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ON A MODIFIED KOVARIK ALGORITHM FOR SYMMETRIC MATRICES *

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To Professor Silviu Sburlan, at his 60's anniversary

Abstract

In some of his scientific papers and university courses, professor Silviu Sburlan has studied integral equations (see the list of references). Beside the theoretical qualitative analysis concerning the existence, uniqueness and other properties of the solution, he was also interested in its numerical approximation. In the case of first kind integral equations with smooth kernel (e.g. continuous) it is well known that, by applying classical discretization techniques (as collocation or projection methods) we get (very) ill-conditioned symmetric positive semi- definite linear systems. This will cause big troubles for both direct or iterative solvers. Moreover, the system matrix is usually dense, thus classical preconditioning techniques, as Incomplete Decomposition can not be used. One possibility to overcome this difficulty is to use orthogonalization algorithms, which also "compress" the spectrum of the system matrix, by transforming it into a well-conditioned one. Unfortunately, the well known Gram-Schmidt method fails in the case of singular matrices or is totally unstable for ill-conditioned ones. In a previous paper, the author extended an iterative approximate orthogonalization algorithm due to Z. Kovarik, to the case of arbitrary rectangular matrices. In the present one, we adapt this algorithm to the class of symmetric (positive semi-definite) matrices. The new algorithm has similar convergence properties as the initial one, but requires much less computational effort per iteration. Some numerical experiments are also described for a "model problem" first kind integral equation.

Key Words: Kovarik algorithm, approximate orthogonalization, symmetric matrices, first kind integral equations.

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1 Kovarik's original algorithm

Let A be an $m \times n$ matrix and $(A)_i, A^t, A^+$ its i-th row, transpose and Moore-Penrose pseudoinverse (see [1]), respectively. By $gk_2(A)$ we shall denote its generalized spectral condition number defined as the square root of the ratio between the biggest and smallest singular values; $\langle \cdot, \cdot \rangle, \parallel \cdot \parallel$ will be the Euclidean scalar product and norm on some space $I\!R^q$. For a square matrix B, $\sigma(B), \rho(B), \parallel B \parallel$ will denote its spectrum, spectral radius and spectral norm, respectively. All the vectors appearing in the paper will be considered as column vectors. Let $(a_k)_{k \geq 0}$ be the sequence of real numbers defined by the Taylor's series

$$(1-t)^{-\frac{1}{2}} = a_0 + a_1 t + a_2 t^2 + \ldots, \quad t \in (-1, 1), \tag{1}$$

i.e.

$$a_j = \frac{1}{2^{2j}} \frac{(2j)!}{(j!)^2}, \quad j \geq 0 \tag{2}$$

and $(q_k)_{k \geq 0}$ a given sequence of positive integers. Then, the "approximate orthogonalization" method proposed by Z. Kovarik in [2] (Algorithm A, page 386) and extended by the author in [6] is the following.
Algorithm KOA. Let $A_0 = A$; for $k = 0, 1, \ldots,$ do

$$H_k = I - A_k A_k^t, \; A_{k+1} = (I + a_1 H_k + a_2 H_k^2 + \ldots + a_{q_k} H_k^{q_k}) A_k, \tag{3}$$

where by I we denoted the corresponding unit matrix. Let us suppose that

$$\parallel A \parallel \; < \; 1. \tag{4}$$

Then, the following result was proved in [6].

Theorem 1 *Let $(A_k)_{k \geq 0}$ be the sequence of matrices defined by $(2) - (4)$. Then*

$$\lim_{k \to \infty} A_k = \left[(AA^t)^{\frac{1}{2}} \right]^+ A = A_\infty. \tag{5}$$

Moreover, we have

$$\parallel A_k - A_\infty \parallel \;\; \leq \;\; \delta^{s_k}, \tag{6}$$

with s_k given by

$$s_k = \prod_{j=0}^{k-1} (1 + q_j) \;\; \geq \;\; 2^k, \;\; k \geq 1 \tag{7}$$

and

$$\delta = 1 - \sigma^2, \tag{8}$$

where σ is the smallest nonzero singular value of A.

