

SOME REMARKS ON THE ELMAN ESTIMATE FOR GMRES

B. BECKERMANN*, S.A. GOREINOV†, AND E.E. TYRTYSHNIKOV‡

Abstract. Starting from a GMRES error estimate proposed by Elman in terms of the ratio of the smallest eigenvalue of the hermitian part and the norm of some non-symmetric matrix, we propose some asymptotically tighter bound in terms of the same ratio. Here we make use of a recent deep result of Crouzeix et al. on the norm of functions of matrices.

Key words. GMRES, non-symmetric systems, error estimates, field of values.

AMS subject classifications. 65F10, 65N22

1. Introduction. A popular method for solving non-hermitian systems $Ax = b$ is given by GMRES [13]. Provided that A has a positive definite hermitian part $(A + A^*)/2$, Elman [9] (see also [8]) pointed out the following upper bound for the norm of the k th residual r_k of GMRES for every $k \geq 0$

$$\frac{\|r_k\|}{\|r_0\|} \leq \sin^k(\beta), \quad \text{where } \cos(\beta) := \frac{\lambda_{\min}((A + A^*)/2)}{\|A\|} \quad (1.1)$$

with $\beta \in [0, \pi/2)$. Here and hereafter we use $\|\cdot\|$ to denote the Euclidean vector norm or spectral matrix norm. Recall that the field of values (or numerical range)

$$W(A) := \{(Ay, y) : y \in \mathbb{C}^n, \|y\| = 1\}$$

of a matrix is bounded by the rectangle defined by the extremal eigenvalues of the hermitian and the skew-hermitian parts of A . Hence $\lambda_{\min}((A + A^*)/2)$ bounds from below the distance between the origin and $W(A)$. More generally, since $W(A)$ is convex by the Hausdorff Theorem, one may show in the case $0 \notin W(A)$ that there is a $t \in \mathbb{R}$ with $\text{dist}(0, W(A)) = \lambda_{\min}((e^{it}A + (e^{it}A)^*)/2)$, and $t \in \{0, \pi\}$ for real matrices A . Since $\|r_k\|$ does not change after multiplying $Ax = b$ by some number of modulus 1, we may rewrite in the case $0 \notin W(A)$ the Elman bound (1.1) as

$$k \geq 0 : \quad \frac{\|r_k\|}{\|r_0\|} \leq \sin^k(\beta), \quad \cos(\beta) = \frac{\text{dist}(0, W(A))}{\|A\|}, \quad (1.2)$$

where we recall that (1.2) can be sharper than (1.1).

Estimates (1.1) or (1.2) are obtained by iterating the inequality for $k = 1$ corresponding to a one-dimensional minimization problem, which should allow for some improvements (compare for instance the approach in [7, Theorem 6.1] in terms of angles between subspaces). Here we propose some asymptotically sharper bounds only in terms of the above angle $\beta \in (0, \pi/2)$ which to our knowledge seems to be new.

*Laboratoire Paul Painlevé UMR 8524 (ANO-EDP), UFR Mathématiques – M3, UST Lille, F-59655 Villeneuve d'Ascq CEDEX, France, e-mail: bbecker@math.univ-lille1.fr. Supported in part by INTAS network NeCCA 03-51-6637, and in part by the Ministry of Science and Technology (MCYT) of Spain and the European Regional Development Fund (ERDF) through the grant BFM2001-3878-C02-02.,

†Institute of Numerical Mathematics, Russian Academy of Sciences, Gubkina Street, 8, Moscow, 119991, Russia, e-mail: serge@inn.ras.ru. Supported in part by RFBR grant No. 02-01-00590a.

‡Institute of Numerical Mathematics, Russian Academy of Sciences, Gubkina Street, 8, Moscow, 119991, Russia, e-mail: tee@inn.ras.ru. Supported in part by RFBR grant No. 02-01-00590a.

