A MIN-MAX PROBLEM ON ROOTS OF UNITY

JÖRG LIESEN[†] AND PETR TICHÝ[†]

Abstract. The worst-case residual norms of the GMRES method for linear algebraic systems [3] can, in case of a normal matrix, be characterized by a min-max approximation problem on the matrix eigenvalues. In [2] we derive a lower bound on this min-max value (worst-case residual norm) for each step of the GMRES iteration. We conjecture that the lower bound and the min-max value agree up to a factor of $4/\pi$, i.e. that the lower bound multiplied by $4/\pi$ represents an upper bound. In this paper we prove for several different iteration steps that our conjecture is true for a special set of eigenvalues, namely the roots of unity. This case is of interest, since numerical experiments indicate that the ratio of the min-max value and our lower bound is maximal when the eigenvalues are the roots of unity.

Key words. min-max problem, polynomial approximation on discrete set, best approximation, best constants, GMRES, evaluation of convergence

AMS subject classifications. 41A10, 41A44, 41A50, 65F10

1. Introduction.

In our paper [2] we study the worst-case residual norm of the GMRES method [3] for normal matrices. In iteration step $i = 1, \ldots, n-1$, this norm is given by the min-max value

$$M_i^L \equiv \min_{p \in \pi_i} \max_{\lambda_j \in L} |p(\lambda_j)|, \tag{1.1}$$

where

$$L = \{\lambda_1, \ldots, \lambda_n\}$$

denotes the set of the n (distinct) matrix eigenvalues, and π_i denotes the set of polynomials of degree at most i and with value one at the origin.

For $i = n-1$, the min-max value M_i^L can be determined as described in [2, Theorem 3.1],

$$M_{n-1}^L = \left(\sum_{j=1}^{n} |l_j(0)| \right)^{-1}, \tag{1.2}$$

where $l_j(\lambda)$, $j = 1, \ldots, n$, denotes the jth Lagrange polynomial,

$$l_j(\lambda) \equiv \prod_{\substack{k=1 \\ k \neq j}}^{n} \frac{\lambda_k - \lambda}{\lambda_k - \lambda_j}. \tag{1.3}$$

In particular,

$$M_{n-1}^L = \left(\sum_{j=1}^{n} \prod_{\substack{k=1 \\ k \neq j}}^{n} \frac{|\lambda_k|}{|\lambda_k - \lambda_j|} \right)^{-1}. \tag{1.4}$$

[†]Institute of Mathematics, Technical University of Berlin, Straße des 17. Juni 136, 10623 Berlin, Germany (`liesen@math.tu-berlin.de`, `tichy@math.tu-berlin.de`). The work was supported by the Emmy Noether-Programm of the Deutsche Forschungsgemeinschaft.

For $i < n-1$, there exist neither a general solution for the min-max problem, nor an explicit formula for the value M_i^L in terms of the eigenvalues of A. Still, we may try to estimate M_i^L (from below, since it already describes a "worst" case) by an easily comprehensible expression involving the eigenvalues. It is clear that the inequality

$$M_i^L \;\geq\; M_i^S \tag{1.5}$$

holds for every subset S of L. When the subset S contains exactly $i+1$ points, we can express the value M_i^S as

$$M_i^S \;=\; \left(\sum_{j=1}^{i+1} |l_j^S(0)| \right)^{-1} \tag{1.6}$$

(see also [2]), where $l_j^S(\lambda)$, for $j = 1, \ldots, i+1$, denotes the jth Lagrange polynomial corresponding to the elements of the set S. Based on (1.5) and (1.6), we receive the following lower bound for M_i^L,

$$B_i^L \;\equiv\; \max_{\substack{S \subseteq L \\ |S| = i+1}} M_i^S \;\leq\; M_i^L\,, \qquad i = 1, \ldots, n-1\,. \tag{1.7}$$

It is natural to ask about the closeness of the lower bound (1.7). Using a classical result from approximation theory, see e.g. [1, Theorem 2.4 and Corollary 2.5], it can be shown that (1.7) is an *equality* if all eigenvalues λ_j, $j = 1, \ldots, n$, are real. But if at least one eigenvalue is non-real, then (1.7) may be a *sharp inequality.* Nevertheless, our numerical experiments with various (complex) eigenvalue distributions in [2, Section 4] indicate that B_i^L is very close to M_i^L. In fact, we conjecture that

$$\boxed{B_i^L \;\leq\; M_i^L \;\leq\; \frac{4}{\pi}\, B_i^L\,, \qquad i = 1, \ldots, n-1\,,} \tag{1.8}$$

holds for *all* sets L containing n distinct complex numbers. (Note that the conjecture is trivial for $i = n-1$; this case is included only for completeness.)

