{-1}$ exists, and let $\kappa = \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\|$.

Theorem

If A is symmetric positive definite, then, for any vector z, the one–term estimate $e_n(z)$ satisfies the following inequalities for $n \in Z$, $n \neq 0$,

$$\mathbf{e_n(z) \le c_n(z) \le \left(\frac{(1+\kappa)^2}{4\kappa}\right)^{2^d-1} e_n(z)},$$

where

$$\mathbf{d} = \begin{cases} n-1, & n > 1 \\ |n|, & n < 0,\ n = 1 \end{cases}$$

Two–term estimates

Estimate $c_q(z)$, $q \in Q$, by keeping **two terms**

$$\mathbf{c_q(z) \simeq e_q(z) = s_1^q a_1^2(z) + s_2^q a_2^2(z)}. \tag{1}$$

The unknowns $\mathbf{s_1, s_2, a_1^2(z)}$ and $\mathbf{a_2^2(z)}$ will be computed by imposing the **interpolation conditions**,

$$\mathbf{c_n(z) = e_n(z) = s_1^n a_1^2(z) + s_2^n a_2^2(z)}, \tag{2}$$

for different integer values of the integer n.

$c_n(z)$'s satisfy **the difference equation** of order 2

$$\mathbf{c_{n+2}(z) - s c_{n+1}(z) + p c_n(z) = 0}, \tag{3}$$

where $\mathbf{s = s_1 + s_2}$ and $\mathbf{p = s_1 s_2}$.

Two–term estimates

Using this relation for $n = 0$ and 1 gives s and p.

$$\mathbf{s} = \frac{\mathbf{c_0(z)c_3(z) - c_1(z)c_2(z)}}{\mathbf{c_0(z)c_2(z) - c_1^2(z)}}, \quad \mathbf{p} = \frac{\mathbf{c_1(z)c_3(z) - c_2^2(z)}}{\mathbf{c_0(z)c_2(z) - c_1^2(z)}} \tag{4}$$

$e_q(z)$ follows with $\mathbf{s_{1,2} = (s \pm \sqrt{s^2 - 4p})/2}$ and

$$\mathbf{a_1^2(z) = \frac{c_0(z)s_2 - c_1(z)}{s_2 - s_1}}, \quad \mathbf{a_2^2(z) = \frac{c_1(z) - c_0(z)s_1}{s_2 - s_1}}, \tag{5}$$

Proposition 2

The moment $c_q(z)$ can be estimated by the **two–term formula**

$$\mathbf{c_q(z) \simeq e_q(z) = s_1^q a_1^2(z) + s_2^q a_2^2(z), \quad q \in Q}, \tag{6}$$

- $\mathbf{e_q(z) \in R},$ if $q \in Q$.

The trace

Theorem

M. Hutchinson, A stochastic estimator of the trace of the influence matrix for Laplacian smoothing splines, Commun. Statist. Simula., 18 (1989) 1059–1076.

Let

- $A \in \mathbb{R}^{p \times p}$ symmetric, $\mathrm{Tr}(A) \neq 0$,
- X a discrete random variable with values 1 , -1 with equal probability 0.5,
- x a vector of p independent samples from X.

Then (x, Ax) is an unbiased estimator of $\mathrm{Tr}(A)$.

$$E((x, Ax)) = \mathrm{Tr}(A),$$

$$\mathrm{Var}((x, Ax)) = 2 \sum_{i \neq j} a_{ij}^2,$$

This Theorem tells us that

$$Tr(\mathbf{A^q}) = \mathbf{E}((\mathbf{x}, \mathbf{A^q x})) = \mathbf{E}(\mathbf{c_q}(\mathbf{x})), \ \mathbf{x} \in \mathbf{X^p}$$

.

Thus, estimates of $Tr(\mathbf{A^q})$ could be obtained by

- **extrapolating the moments** at the point q,
- computing the **expectation** $\mathbf{E}(\mathbf{e_q}(\mathbf{x}))$ of $\mathbf{e_q}(\mathbf{x})$, $x \in X^p$.