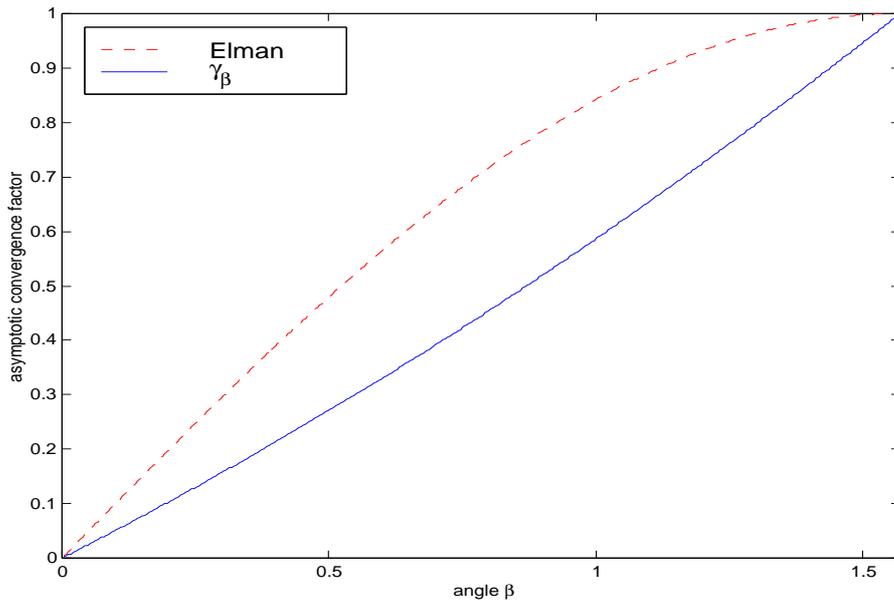


FIG. 1. Elman’s asymptotic convergence factor $\sin(\beta)$ (dashed) versus the new asymptotic convergence factor γ_β of Theorem 2.1 (solid).

2. Main result. THEOREM 2.1. *Let A be a matrix with $0 \notin W(A)$, and let $\beta \in (0, \pi/2)$ be as in (1.2). Then for the k th relative residual, $k \geq 1$, of GMRES we have*

$$\frac{\|r_k\|}{\|r_0\|} \leq (2 + 2/\sqrt{3})(2 + \gamma_\beta) \gamma_\beta^k, \quad (2.1)$$

where

$$\gamma_\beta := 2 \sin\left(\frac{\beta}{4 - 2\beta/\pi}\right) < \sin(\beta).$$

All convergence bounds (1.1), (1.2), (2.1) are of the form $C \gamma^k$, where we will call C the constant factor, and γ the asymptotic convergence factor. We have drawn in Figure 1 the two different asymptotic convergence factors of (1.1) and of Theorem 2.1. Especially for β close to $\pi/2$ (i.e., the critical case where the origin is close to the field of values), the asymptotic convergence factor of Theorem 2.1 is clearly more interesting. However, the constant factor of (2.1) (which can be shown to be not optimum) slightly deteriorates the sharpness of the new convergence bound, see Figure 2. Notice that bounds of type (2.1) do not capture the range of superlinear convergence of GMRES.

Before entering in the proof of Theorem 2.1, let us briefly recall some well-known facts on the convergence of GMRES. Starting from the observation

$$\frac{\|r_k\|}{\|r_0\|} \leq \min\{\|p(A)\| : p \text{ a polynomial of degree } \leq k, p(0) = 1\},$$

there are many classical GMRES estimates not involving special properties of the right-hand side b of the system, see for instance [14, Chapter 6.11] or [10, Chapter 3].