The purpose of this this paper is to discuss the inequality in (1.8) for a special set of eigenvalues, namely the nth roots of unity. We give proofs that in this case the inequality holds for $i = 1, 2, n-3, n-2$. We did not find a proof for all i yet, but we suggest a possible approach for such a proof.

The case of the nth roots of unity seems to be very important for proving our conjecture in general. A variety of numerical experiments we performed indicates that the nth roots of unity represent the "worst" distribution in the sense that the ratio M_i^L/B_i^L tends to be maximal on this set. In other words, we were unable to find a set L containing n distinct complex numbers for which the ratio of the min-max value M_i^L and its lower estimate B_i^L was larger than for the nth roots of unity.

The paper has 9 Sections. In Section 2 we give a precise definition of the problem we intend to study. In Section 3 we give an alternative proof of the result from [4] that $M_{n-1}^L = 1$ (for $L = n$th roots of unity) and derive an important formula that will be used in the following sections. Sections 4–7 give proofs of the inequality in (1.8) for L consisting of the nth roots of unity and the special cases $i = n-2, n-3, 2, 1$ (in this order, one case in each section). In Section 8 we suggest a way for proving this inequality for every i. Finally, numerical experiments supporting our conjecture are given in Section 9.

2. Min-max problem on roots of unity. Consider the complex numbers

$$\lambda_k \;=\; e^{\mathbf{i}\frac{2k\pi}{n}}, \quad k = 1, \ldots, n\,, \tag{2.1}$$

where $\mathbf{i}$ denotes the imaginary unit. These numbers are the well known nth roots of unity, i.e. they are roots of the polynomial

$$z^n - 1\,. \tag{2.2}$$

Denote the set of points (2.1) by L. In [4] it was shown that

$$M_i^L \;=\; 1, \qquad i = 1, \ldots, n-1\,,$$

where M_i^L is defined as in (1.1). In this paper we are interested in the value B_i^L, which represents a lower bound on M_i^L, cf. (1.7). We conjecture that B_i^L is always close to M_i^L (i.e. close to one), and in particular that the inequality

$$\boxed{B_i^L \;=\; \max_{\substack{S\subseteq L\\ |S|=i+1}} \left(\sum_{j=1}^{i+1} \prod_{\substack{k=1\\ k\neq j}}^{i+1} \frac{1}{|\lambda_k^S - \lambda_j^S|} \right)^{-1} \;\geq\; \frac{\pi}{4}} \tag{2.3}$$

holds for every $i < n$. Here λ_k^S denotes the elements of the subset $S \subseteq L$.

To compute the value of B_i^L it is desirable to express the distance between the roots of unity in some convenient way. Note that the vectors determined by the numbers $e^{\mathbf{i}\frac{2j\pi}{n}}$ and $e^{\mathbf{i}\frac{2k\pi}{n}}$ form the angle $|j-k|\frac{2\pi}{n}$. It can be easily shown that

$$|e^{\mathbf{i}\frac{2j\pi}{n}} - e^{\mathbf{i}\frac{2k\pi}{n}}| \;=\; 2\sin\left(\frac{|j-k|\,\pi}{n}\right)\,, \tag{2.4}$$

see Fig. 2.1.

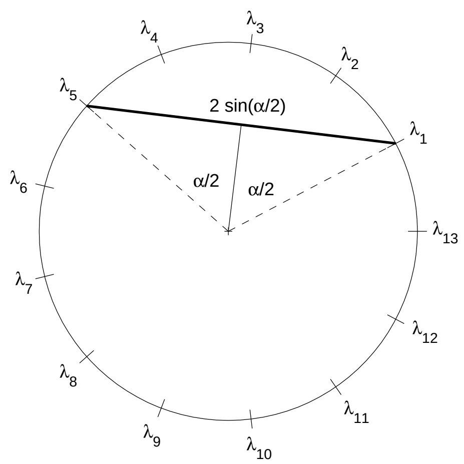

FIG. 2.1. *The distance between 2 roots of unity.*

For every subset $S \subseteq L$, $|S| = i+1$, there are indices $m_1, \ldots, m_{i+1}$, $1 \leq m_j \leq n$, such that

$$S \;=\; \{\lambda_1^S, \ldots, \lambda_{i+1}^S\} \;=\; \{\lambda_{m_1}, \ldots, \lambda_{m_{i+1}}\}.$$