For the **one–term estimates**, for $x \in X^p$ and $q = n \in Z$, we have

Proposition 3

If the matrix A is symmetric positive definite, then, for the one–term estimates, we have the bounds

$$\mathbf{E}(\mathbf{e_n}(\mathbf{x})) \leq Tr(\mathbf{A^n}) \leq \left(\frac{(\mathbf{1}+\kappa)^{\mathbf{2}}}{\mathbf{4}\kappa}\right)^{\mathbf{2^d-1}} \mathbf{E}(\mathbf{e_n}(\mathbf{x})),$$

where

$$\mathbf{d} = \begin{cases} n-1, & n > 1 \\ |n|, & n < 0, \; n = 1 \end{cases}$$

$\hookrightarrow$ If $\mathbf{A}$ is **orthogonal**, then $\kappa(A) = 1 \rightarrow \mathbf{Tr}(\mathbf{A^n}) = \mathbf{E}(\mathbf{e_n}(\mathbf{x}))$.

When $q \in Q$, estimates of $Tr(A^q)$ could be obtained by **realizing N experiments**, and then **computing the mean value** of the quantities $e_q(x_i)$ for $x_i \in X^p$.

We set

$$\mathbf{t_q} = \frac{\mathbf{1}}{\mathbf{N}} \sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{e_q(x_i)},$$

where the x_i's are N realizations of $x \in X^p$. Thus, we have

- the **one term estimates**,

$$\mathbf{t_q} = \frac{\mathbf{1}}{\mathbf{N}} \sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{c_1^q(x_i)/c_0^{q-1}(x_i)}, \quad \mathbf{q} \in \mathbf{Q}, \tag{7}$$

- and the **two term estimates**

$$\mathbf{t_q} = \frac{\mathbf{1}}{\mathbf{N}} \sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{s_1^q a_1^2(x_i) + s_2^q a_2^2(x_i)}, \quad \mathbf{q} \in \mathbf{Q}, \tag{8}$$

Specification of **confidence interval** for the estimates

Theorem

$$Pr\left(\left|\frac{\mathbf{t_q} - Tr(\mathbf{A^q})}{\sqrt{\mathbf{Var}((\mathbf{x}, \mathbf{A^q x}))/\mathbf{N}}}\right| < \mathbf{Z_{a/2}}\right) = \mathbf{1 - a}.$$

where N is the number of trials, a is the significance level, $Z_{a/2}$ the upper $a/2$ percentage point of the distribution $N(0,1)$.

For a significance level $a = 0.01$, we have the confidence interval $100(1-a)\% = 99\%$.

The norm of the error

We consider the **symmetric linear system** $\mathbf{A}\mathbf{x} = \mathbf{f}$.

Let $\mathbf{y}$ **be an approximation of** $\mathbf{x}$, obtained either directly or as an iterate of an iterative method.

We define the **residual** as $\mathbf{r} = \mathbf{f} - \mathbf{A}\mathbf{y}$.

Thus

$$\mathbf{c}_{-2}(\mathbf{r}) = (\mathbf{A}^{-1}\mathbf{r}, \mathbf{A}^{-1}\mathbf{r}) = (\mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y}) = \|\mathbf{x}-\mathbf{y}\|^2,$$

which is the square of the norm of the error.

The norm of the error

For $q = -2$, the **one–term estimate**

$$\mathbf{e_{-2}(r) = c_0^3(r)/c_1^2(r)}$$

will be an approximation of $\|x - y\|^2$.

We also get the **two–term estimate**

$$c_{-2}(z) \quad \simeq \quad \mathbf{e_{-2}(z) = N_{-2}(z)/(c_1(z)c_3(z) - {c_2}^2(z))^2}$$

$$\begin{aligned} N_{-2}(z) \quad = \quad & {c_0}^3(z){c_3}^2(z) + {c_1}^2(z){c_2}^2(z)c_0(z) + 2{c_1}^3(z)c_0(z)c_3(z \\ & -{c_1}^4(z)c_2(z) + {c_2}^3(z)c_0^2(z) - 4{c_0}^2(z)c_1(z)c_2(z)c_3(z) \end{aligned}$$

Numerical results

Complexity

The estimates require only **few matrix–vector products** and **some inner products**.

For a spd matrix $\mathbf{A} \in \mathbf{R}^{\mathbf{p} \times \mathbf{p}}$,

- the **one-term** estimate e_q needs only $\mathbf{O(p^2)}$ flops,
- the **two-term** one requires $\mathbf{O(2p^2)}$ flops.

Random vector generation sampling method

For the vectors $x \in X^p$, we used the uniform generator of random numbers between 0 and 1 of MATLAB.

If the value was less or equal to $\mathbf{0.5} \xrightarrow{\text{component of x}} \mathbf{-1}$;

if it was greater than $\mathbf{0.5} \xrightarrow{\text{component of x}} \mathbf{+1}$;

Numerical results

Statistical techniques

Trimmed mean value $\longrightarrow$ to exclude extreme values

In this technique, all the estimates $e_q(x_i)$ are put in ascending order, and we discard 2% of the values from the two edges.
This technique reduces the variance.