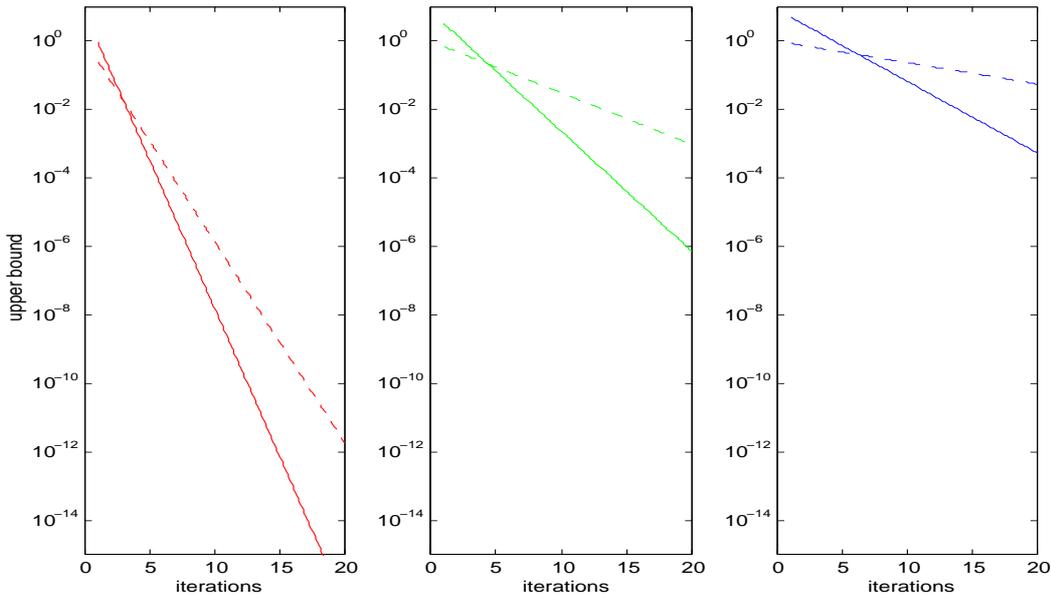


FIG. 2. Upper bounds for the relative residuals of the k th iterate ($k = 1, \dots, 20$) of GMRES for $\beta = \pi/12$, $\beta = \pi/4$, $\beta = \pi/3$ (from the left to the right), the curve corresponding to Elman's bound is dashed, the one of Theorem 2.1 is solid.

Here usually the quantity on the right is estimated in terms of a polynomial extremal problem: for a compact set K , consider the constrained Chebyshev approximation problem

$$E_k(K) := \min\{\|p\|_K : p \text{ a polynomial of degree } \leq k, p(0) = 1\},$$

where by $\|\cdot\|_K$ we denote the maximum norm on K . For instance, for diagonalizable A one immediately obtains the classical bound

$$k \geq 0 : \quad \frac{\|r_k\|}{\|r_0\|} \leq \|V\| \|V^{-1}\| E_k(\sigma(A)) \quad (2.2)$$

in terms of the spectrum $\sigma(A)$ and the matrix of eigenvectors V of A . Other more sophisticated estimates are based for instance on the pseudo-spectrum, but in general the shape of these sets are difficult to predict. A third group of estimates are obtained via the field of values, starting perhaps with a paper of Eiermann [6], see also [10]. These estimates are based on the observation that, given a convex set $K \neq \mathbb{C}$, there exists a constant $C(K) < \infty$ such that for all matrices A and for all rational functions f having no pole in K there holds

$$W(A) \subset K \quad \implies \quad \|f(A)\| \leq C(K) \|f\|_K. \quad (2.3)$$

Recently, Crouzeix and his co-workers [1, 3, 4, 5] gave quite deep results concerning (2.3). For instance, the existence of such a finite constant in (2.3) only depending on the set K was established in [5]. In [1, Corollary 2.3], it was shown that for the optimal constant in (2.3) (also denoted by $C(K)$) one has

$$C(K) \leq 2 + \pi + \int_0^{2\pi} \frac{|\rho'(t)|}{\rho(t)} dt, \quad (2.4)$$

where $[0, 2\pi] \ni t \mapsto z_0 + \rho(t)e^{it} \in \partial K$, $\rho(t) > 0$, is any polar parametrization of the boundary of K for some z_0 in the interior of K (the case of a segment K is trivial, here $aI + bA$ is hermitian for some $a, b \in \mathbb{C}$ and thus $C(K) = 1$). The authors also give improved estimates for particular K , e.g., for a sector [4]

$$C(S_\alpha) \leq 2 + 2/\sqrt{3}, \quad S_\alpha = \{z \in \mathbb{C} : 0 \leq \arg(z) \leq \alpha\}, \quad 0 \leq \alpha \leq \pi. \quad (2.5)$$

In some recent manuscript [3], Crouzeix showed that

$$C(K) \leq 33.75 \quad (2.6)$$

for any convex compact set K , independently of its shape. It is a conjecture of Crouzeix that $C(K)$ in (2.3) can be replaced by the number 2.