Hence

$$l_j^S(0) \;=\; \left[2^i \prod_{\substack{k=1\\k\neq j}}^{i+1} \sin\left(\frac{|m_j - m_k|\,\pi}{n}\right)\right]^{-1}, \tag{2.5}$$

and B_i^L can be written in the form

$$B_i^L \;=\; 2^i \max_{\substack{S\subseteq L\\|S|=i+1}} \left(\sum_{j=1}^{i+1} \left[\prod_{\substack{k=1\\k\neq j}}^{i+1} \sin\left(\frac{|m_j - m_k|\,\pi}{n}\right)\right]^{-1}\right)^{-1}. \tag{2.6}$$

Using this formula we will in this paper prove the inequality (2.3) for $i = 1, 2, n-3, n-2$, and suggest a way for finding a general proof for all i.

3. Evaluation of M_{n-1}^L. From [4] we know that $M_{n-1}^L = 1$. Here we give an alternative proof of this relation. It can be easily seen by rotation that

$$\prod_{\substack{k=1\\k\neq 1}}^{n} |\lambda_1 - \lambda_k| \;=\; \prod_{\substack{k=1\\k\neq 2}}^{n} |\lambda_2 - \lambda_k| \;=\; \ldots \;=\; \prod_{\substack{k=1\\k\neq n}}^{n} |\lambda_n - \lambda_k|\,,$$

and therefore

$$M_{n-1}^L \;=\; \frac{1}{n} \prod_{\substack{k=1\\k\neq n}}^{n} |\lambda_n - \lambda_k| \;=\; \frac{1}{n} \prod_{k=1}^{n-1} |1 - \lambda_k|\,. \tag{3.1}$$

Since the numbers λ_k, $k = 1, \ldots, n$, are the nth roots of unity, i.e. the roots of the polynomial $z^n - 1$, and since $\lambda_n = 1$,

$$(z-1)(z^{n-1} + \cdots + z + 1) \;=\; z^n - 1 \;=\; \prod_{k=1}^{n} (z - \lambda_k) \;=\; (z-1) \prod_{k=1}^{n-1} (z - \lambda_k)\,.$$

We conclude that

$$\sum_{k=1}^{n-1} z^k + 1 \;=\; \prod_{k=1}^{n-1} (z - \lambda_k)$$

holds for each $z \in \mathbb{C}$. For $z = 1$ we obtain

$$n \;=\; \prod_{k=1}^{n-1} (1 - \lambda_k)\,. \tag{3.2}$$

A comparison with (3.1) shows that $M_{n-1}^L = 1$. Using (2.4), the formula (3.2) can be expressed as

$$n \;=\; 2^{n-1} \prod_{j=1}^{n-1} \sin\left(\frac{j\pi}{n}\right). \tag{3.3}$$

4. Proof of (2.3) for $i = n-2$. Since all subsets S of L, $|S| = n-1$, can be obtained by rotation of the set $L - \{\lambda_n\}$, it holds

$$B_{n-2}^{L} = \max_{\substack{S \subseteq L \\ |S|=n-1}} M_{n-2}^{S} = M_{n-2}^{L-\{\lambda_n\}} = \left(\sum_{k=1}^{n-1} \prod_{\substack{j=1 \\ j\neq k}}^{n-1} \frac{1}{|\lambda_j - \lambda_k|} \right)^{-1} .$$

The formula (2.6) gives

$$M_{n-2}^{L-\{\lambda_n\}} = 2^{n-2} \left(\sum_{k=1}^{n-1} \prod_{\substack{j=1 \\ j\neq k}}^{n-1} \frac{1}{\sin\left(\frac{j\pi}{n}\right)} \right)^{-1} = 2^{n-2} \left(\frac{\sum\limits_{k=1}^{n-1} \sin\left(\frac{k\pi}{n}\right)}{\prod\limits_{j=1}^{n-1} \sin\left(\frac{j\pi}{n}\right)} \right)^{-1} .$$

Using (3.3) we obtain

$$M_{n-2}^{L-\{\lambda_n\}} = \left[\frac{2}{n} \sum_{k=1}^{n-1} \sin\left(\frac{k\pi}{n}\right) \right]^{-1} = \frac{\pi}{2} \left[\frac{\pi}{n} \sum_{k=1}^{n-1} \sin\left(\frac{k\pi}{n}\right) \right]^{-1} . \tag{4.1}$$

Note that the right hand side of (4.1) represents a lower bound for an integral, namely

$$\frac{\pi}{n} \sum_{k=1}^{n-1} \sin\left(\frac{k\pi}{n}\right) < \int_0^\pi \sin(x)\, dx = 2 , \qquad \lim_{n\to\infty} \left[\frac{\pi}{n} \sum_{k=1}^{n-1} \sin\left(\frac{k\pi}{n}\right) \right] = 2 . \tag{4.2}$$

Fig. 4.1 gives an illustration of this approximation.