Remark 1 *Relations* $(6)-(7)$ *tell us that the algorithm* ***KOA*** *converges at least quadratically. Moreover, the assumption* (4) *is not restrictive. It can be obtained by a scaling of the matrix A, of the form*

$$A := \frac{1}{\sqrt{\| A \|_\infty \| A \|_1 + 1}} A, \tag{9}$$

where $\| \cdot \|_\infty$, $\| \cdot \|_1$ *are the well known matrix norms (see e.g. [1]).*

Remark 2 *If* $U^t AV = diag(\sigma_1, \ldots, \sigma_r, 0, \ldots, 0)$, $r = rank(A)$ *is a singular value decomposition of* A *and* $\tilde{I}$ *is the* $m \times m$ *matrix defined by*

$$\tilde{I} = diag(1, 1, \ldots, 1, 0, \ldots, 0) \tag{10}$$

(with 1's in the first r positions) then, the following "approximate orthogonalization" relation holds with respect to the rows of the matrix A_∞ *from* (5) *(see [6])*

$$\langle (A_\infty)_i, (A_\infty)_j \rangle = \langle \tilde{I}(U)_i, (U)_j \rangle, \tag{11}$$

which for $\tilde{I} = I$ *(i.e. for A with linearly independent rows) becomes a classical orthogonality (because the matrix U is orthogonal), as for the Gram-Schmidt algorithm (see e.g. [1]). Moreover, the following result can be proved with respect to the generalized spectral condition number of the matrices* A_k

$$\lim_{k \to \infty} gk_2(A_k) = gk_2(A_\infty) = 1. \tag{12}$$

This tells us that the generalized spectral condition number of A improves during the application of (3)*, by reaching at the limit the ideal value* 1.

2 The case of symmetric matrices

Let us now suppose that A is an $n \times n$ symmetric matrix. Then, if A satisfies (4) the above algorithm **KOA** applies for it and all the results from the previous section rest true. Moreover, it can be easily proved that all the matrices A_k will be symmetric, thus (3) will become

$$H_k = I - A_k^2, \; A_{k+1} = (I + a_1 H_k + a_2 H_k^2 + \ldots + a_{q_k} H_k^{q_k}) A_k. \tag{13}$$

Unfortunately, a big computational effort will be required for the product A_k^2. We can eliminate this by considering the following modified version.
Algorithm KOAS. Let $A_0 = A$; for $k = 0, 1, \ldots,$ do

$$H_k = I - A_k, \; A_{k+1} = (I + a_1 H_k + a_2 H_k^2 + \ldots + a_{q_k} H_k^{q_k}) A_k \tag{14}$$

Remark 3 *We have to observe that the above algorithm can not be derived from the former **KOA**; indeed H_k from* (14) *is different from H_k in* (3)*, but A_{k+1} is computed with a similar formula as*

$$A_{k+1} = f(H_k)A_k, \tag{15}$$

with $f_k : \mathbb{R} \longrightarrow \mathbb{R}$ the function defined by

$$f_k(x) = 1 + a_1 x + \cdots + a_{q_k} x^{q_k}, \; k \geq 0. \tag{16}$$

Concerning the convergence of the new algorithm **KOAS**, we have the following main result of the paper.

Theorem 2 *Let us suppose that A is symmetric, satisfies* (4) *and is positive semi-definite, i.e.*

$$\langle Ax, x \rangle \; \geq \; 0, \; \forall x \in \mathbb{R}^n. \tag{17}$$

*Then, the sequence $(A_k)_{k \geq 0}$ generated with the algorithm **KOAS** converges and*

$$\lim_{k \to \infty} A_k = A^+ A. \tag{18}$$

Proof. Because A is symmetric it exists an orthogonal $n \times n$ matrix Q such that

$$Q^t A Q = Q^t A_0 Q = D_0 = diag(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0), \tag{19}$$

where $r = rank(A)$ and (see(4) and (17))

$$\lambda_i \in (0, 1), \forall i = 1, \ldots, r. \tag{20}$$

Then, by using (14)-(16) and (19) we obtain

$$Q^t(f_0(H_0))Q = diag(f_0(\delta_1), \ldots, f_0(\delta_r), f_0(1), \ldots, f_0(1)) \tag{21}$$

with δ_i given by

$$\delta_i = 1 - \lambda_i \in (0, 1), \forall i = 1, \ldots, r. \tag{22}$$

Thus, from (21) and (15) (for $k = 0$) we get

$$A_1 = f_0(H_0)A_0 = QD_1Q^t, \tag{23}$$

with

$$D_1 = diag(f_0(\delta_1)\lambda_1, \ldots, f_0(\delta_r)\lambda_r, 0, \ldots, 0). \tag{24}$$