Let us return to the proof of Theorem 2.1. By possibly multiplying A with some complex number of modulus 1, we may suppose without loss of generality that the element of $W(A)$ closest to 0 is real positive, and thus

$$W(A) \subset \{z : \operatorname{Re}(z) \geq \|A\| \cos(\beta)\},$$

with β as in (1.2). Define K_β to be the (convex) intersection between the closed unit disk and the half plane $\{\operatorname{Re}(z) \geq \cos(\beta)\}$. Since $W(A) \subset \{|z| \leq \|A\|\}$, we see that $W(A) \subset \|A\| K_\beta$. Moreover, by constructing block-diagonal matrices with blocks

$$B(\phi) = \begin{bmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{bmatrix}, \quad 0 \leq \phi \leq \beta,$$

we find unitary matrices $A_n \in \mathbb{R}^{2^n \times 2^n}$ with $W(A_n) \subset W(A_{n+1}) \subset K_\beta$, and the closure of $\bigcup_n W(A_n)$ coinciding with K_β . Hence in general the relation $W(A) \subset \|A\| K_\beta$ cannot be improved without further knowledge on A .

We have the following result for our constrained Chebyshev approximation problem.

LEMMA 2.2. *There holds for any $k \geq 1$ for any $\beta \in (0, \pi/2)$*

$$\gamma_\beta^k < E_k(K_\beta) \leq \min\left\{2 + \gamma_\beta, \frac{2}{1 - \gamma_\beta^{k+1}}\right\} \gamma_\beta^k,$$

with $\gamma_\beta = 2 \sin(\frac{\beta}{4 - 2\beta/\pi})$ as in Theorem 1.

Proof. Let K be some convex compact set containing at least 2 elements, $0 \notin K$, and denote by ϕ the Riemann conformal map mapping from $\mathbb{C} \setminus K$ onto the exterior of the closed unit disk, with $\phi(\infty) = \infty$. In the first part of the proof we claim that

$$k \geq 1 : \quad \gamma^k \leq E_k(K) \leq \min\left\{2 + \gamma, \frac{2}{1 - \gamma^{k+1}}\right\} \gamma^k, \quad \gamma := 1/|\phi(0)|. \quad (2.7)$$

The inequality $\gamma^k \leq E_k(K)$ follows by applying the maximum principle to the function p/ϕ^k for an arbitrary polynomial p of degree $\leq k$, see also the classical Bernstein-Walsh inequality [12]. Notice also that, again by the maximum principle, we have $\gamma^k = E_k(K)$ for some $k > 0$ if and only if ϕ^k is a polynomial of degree k or, in other words, if K is a lemniscate, which is certainly not true for our set K_β .

For the other inequality of (2.7) we need a good candidate p of degree k . Consider the Faber polynomial F_k being the polynomial part of the Laurent expansion of ϕ^k at ∞ , see, e.g., [15, 16]. It is shown in [11, Theorem 2] for general convex sets K that

$$\delta_k := \|F_k - \phi^k\|_{\partial K} \leq 1. \quad (2.8)$$

From the maximum principle applied to $\phi F_k - \phi^{k+1}$ we know that $|\phi(0)| |F_k(0) - \phi(0)^k| < \|\phi F_k - \phi^{k+1}\|_{\partial K} \leq \delta_k$, and hence for the polynomial depending on some parameter $v \in [0, 1]$

$$p_v(z) = F_k(z) + v(\phi(0)^k - F_k(0))$$

we obtain $|p_v(0)| \geq |\phi(0)^k - (1-v)\delta_k/|\phi(0)|$, and

$$\|p_v\|_K = \|p_v\|_{\partial K} \leq \|\phi^k\|_{\partial K} + \|\phi^k - F_k\|_{\partial K} + v|\phi(0)^k - F_k(0)| \leq 1 + \delta_k + v\delta_k/|\phi(0)|,$$

and thus

$$E_k(K_\beta) \leq \min_{v \in [0,1]} \frac{\|p_v\|_K}{|p_v(0)|} \leq \min_{v \in [0,1]} \gamma^k \frac{1 + \delta_k(1 + v\gamma)}{1 - (1-v)\delta_k\gamma^{k+1}},$$

leading to the other inequality of (2.7).