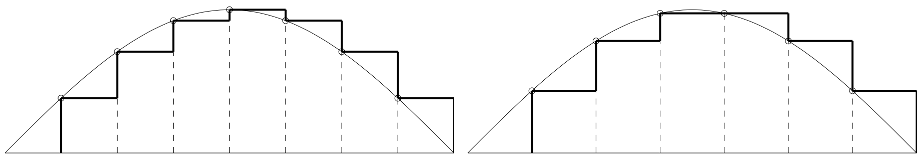

FIG. 4.1. *The approximation of the integral for n even (left part) and n odd (right part).*

From (4.1) and (4.2) it follows that

$$B_{n-2}^{L} = M_{n-2}^{L-\{\lambda_n\}} > \frac{\pi}{4} , \qquad \lim_{n\to\infty} B_{n-2}^{L} = \frac{\pi}{4} .$$

This relation shows that (2.3) is sharp for $i = n-2$. Hence the constant $C = \pi/4$ is the smallest for which (2.3) may possibly hold for every $i = 1, \ldots, n-1$.

5. Proof of (2.3) for $i = n-3$. The situation here is more complicated than for $i = n-2$ since the subsets S of L with $|S| = n-2$ are not equivalent modulo rotation. It suffices, however, to find one subset S of L with $|S| = n-2$, that satisfies $M_{n-3}^{S} \geq \pi/4$. We distinguish two cases, 1. n is even and 2. n is odd.

Case 1: n is even. Consider even n and define $S \equiv L - \{\lambda_1, \lambda_{\frac{n}{2}+1}\}$, see Fig. 5.1. We shall compute the values $l_1^S(0), \ldots, l_{n-2}^S(0)$. Since the set S is symmetric, it holds

$$l_j^S(0) = l_{j+\frac{n-2}{2}}^S(0) , \qquad j = 1, \ldots, \frac{n-2}{2} . \tag{5.1}$$

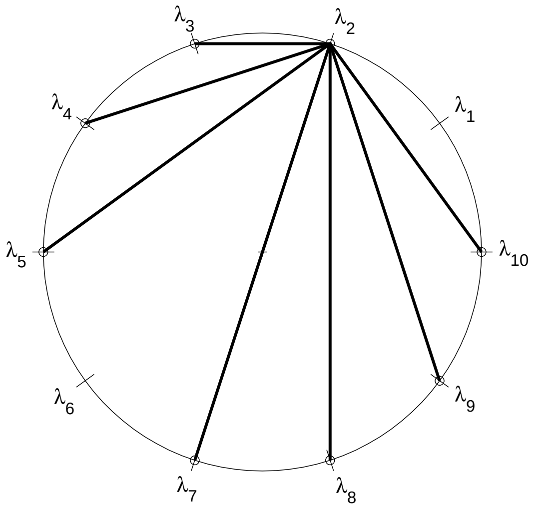

FIG. 5.1. *The choice of $n-2$ points when n is even.*

Next, $(l_j^S(0))^{-1}$ is, according to (2.5), given by

$$(l_j^S(0))^{-1} \;=\; 2^{n-3}\prod_{\substack{k=1\\ k\neq j}}^{n-2}\sin\left(\frac{|m_j-m_k|\,\pi}{n}\right) \;=\; 2^{n-3}\prod_{\substack{k=1\\ k\neq j,\, k\neq \frac{n}{2}+j}}^{n-1}\sin\left(\frac{k\,\pi}{n}\right) \qquad (5.2)$$

for $j=1,\dots,\frac{n-2}{2}$ (cf. Fig. 5.1 for $l_1^S(0)$). From (1.6), (5.1) and (5.2) we obtain

