Estimates for the bilinear form $x^T A^{-1} y$ by extrapolating the moments of the matrix A

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Motivation for the problem

Evaluation of $x^T A^{-1} y$

A: a real nonsingular matrix of order p

x, y: real vectors of length p

Estimates for the quantities:

- Elements of the matrix A^{-1}
- The trace of the matrix A^{-1}

Applications:

- ✓ Networks analysis
- ✓ Signal processing
- ✓ Nuclear physics
- ✓ Quantum mechanics
- ✓ Computational fluid dynamics

Estimates for $x^T A^{-1} y$ via an extrapolation procedure

Estimates for $x^T A^{-1} x$

SVD of A: $A = U\Sigma V^T = \sum_{k=1}^{p} \sigma_k u_k v_k^T$

Moments of A:

$c_{2n}(x) = (x,(A^TA)^n x)$, $c_{2n+1}(x) = (x, A(A^TA)^n x)$, $n \geq 0$

$c_{2n}(x) = (x,(AA^T)^n x)$, $c_{2n+1}(x) = (x, A^T(AA^T)^n x)$, $n \leq 0$

$$c_{-1}(x) = (x, A^T(AA^T)^{-1} x) = (x, A^{-1} x) =$$
$$\sum_k \sigma_k^{-1}(x, vk)(x, uk) = \sum_k \sigma_k^{-1} a_k b_k$$

One term estimates

$$c_{-1} = (x, A^{-1}x) \approx s^{-1}\alpha\beta$$

s, α and β are determined by the interpolation conditions

$$c_0 = \alpha^2, \;\; c_0 = \beta^2$$

$$c_1 = s\alpha\beta, \;\; c_2 = s^2\alpha^2$$

Family of one term estimates for the moment c_{-1}

$$\mathbf{e_\nu = c_0^{\nu+2} c_1^{-2\nu-1} c_2^{\nu}, \;\; \nu \in R}$$

- ✓ $e_\nu = \rho^\nu e_0$, $e_\nu = \rho\, e_{\nu-1}$, where $\rho = c_0 c_2 / c_1^{\,2}, \nu \in R$
- ✓ non decreasing function of $\nu \in R$ for $c_1 > 0$
- ✓ non increasing for $c_1 < 0$

Lemma

Let $A \in R^{p \times p}$ be a positive real matrix i.e. $(x, Ax) > 0,\ \forall\ x \neq 0$.

- There exists a value ν_0 given by

$$\nu_0 = \frac{\log(c_{-1}/e_0)}{\log(\rho)}, \quad \rho = c_0 c_2 / c_1^2,$$

such that $e_{\nu_0} = c_{-1}$.

- It holds that $\nu_0 \leq \dfrac{\log(c_1/(c_0 \sigma_p))}{\log(p)}$,

$\boldsymbol{\sigma_p}$**:** the minimum singular value of the matrix $A \in R^{p \times p}$.

- **Two term estimates**

$$c_{-1} = (x, A^{-1}x) \approx \hat{e}_\nu = s_1^{-1}\alpha_1\beta_1 + s_2^{-1}\alpha_2\beta_2$$

Family of two term estimates for the moment c_{-1}

$$\hat{e}_\nu = e_0 + \frac{c_0 c_2 - c_1^2}{c_1} \frac{c_o \tilde{c}_{\nu+2} - c_1 c_{\nu+1}}{c_1 c_{\nu+3} - c_2 \tilde{c}_{\nu+2}}, \ \nu \in \mathbb{N}$$

$\mathbf{e_0}$: the one term estimate for $\nu = 0$.

❖ Estimates for $x^T A^{-1} y$

For $x \neq y$,

⇨ we define the bilinear moment

$$c_{-1}(x,y)=(x,A^{-1}y)$$

⇨ polarization identity

$$x^T(A^TA)^{-1}u = \frac{1}{4}(w^T(A^TA)^{-1}w - z^T(A^TA)^{-1}z),$$

where $u=A^Ty$, $w=x+u$ and $z=x-u$

⇨ we set the moments $g_n(x) = (x,(A^TA)^n x)$, $n \in \mathbb{Z}$

⇩

$$\mathbf{c_{-1}(x,y) = \frac{1}{4}(g_{-1}(w)-g_{-1}(z))}$$

❖ Estimates for symmetric matrices

$A \in R^{pxp}$ a symmetric matrix

one term estimate e_0 $=$ lower bound of $(x, A^{-1}x)$ Gauss quadrature - **one** Lanczos iteration

two term estimate $\hat{e}_0$ $=$ lower bound of $(x, A^{-1}x)$ Gauss quadrature - **two** Lanczos iterations

Proposition

Let $A \in R^{pxp}$ be a symmetric positive definite matrix. It holds that

$$0 \le v_0 \le \frac{\log(m)}{\log(\rho)},$$

where $m = \frac{(1+\kappa(A))2}{4\kappa(A)}$ and $\kappa(A)$ is the spectral condition number of A.