Now the assertion of the Lemma follows from (2.7) once we have shown that the Riemann conformal map ϕ for $K = K_\beta$ satisfies $1/|\phi(0)| = \gamma_\beta$. Indeed, this map can be explicitly constructed as a composition $\phi = T_3 \circ T_2 \circ T_1$, with

$$T_1(z) = \frac{z - e^{i\beta}}{z - e^{-i\beta}}, \quad T_2(z) = (e^{i(\pi-\beta)}z)^{\pi/(2\pi-\beta)}, \quad T_3(z) = \frac{z - \overline{T_2(1)}}{z - T_2(1)},$$

where T_1 maps the complement of K_β conformally onto $\{z \in \mathbb{C} : -\pi + \beta < \arg(z) < \pi\}$, T_2 maps $\{z \in \mathbb{C} : -\pi + \beta < \arg(z) < \pi\}$ conformally onto the upper half plane $\{z \in \mathbb{C} : 0 < \arg(z) < \pi\}$, and finally T_3 maps the upper half plane conformally onto the complement of the exterior of the closed unit disk. Finally, notice that

$$\frac{1}{|\phi(0)|} = \left| \frac{\exp(i\pi \frac{\pi+\beta}{2\pi-\beta}) - \exp(i\pi \frac{\pi-\beta}{2\pi-\beta})}{\exp(i\pi \frac{\pi+\beta}{2\pi-\beta}) - \exp(-i\pi \frac{\pi-\beta}{2\pi-\beta})} \right| = \frac{\sin(\frac{2\beta}{4-2\beta/\pi})}{\sin(\frac{\pi}{2} + \frac{\beta}{4-2\beta/\pi})} = \gamma_\beta,$$

as required for the assertion of Lemma 2.2. \square

By means of elementary computations one checks that the asymptotic convergence factor $\sin(\beta)$ found by Elman coincides with $E_1(K_\beta)$, which by Lemma 2.2 is larger than our constant γ_β . Thus (2.1) is asymptotically sharper than (1.1), (1.2), compare with Figure 1 and Figure 2.

The second ingredient in our proof of Theorem 2.1 is the following observation.

LEMMA 2.3. *With $\beta \in (0, \pi/2)$ as in (1.2) there holds for any polynomial $p \neq 0$*

$$\|p(A)\| \leq (2 + 2/\sqrt{3}) \|p\|_K, \quad K := \|A\| K_\beta.$$

Proof. Choose $\alpha \in (\beta, \pi/2)$, and consider the linear fractional transformation

$$r(z) = \frac{\|A\| e^{i\alpha} - z}{z - \|A\| e^{-i\alpha}}.$$

Then $f := p \circ r^{-1}$ is a rational function with all poles at $-1 \notin S_\alpha$. Also, observe that $r(K) \subset r(\|A\| K_\alpha) = S_\alpha$. According to the Crouzeix results (2.3) and (2.5), for the claim of Lemma 2.3 it is sufficient to show the relation $W(r(A)) \subset S_\alpha$. For a vector $y \neq 0$, we define $\tilde{y} := (A - \|A\| e^{-i\alpha} I)^{-1} y \neq 0$, and consider

$$\begin{aligned} d &:= \frac{(r(A)y, y)}{(\tilde{y}, \tilde{y})} = \frac{((A - \|A\| e^{-i\alpha} I)^*(\|A\| e^{i\alpha} I - A)\tilde{y}, \tilde{y})}{(\tilde{y}, \tilde{y})} \\ &= -\|A\|^2 e^{2i\alpha} - \frac{\|A\tilde{y}\|^2}{\|\tilde{y}\|^2} + 2\|A\| e^{i\alpha} \operatorname{Re}\left(\frac{(A\tilde{y}, \tilde{y})}{(\tilde{y}, \tilde{y})}\right). \end{aligned}$$

Thus $\text{Im}(d) \geq 2 \|A\|^2 \sin(\alpha) [-\cos(\alpha) + \cos(\beta)] > 0$, and $\text{Im}(e^{-i\alpha}d) = \sin(\alpha) [-\|A\|^2 + \|A\tilde{y}\|^2/\|\tilde{y}\|^2] \leq 0$, implying that $W(r(A)) \subset S_\alpha$. \square

Since the quantity $E_k(K)$ is invariant under a scaling of the set K , we obtain from Lemma 2.3

$$\begin{aligned} & \min\{\|p(A)\| : p \text{ a polynomial of degree } \leq k, p(0) = 1\} \\ & \leq (2 + 2/\sqrt{3}) E_k(\|A\| K_\beta) = (2 + 2/\sqrt{3}) E_k(K_\beta), \end{aligned}$$

and Lemma 2.2 allows us to conclude the proof of Theorem 2.1.