$$\begin{aligned}
(M_{n-3}^S)^{-1} &= \sum_{j=1}^{n-2}|l_j^S(0)| \;=\; 2\sum_{j=1}^{\frac{n-2}{2}}|l_j^S(0)| \\
&= \frac{2}{2^{n-3}}\sum_{j=1}^{\frac{n-2}{2}}\prod_{\substack{k=1\\ k\neq j,\, k\neq \frac{n}{2}-j}}^{n-1}\frac{1}{\sin\left(\frac{k\,\pi}{n}\right)} \\
&= \frac{\sum\limits_{j=1}^{\frac{n-2}{2}}\sin\left(\frac{j\pi}{n}\right)\sin\left(\frac{\pi}{2}-\frac{j\pi}{n}\right)}{2^{n-4}\prod\limits_{k=1}^{n-1}\sin\left(\frac{k\pi}{n}\right)} \\
&= \frac{8}{n}\sum_{j=1}^{\frac{n-2}{2}}\sin\left(\frac{j\pi}{n}\right)\sin\left(\frac{\pi}{2}-\frac{j\pi}{n}\right).
\end{aligned}$$

Using the formula $\sin(\alpha)\sin(\beta) = \frac{1}{2}\left[\cos(\alpha-\beta) - \cos(\alpha+\beta)\right]$, we receive

$$\begin{aligned}
(M^S_{n-3})^{-1} &= \frac{8}{n}\sum_{j=1}^{\frac{n-2}{2}} \frac{1}{2}\left[\cos\left(-\frac{\pi}{2}+\frac{2j\pi}{n}\right) - \cos\left(\frac{\pi}{2}\right)\right] \\
&= \frac{4}{n}\sum_{j=1}^{\frac{n-2}{2}} \cos\left(\frac{\pi}{2}-\frac{2j\pi}{n}\right) \\
&= \frac{4}{n}\sum_{j=1}^{\frac{n-2}{2}} \sin\left(\frac{2j\pi}{n}\right) \\
&= \frac{4}{\pi}\left[\frac{\pi}{n}\sum_{j=1}^{\frac{n-2}{2}} \sin\left(\frac{2j\pi}{n}\right)\right].
\end{aligned}$$

Again, the last quantity on the right hand side approximates a sine integral from below,

$$\frac{\pi}{n}\sum_{j=1}^{\frac{n-2}{2}} \sin\left(\frac{2j\pi}{n}\right) \;<\; \int_0^{\frac{\pi}{2}} \sin(x)dx \;=\; 1 \quad\Rightarrow\quad B^L_{n-3} \geq M^S_{n-3} > \frac{\pi}{4}.$$

Fig. 5.2 gives an illustration of this approximation.

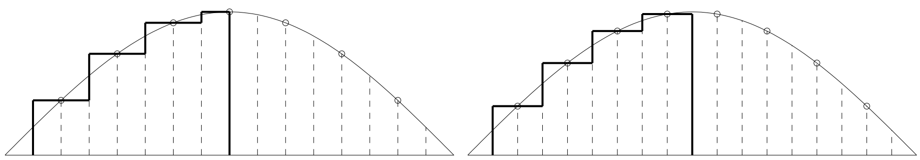

FIG. 5.2. *The approximation of the sine integral when n is even and $n \bmod 4 = 0$ (left part: $n = 16$) and $n \bmod 4 = 2$ (right part: $n = 18$).*

Case 2: n is odd. For odd n we choose $S = L - \{\lambda_1, \lambda_{\frac{n+1}{2}+1}\}$, see Fig. 5.3, and the inequality can be proven in a similar way as for even n,