Estimates for the elements of the matrix A^{-1}

$A = [\alpha_{ij}] \in R^{pxp}$ i, j = 1, …, p

Proposition

The families of one term estimates for the diagonal elements of the matrix A^{-1} are

$$(A^{-1})_{ii} \cong \rho^{\nu}\frac{1}{\alpha_{ii}}, \quad \rho = \frac{s_i}{\alpha_{ii}^{\ 2}} \quad \textbf{or} \quad (A^{-1})_{ii} \cong \tilde{\rho}^{\nu}\frac{1}{\alpha_{ii}}, \quad \tilde{\rho} = \frac{\tilde{s}_i}{\alpha_{ii}^{\ 2}}, \quad \nu \in R,$$

where $s_i = \sum_{k=1}^{p} a_{ki}^{\ 2}$ and $\tilde{s}_i = \sum_{k=1}^{p} a_{ik}^{\ 2}$.

Proposition

The one term estimates for the elements of the matrix A^{-1}, using the one term estimates e_0 are

$$(A^{-1})_{ii} \cong \frac{1}{\alpha_{ii}},$$

$$(A^{-1})_{ij} \cong \frac{1}{4}\left(\frac{(\tilde{s}_j+2aji+1)^2}{\sum_{t=1}^{p}(s_{tj}+ati)^2} - \frac{(\tilde{s}_j-2aji+1)^2}{\sum_{t=1}^{p}(-st_j+ati)^2}\right),$$

where $s_{tj} = \sum_{k=1}^{p} a_{tk}a_{jk}$ and $\tilde{s}_j = \sum_{k=1}^{p} a_{jk}{}^2$.

❖ Estimates for the elements of symmetric matrices

- **one term estimate:**

$(A^{-1})_{ij} \cong \frac{-4aij}{(a_{ii}+ajj)^2-4aij^2}$, i≠j

$(A^{-1})_{ii} \cong \frac{1}{\alpha_{ii}}$ ⟶ lower bound of $(A^{-1})_{ii}$ - Gauss quadrature

- **one** Lanczos iteration

- **two term estimate:**

$\hat{e}_0$ for $x=\delta_i$ ⟶ lower bound of $(A^{-1})_{ii}$ - Gauss quadrature

- **two** Lanczos iterations

Family of estimates for the trace of the matrix A^{-1}

$A \in R^{pxp}$ a nonsingular matrix

$M = \frac{1}{2}(A^{-1} + A^{-T}) = \frac{1}{2}((A^TA)^{-1}A^T + A(A^TA)^{-1})$ symmetric

$$\mathbf{Tr(M) = Tr(A^{-1})}$$

Moments:

$$d_n = d_n(x) = (x, (((A^TA)^n A^T + A(A^TA)^n)/2)x), \; n=-1,0,1,\ldots$$

$$d_n = \sum_{k=1}^{p} \sigma_k^{2n+1} a_k b_k$$

$$s^2 = d_0^{-\nu/2-1} d_1^{\nu+1} d_2^{-\nu/2}, \; \nu \in R$$

$$d_{-1} \cong s^{-4} d_1 \longrightarrow \mathbf{t_\nu = d_0^{\nu+2} d_1^{-2\nu-1} d_2^{\nu} \cong d_{-1}, \; \nu \in R}$$