Bootstrapping-like technique

We construct the samples by only permuting the elements of the first sample vector, keeping half of the elements equal to $+1$ and half to -1.
If we have a good initial selection this technique can improve the results, and reduce the variance.

Example 1

The **Prolate** matrix

This matrix is symmetric Toeplitz.

Using as calling parameter a variable w in the range $0 < w < 0.5$, then $\mathbf{P}$ is positive definite.
The eigenvalues of $\mathbf{P}$ are distinct, lie in (0,1], and tend to cluster around 0 and 1.

We compute the $Tr(\mathbf{P^{1/2}})$, $Tr(\mathbf{P^{12}})$.

For matrices $\mathbf{P}$ of dimensions $100, 200, 500, 1000$, the variance of the estimate for $\mathbf{q = 1/2}$ is $2.29, 3.27, 5.21, 7.39,$ respectively.

These values are small, so we expect good estimates even for a small size of the samples.

Dim	Exact	1-term est		
	$Tr(\mathbf{P^{1/2}})$,	1-term est	rel1	conf interval
100	1.33183e2	1.34049e2	6.5047e-3	[1.33219e2, 1.34880e2]
200	2.66325e2	2.67551e2	4.6034e-3	[2.66389e2, 2.68714e2]
500	6.65743e2	6.69844e2	6.1598e-3	[6.68274e2, 6.71413e2]
1000	1.33143e3	1.34147e3	7.5353e-3	[1.33912e3, 1.34381e3]

Dim	Exact	2-term est		
	$Tr(\mathbf{P^{1/2}})$,	2-term est	rel2	conf interval
100	1.33183e2	1.33188e2	3.4839e-5	[1.32463e2, 1.33912e2]
200	2.66325e2	2.66245e2	3.0015e-4	[2.65088e2, 2.67402e2]
500	6.65743e2	6.65605e2	2.0770e-4	[6.63429e2, 6.67780e2]
1000	1.33143e3	1.33160e3	1.2375e-4	[1.32892e3, 1.33428e3]

Dim	Exact	2-term est		
		2-term est	rel2	conf interval
100	3.21895e5	3.21982e5	2.7162e-4	[3.11421e5, 3.32544e5]
200	6.48958e5	6.49168e5	3.2310e-4	[6.36575e5, 6.61760e5]
500	1.63121e6	1.62928e6	1.1828e-3	[1.60884e6, 1.64973e6]
1000	3.26907e6	3.26318e6	1.8031e-3	[3.23330e6, 3.29306e6]

Table: Estimating $Tr(P^{12})$, $w = 0.9$, cond= 2, (sample=50)

Example 2

Comparison with other methods estimating $Tr(\mathbf{A}^{-1})$

We compare our estimates for $\mathbf{q = -1}$ developed in

C. Brezinski, P. Fika, M. Mitrouli, Moments of a linear operator on a Hilbert space, with applications to the trace of the inverse of matrices and the solution of equations, Numerical Linear Algebra with Applications, (to appear).

with the **Monte–Carlo approach** presented in
G.H. Golub, G. Meurant, *Matrices, Moments and Quadrature with Applications*, Princeton University Press, Princeton, **2010**.

and the **modified Chebyshev algorithm** of
G. Meurant, Estimates of the trace of the inverse of a symmetric matrix using the modified Chebyshev algorithms, **Numer. Algorithms**, 51 (**2009**) 309–318.

The **Poisson** matrix

We consider the block tridiagonal (sparse) matrix P of dimension p, resulting from discretizing the Poisson's equation with the 5–point operator on a $\sqrt{p} \times \sqrt{p}$ mesh.

Dim	exact	2-term est	M-C	mod Chebyshev
36	1.37571e1	1.37106e1	1.39216e1	1.37568e1 (k=10)
900	5.12644e2	5.12614e2	5.02012e2	5.12547e2 (k=40)

Table: $Tr(P^{-1})$ for *Poisson* matrices

Further work

- Estimation of $Tr(A^q)$ for any matrix A.
- Further study of sampling methods and statistical techniques.
- Thorough comparison of our estimates with other methods.
- The derivation of estimates of the trace of functions of matrices.
- Application of our estimates to the partial eigenvalue sum.
- Application of our estimates for the error in the solution of an operator equation or, more generally, of any functional equation in a Hilbert space under appropriate conditions.

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