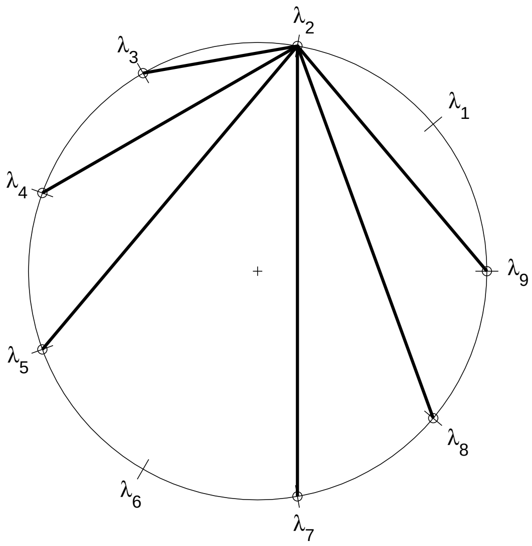

FIG. 5.3. *The choice of $n-2$ points when n is odd.*

$$
\begin{aligned}
(M^{S}_{n-3})^{-1} &= \frac{1}{2^{n-3}} \sum_{j=1}^{\frac{n-1}{2}} \prod_{\substack{k=1 \\ k\neq j,\, k\neq \frac{n+1}{2}-j}}^{n-1} \frac{1}{\sin\left(\frac{k\pi}{n}\right)} + \frac{1}{2^{n-3}} \sum_{j=1}^{\frac{n-1}{2}-1} \prod_{\substack{k=1 \\ k\neq j,\, k\neq \frac{n-1}{2}-j}}^{n-1} \frac{1}{\sin\left(\frac{k\pi}{n}\right)} \\
&= \frac{\sum_{j=1}^{\frac{n-1}{2}} \sin\left(\frac{j\pi}{n}\right)\sin\left(\frac{\pi}{2}-\frac{j\pi}{n}+\frac{\pi}{2n}\right) + \sum_{j=1}^{\frac{n-1}{2}-1} \sin\left(\frac{j\pi}{n}\right)\sin\left(\frac{\pi}{2}-\frac{j\pi}{n}-\frac{\pi}{2n}\right)}{2^{n-3}\prod_{k=1}^{n-1}\sin\left(\frac{k\pi}{n}\right)} \\
&= \frac{4}{n}\sum_{j=1}^{\frac{n-1}{2}} \sin\left(\frac{j\pi}{n}\right)\sin\left(\frac{\pi}{2}-\frac{j\pi}{n}+\frac{\pi}{2n}\right) \\
&\quad + \frac{4}{n}\sum_{j=1}^{\frac{n-1}{2}-1} \sin\left(\frac{j\pi}{n}\right)\sin\left(\frac{\pi}{2}-\frac{j\pi}{n}-\frac{\pi}{2n}\right) \\
&= \frac{2}{n}\sum_{j=1}^{\frac{n-1}{2}} \left[\cos\left(-\frac{\pi}{2}+\frac{2j\pi}{n}-\frac{\pi}{2n}\right) - \cos\left(\frac{\pi}{2}+\frac{\pi}{2n}\right)\right] \\
&\quad + \frac{2}{n}\sum_{j=1}^{\frac{n-1}{2}-1} \left[\cos\left(-\frac{\pi}{2}+\frac{2j\pi}{n}+\frac{\pi}{2n}\right) - \cos\left(\frac{\pi}{2}-\frac{\pi}{2n}\right)\right] \\
&= \frac{2}{n}\sum_{j=1}^{\frac{n-1}{2}} \cos\left(\frac{\pi}{2}-\frac{2j\pi}{n}+\frac{\pi}{2n}\right) + \frac{2}{n}\sum_{j=1}^{\frac{n-1}{2}-1} \cos\left(\frac{\pi}{2}-\frac{2j\pi}{n}-\frac{\pi}{2n}\right) \\
&\quad - \frac{2}{n}\cos\left(\frac{\pi}{2}+\frac{\pi}{2n}\right) \\
&= \frac{2}{n}\left[\sum_{j=1}^{\frac{n-1}{2}} \sin\left(\frac{2j\pi}{n}-\frac{\pi}{2n}\right) + \sum_{j=1}^{\frac{n-1}{2}-1} \sin\left(\frac{2j\pi}{n}+\frac{\pi}{2n}\right) + \sin\left(\frac{\pi}{2n}\right)\right] \\
&= \frac{2}{n}\sum_{j=0}^{n-2} \sin\left(\frac{j\pi}{n}+\frac{\pi}{2n}\right) \\
&= \frac{2}{\pi}\left[\frac{\pi}{n}\sum_{j=1}^{n-1} \sin\left(\frac{j\pi}{n}-\frac{\pi}{2n}\right)\right].
\end{aligned}
$$

Since

$$\frac{\pi}{n}\sum_{j=1}^{n-1}\sin\left(\frac{j\pi}{n}-\frac{\pi}{2n}\right) < \int_0^{\pi}\sin(x)\,dx = 2,$$

see Fig. 5.4, $B^L_{n-3} > \pi/4$ also holds for odd n.