From (19)-(24), by mathematical induction we get that, if

$$A_k = QD_kQ^t, \tag{25}$$

with

$$D_k = diag(\lambda_1^{(k)}, \ldots, \lambda_r^{(k)}, 0, \ldots, 0), \tag{26}$$

then

$$A_{k+1} = QD_{k+1}Q^t, \tag{27}$$

with

$$D_{k+1} = diag(f_k(1-\lambda_1^{(k)})\lambda_1^{(k)}, \ldots, f_k(1-\lambda_r^{(k)})\lambda_r^{(k)}, 0, \ldots, 0). \tag{28}$$

Thus, for the convergence of the sequence $(A_k)_{k\geq 0}$ it suffices to analyse the behaviour of the sequence of real numbers $(x_k)_{k\geq 0}$, recursively defined by

$$x_0 \in (0,1), x_k1 = f_k(1-x_k)x_k, k \geq 0. \tag{29}$$

Because $x_0 > 0$ and $f_k(x) > 1, \forall x > 0, k \geq 0$ we obtain

$$x_1 - x_0 = (f_0(1-x_0) - 1)x_0 > 0.$$

Now, because $f_k(x) < \frac{1}{\sqrt{1-x}}, \forall x \in (0,1), k \geq 0$ we obtain

$$x_1 - 1 = f_0(1-x_0)x_0 - 1 < \frac{x_0}{\sqrt{1-(1-x_0)}} - 1 = \sqrt{x_0} - 1 < 0,$$

thus

$$x_1 > x_0 \ \text{ and } \ x_1 \in (0,1). \tag{30}$$

Then, by an induction argument we get

$$x_0 \leq x_k < x_k1 < 1, \ \forall k \geq 0, \tag{31}$$

thus

$$\exists \lim_{k\to\infty} x_k = x^* \in (0,1]. \tag{32}$$

We shall prove that $x^* = 1$. Let us suppose that this is not true, i.e.

$$x^* < 1 \tag{33}$$

and let q^* be the integer defined by

$$q^* = \min\{q_k, k \geq 0\} \geq 1. \tag{34}$$

Let $g_k(x) = 1 + a_1x + \cdots + a_kx^k, x \in I\!R, k \geq 0$. Then (see (1))

$$\lim_{k\to\infty} g_k(x) = \frac{1}{\sqrt{1-x}}, \ g_k(x) < \frac{1}{\sqrt{1-x}}, \ k \geq 0, x \in (-1,1). \tag{35}$$

Then, for an arbitrary fixed $k \geq 0$ and $y_k = 1 - x_k \in (0, 1)$ we would obtain (by also using (16) and (34))

$$f_k(y_k) \geq 1 + a_1 y_k + \cdots + a_{q^*}(y_k)^{q^*} = g_{q^*}(y_k), \tag{36}$$

thus

$$x_k 1 - x_k = (f_k(y_k) - 1)x_k \geq (g_{q^*}(y_k) - 1)x_k = (g_{q^*}(1 - x_k) - 1)x_k. \tag{37}$$

By taking the limit in (37) we would obtain (also using (32))

$$0 = x^* - x^* \geq (g_{q^*}(1 - x^*) - 1)x^* > 0, \tag{38}$$

where the last strict inequality holds because $x^* > 0$ and $x^* < 1$ (and thus $g_{q^*}(1 - x^*) > 1$). But, the conclusion (38) is false, thus our assumption (33) is so. It then results that $x^* = 1$ and (see (25) - (28))

$$\lim_{k \to \infty} A_k = Qdiag(1, \ldots, 1, 0, \ldots, 0)Q^t. \tag{39}$$

But, from (19) we obtain that (see also [1])

$$A^+ = Qdiag(\frac{1}{\lambda_1}, \ldots, \frac{1}{\lambda_r}, 0, \ldots, 0)Q^t, \tag{40}$$

thus A^+A will be exactly the matrix in the right hand side of (39) and the proof is complete.