Since the method of proof of (2.7) does not depend on the particular choice of the shape of the domain including the field of values, we have shown implicitly the following result complementary to Theorem 2.1 (compare with [3, Section 9]).

COROLLARY 2.4. *Let K be some compact convex set not including the origin, and A some matrix with $W(A) \subset \|A\| K$. Then for the k th relative residual, $k \geq 1$, of GMRES we have*

$$\frac{\|r_k\|}{\|r_0\|} \leq [2 + \gamma] C(K) \gamma^k < [2 + \gamma] C(K) E_k(K),$$

where $C(K)$ can be chosen as in (2.4) or in (2.6), and $\gamma = 1/|\phi(0)| < 1$, ϕ denoting the Riemann conformal map mapping from $\overline{\mathbb{C}} \setminus K$ onto the exterior of the unit disk, with $\phi(\infty) = \infty$.

In particular, we get from Corollary 2.4 that the norm of the k th relative residual of GMRES is bounded above by $101.25 \gamma^k$, with $\gamma < 1$ as before.

Note added in proof. After finishing this paper, one of the authors [2] was able to show an improvement of Corollary 2.4: for a convex compact set E and a matrix A with $W(A) \subset E$ it is shown in [2, Theorem 1] that $\|F_n(A)\| \leq 2$, where F_n denotes the n th Faber polynomial corresponding to the set E . As a consequence [2, Theorem 2 and Corollary 3], Corollary 2.4 remains valid after replacing the constant $C(K)$ by 1.

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REFERENCES

- [1] C. Badea, M. Crouzeix, B. Delyon, Convex domains and K-spectral sets. To appear in *Mathematische Zeitschrift* (2005).
- [2] B. Beckermann, Image numérique, GMRES et polynômes de Faber, *C.R. Acad. Sci. Paris, Ser. I* **340** (2005) 855-860.
- [3] M. Crouzeix, Numerical range, holomorphic calculus and applications. Manuscript (2004).
- [4] M. Crouzeix, B. Delyon, Some estimates for analytic functions of strip or sectorial operators, *Arch. Math.* **81** (2003) 553-566.
- [5] B. Delyon, F. Delyon, Generalization of Von Neumann's spectral sets and integral representation of operators, *Bull. Soc. Math. France* **1** (1999) 25-42.
- [6] M. Eiermann, Fields of Values and Iterative Methods, *Lin. Alg. Applics* **180** (1993) 167-197.
- [7] M. Eiermann, O.G. Ernst, Geometric aspects in the theory of Krylov subspace methods, *Acta Numerica* **10** (2001) 251-312.
- [8] S.C. Eisenstat, H.C. Elman, M.H. Schultz, Variational Iterative Methods for Nonsymmetric Systems of Linear Equations, *SIAM J. Numer. Anal.* **20** (1983) 345-357.
- [9] H.C. Elman, Iterative Methods for Sparse Nonsymmetric Systems of Linear Equations, PhD Thesis, Yale University, Department of Computer Science, 1982.

- [10] A. Greenbaum, *Iterative Methods for Solving Linear Systems*, *Frontiers in Applied Mathematics*, **17**, SIAM (1997).
- [11] T. Kövari & Ch. Pommerenke, On Faber Polynomials and Faber Expansions, *Math. Zeitschrift* **99** (1967) 193–206.
- [12] E.M. Nikishin & V.N. Sorokin, *Rational Approximations and Orthogonality*, Nauka, Moscow, 1988. Engl. transl. in *Translations of Mathematical Monographs* **92**, Am. Math. Soc., Providence, R.I. (1991).
- [13] Y. Saad & M.H. Schultz, GMRES: A generalized minimal residual algorithm for solving non-symmetric linear systems, *SIAM J. Sci. Comput.* **7** (1986) 856-869.
- [14] Y. Saad, *Iterative methods for sparse linear systems*, PWS Publishing, Boston, MA, 1996.
- [15] V.I. Smirnov & N.A. Lebedev, *Functions of a Complex Variable*, M.I.T. Press, Cambridge, Massachusetts (1968).
- [16] P.K. Suetin, Polynomials Orthogonal over a Region and Bieberbach polynomials, *Proc. of the Steklov Inst. of Maths.* **100** (1971) 1–89.