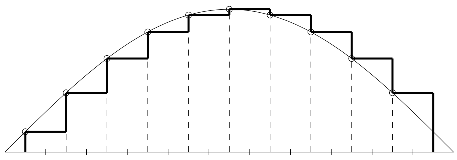

FIG. 5.4. *The approximation of the integral from sinus when n is odd.*

6. Proof of (2.3) for $i=2$ and $n>3$. To show this, it suffices to find a subset $S\subset L$, such that $|S|=3$, and

$$M_2^S \geq \frac{\pi}{4}$$

for every $n>3$. (Note that everything is trivial for $n=3$, and not defined for $i=2$ and $n<3$.) Consider a subset S,

$$S\equiv\{\lambda_{m_1},\lambda_{m_2},\lambda_{m_3}\}\subset L\,,$$

and denote angles between the pairs of vectors $(\lambda_{m_1},\ \lambda_{m_2})$, $(\lambda_{m_2},\ \lambda_{m_3})$, and $(\lambda_{m_3},\ \lambda_{m_1})$ by α_1, α_2, and α_3, respectively (see Fig. 6.1 for an example). Then it can be easily shown that

$$\begin{aligned}(M_2^S)^{-1} = {} & \frac{1}{4\sin\left(\frac{\alpha_1}{2}\right)\sin\left(\frac{\alpha_1+\alpha_2}{2}\right)}+\frac{1}{4\sin\left(\frac{\alpha_2}{2}\right)\sin\left(\frac{\alpha_2+\alpha_3}{2}\right)} \\ & +\frac{1}{4\sin\left(\frac{\alpha_3}{2}\right)\sin\left(\frac{\alpha_3+\alpha_1}{2}\right)}.\end{aligned} \tag{6.1}$$

We are going to choose the three elements of S among the elements of L such that they are "maximally" uniformly distributed. According to the value of n we distinguish 3 situations: 1. $n \bmod 3=0$, 2. $n \bmod 3=1$ and 3. $n \bmod 3=2$.

Case 1: $n \bmod 3=0$. In this case we can choose 3 of the given n points such that they are uniformly distributed, e.g.

$$m_1=1,\quad m_2=\frac{n}{3}+1,\quad m_3=\frac{2n}{3}+1.$$

The halfs of central angles are given by

$$\frac{\alpha_1}{2}=\frac{\alpha_2}{2}=\frac{\alpha_3}{2}=\frac{\pi}{3}$$

and from (3.3) and (6.1) it follows that $1 = M_2^S = B_2^L = M_2^L$.

Case 2: $n \bmod 3=1$. Consider the subset S that contains points from L with indices

$$m_1=1,\quad m_2=\frac{n-1}{3}+1,\quad m_3=\frac{2n+1}{3}+1,$$

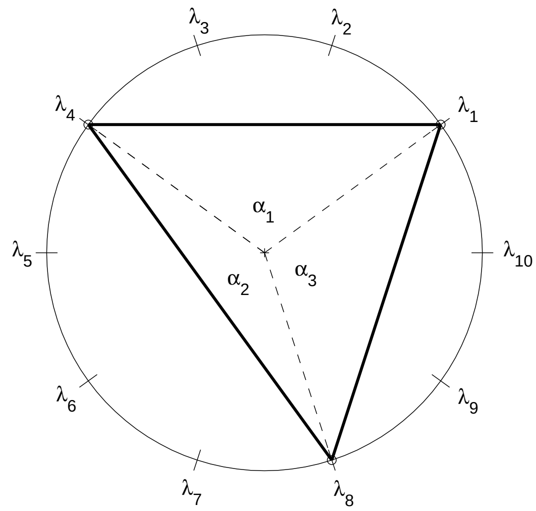

FIG. 6.1. *The choice of 3 points when* $n \bmod 3 = 1$.

see Fig. 6.1 for $n = 10$. The halfs of central angles are given by

$$\frac{\alpha_1}{2} = \frac{\frac{n-1}{3}\pi}{n} = \frac{\pi}{3} - \frac{\pi}{3n}, \qquad \frac{\alpha_2}{2} = \frac{\frac{2n+1}{3}\pi}{n} - \frac{\alpha_1}{2} = \frac{\pi}{3} + \frac{2\pi}{3n}, \qquad \frac{\alpha_3}{2} = \frac{\pi}{3} - \frac{\pi}{3n}$$