Corollary 3 *If the matrix A is not positive semi-definite, then the sequence $(A_k)_{k \geq 0}$ generated with the **KOAS** algorithm is divergent.*

Proof. In this case, at least one eigenvalue λ_i in (19)-(20) will be in $(-1, 0)$. This means that in the recursion (29) we shall start with $x_0 \in (-1, 0)$, thus

$$1 - x_0 \ > \ 1. \tag{41}$$

Then, by using (16), (41) and (34) we shall obtain

$$f_0(1 - x_0) = 1 + a_1(1 - x_0) + \cdots + a_{q_0}(1 - x_0)^{q_0} \geq$$

$$1 + a_1(1 - x_0) + \cdots + a_{q^*}(1 - x_0)^{q^*} \geq 1 + a_1(1 - x_0) > 1 + a_1 > 1. \tag{42}$$

From (41)-(42) we shall get

$$x_1 = f_0(1 - x_0)x_0 < (1 + a_1)x_0 < x_0 < 0.$$

Then, using similar arguments as before we shall obtain

$$f_1(1-x_1) \geq 1 + a_1(1-x_1) + \cdots + a_{q^*}(1-x_1)^{q^*} \geq 1 + a_1(1-x_1) > 1 + a_1$$

and

$$x_2 = f_1(1-x_1)x_1 < (1+a_1)x_1 < (1+a_1)^2 x_0.$$

A recursive argument will give us that

$$x_k < (1+a_1)^k x_0 < 0, \ \forall k \geq 1,$$

from which we shall obtain

$$\lim_{k\to\infty} x_k = -\infty,$$

i.e. $(x_k)_{k\geq 0}$ diverges and the proof is complete.

Corollary 4 *For the generalized spectral conditions numbers of the matrices $A_k, k \geq 0$ generated with the algorithm **KOAS**, the following holds*

$$\lim_{k\to\infty} gk_2(A) = gk_2(A^+A) = 1. \tag{43}$$

Proof. It results directly from Theorem 1 and the definition of $gk_2(A)$.

Remark 4 *A similar approximate orthogonalization property as in* (11) *holds for the rows of the limit matrix A^+A from* (18).

Remark 5 *Unfortunately, we have not yet a theoretical analysis of the convergence rate of the algorithm **KOAS**. But, numerical experiments show that it is of an order smaller with one unit than that of the original **KOA** algorithm.*

3 Numerical experiments

We considered in our tests the following first kind integral equation: for a given function $y \in L^2([0,1])$, find $x^* \in L^2([0,1])$ such that

$$\int_0^1 k(s,t)x(t)dt \ = \ y(s), \ s \in [0,1], \tag{44}$$

with

$$k(s,t) = \frac{1}{1+|s-t|}, \quad y(s) = ln[(1+s)(2-s)]. \tag{45}$$

Remark 6 *The equation* $(44)-(45)$ *has the solution* $x(t) = 1, \forall t \in [0,1]$.

We discretized (44)-(45) by a collocation algorithm (see [3]) with the collocation points

$$s_i = (i-1)\frac{1}{n-1}, \ i = 1, 2, \dots, n. \tag{46}$$

Thus, we obtained the symmetric (positive definite) system

$$Ax = b, \tag{47}$$

with the $n \times n$ matrix A and $b \in I\!R^n$ given by

$$A_{ij} = \int_0^1 k(s_i, t)k(s_j, t)dt, \quad b_i = y(s_i). \tag{48}$$

The values $gk_2(A))$, for different values of n are presented in Table 1. They indicate that, for relatively small values of n the matrix A is very ill-conditioned. We then tested the algorithms **KOA** and **KOAS** with

$$q_k = 2, \ \forall k \geq 0 \tag{49}$$

and using the following three stopping rules

$$\| A_{k+1} - A_k \|_\infty \ \leq \ 10^{-6}, \tag{50}$$

$$gk_2(A) \ \leq \ 10, \tag{51}$$

$$gk_2(A) \ \leq \ 100. \tag{52}$$

Because of its symmetry, the matrix A was scaled by (see (19))

$$A := \frac{1}{\| A \|_\infty + 1} A, \tag{53}$$

in order to obtain (4). The numbers of iterations neccessary to fulfill one the stopping rules (50)-(52) are described in Tables 2 and 3.

Note. All the computations have been made with the Numerical Linear Algebra software package OCTAVE, freely available under the terms of the GNU General Public License, see `www.octave.org`.

Table 1. Conditioning of of A

n	$gk_2(A)$
16	$3.7 \ 10^5$
32	$6.7 \ 10^6$
64	$1.14 \ 10^8$
128	$1.8 \ 10^9$
256	$3.0 \ 10^{10}$

Table 2. Results for algorithm KOA

n	stop (50)	stop (51)	stop (52)
16	18	10	8
32	21	14	10
64	24	17	13
128	27	20	16

Table 3. Results for alg. KOAS

n	stop (50)	stop (51)	stop (52)
16	37	14	11
32	41	18	15
64	45	22	19
128	49	26	23

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