Implementation and numerical examples

❖ Computational complexity of the estimates

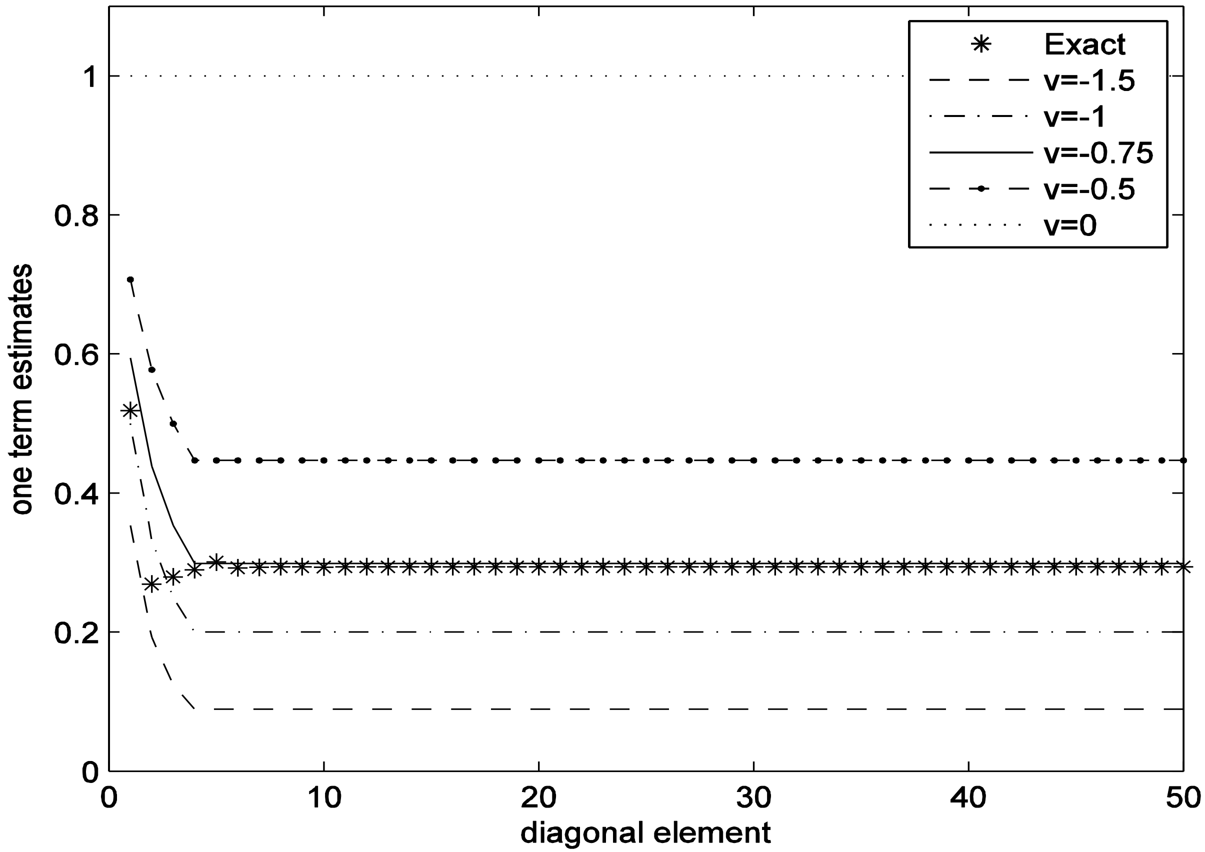
Matrix A	e_ν	$\tilde{e}_\nu$	$\hat{e}_\nu$, ν even	$\hat{e}_\nu$, ν odd
Dense	$O(p^2)$	$O(2p^2)$	$O((\nu+3)p^2)$	$O((\nu+2)p^2)$
Symmetric dense	$O(p^2)$	$O(p^2)$	$O((\nu/2+2)p^2)$	$O((\nu/2+3/2)p^2)$
Banded	$O(qp)$	$O(2qp)$	$O((\nu+3)qp)$	$O((\nu+2)qp)$
Symmetric banded	$O(qp)$	$O(qp)$	$O((\nu/2+2)qp)$	$O((\nu/2+3/2)qp)$

Arithmetic operations for the estimation of the moment $x^TA^{-1}x$.

Matrix A	e_0	E_ν	$\tilde{e}_\nu$	$\hat{e}_\nu$
nonsymmetric	$O(3p^2)$	$O(5p^2)$	$O(9p^2)$	$O((2\nu+7)p^2)$

Arithmetic operations for the estimation of the bilinear form $x^TA^{-1}y$.

- *Monotonic behavior of the one term estimates*



Estimating the diagonal of the inverse of *grcar* matrix of order 4000.

Grcar matrix:

- Toeplitz
- well conditioned, κ(A)=3.6277
- First 50 diagonal elements
- $e_{-0.75}$ good estimate
- e_ν increases as ν increases