and, using (6.1),

$$\begin{aligned}
(M_2^s)^{-1} &= \frac{1}{4\sin\left(\frac{\pi}{3} - \frac{\pi}{3n}\right)\sin\left(\frac{2\pi}{3} + \frac{\pi}{3n}\right)} + \frac{1}{4\sin\left(\frac{\pi}{3} + \frac{2\pi}{3n}\right)\sin\left(\frac{2\pi}{3} + \frac{\pi}{3n}\right)} \\
&\quad + \frac{1}{4\sin\left(\frac{\pi}{3} - \frac{\pi}{3n}\right)\sin\left(\frac{2\pi}{3} - \frac{2\pi}{3n}\right)} \\
&= \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3} + \frac{2\pi}{3n}\right) + 1} + \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3} - \frac{\pi}{3n}\right) - \cos\left(\pi + \frac{\pi}{n}\right)} \\
&\quad + \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3} - \frac{\pi}{3n}\right) - \cos\left(\pi - \frac{\pi}{n}\right)} \\
&= \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3} + \frac{2\pi}{3n}\right) + 1} + \frac{1}{\cos\left(\frac{\pi}{3} - \frac{\pi}{3n}\right) + \cos\left(\frac{\pi}{n}\right)} \,.
\end{aligned} \tag{6.2}$$

Now realize that the first n with $n > 3$, and n mod $3 = 1$, that comes into play is $n = 4$. Therefore, for $n > 3$,

$$\cos\left(\frac{\pi}{3} + \frac{2\pi}{3n}\right) \;\geq\; \cos\left(\frac{\pi}{3} + \frac{2\pi}{12}\right) . \tag{6.3}$$

Next

$$\cos\left(\frac{\pi}{3} - \frac{\pi}{3n}\right) \;\geq\; \cos\left(\frac{\pi}{3}\right) . \tag{6.4}$$

Using (6.2), (6.3) and (6.4), $(M_2^s)^{-1}$ can be bounded as

$$(M_2^S)^{-1} \le \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3}+\frac{2\pi}{12}\right)+1} + \frac{1}{\cos\left(\frac{\pi}{3}\right)+\cos\left(\frac{\pi}{5}\right)} < \frac{4}{\pi}.$$

The last inequality was determined by computation.

Case 3: $n \bmod 3 = 2$. Consider the subset S that contains points from L with indices

$$m_1 = 1, \quad m_2 = \frac{n+1}{3}+1, \quad m_3 = \frac{2n-1}{3}+1,$$

see Fig. 6.2 for $n = 11$. The halfs of the central angles are given by

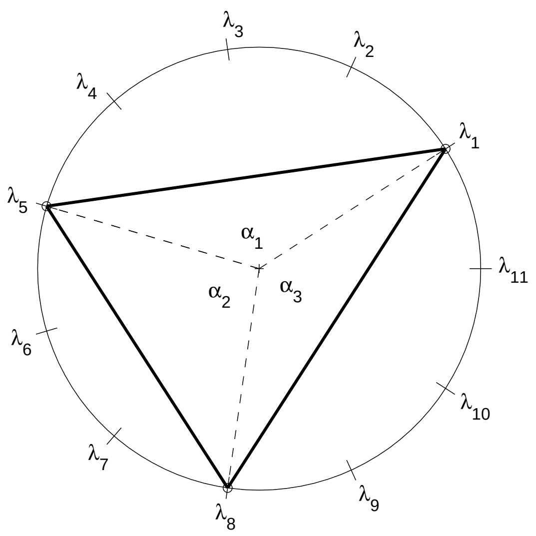

FIG. 6.2. *The choice of 3 points when* $n \bmod 3 = 2$.

$$\frac{\alpha_1}{2} = \frac{\frac{n+1}{3}\pi}{n} = \frac{\pi}{3}+\frac{\pi}{3n}, \qquad \frac{\alpha_2}{2} = \frac{\frac{2n-1}{3}\pi}{n} - \frac{\alpha_1}{2} = \frac{\pi}{3}-\frac{2\pi}{3n}, \qquad \frac{\alpha_3}{2} = \frac{\pi}{3}+\frac{\pi}{3n}$$

and, using (6.1),

$$\begin{aligned}
(M_2^S)^{-1} &= \frac{1}{4\sin\left(\frac{\pi}{3}+\frac{\pi}{n3}\right)\sin\left(\frac{2\pi}{3}-\frac{\pi}{3n}\right)} + \frac{1}{4\sin\left(\frac{\pi}{3}-\frac{2\pi}{n3}\right)\sin\left(\frac{2\pi}{3}-\frac{\pi}{3n}\right)} \\
&\quad + \frac{1}{4\sin\left(\frac{\pi}{3}+\frac{\pi}{n3}\right)\sin\left(\frac{2\pi}{3}+\frac{2\pi}{3n}\right)} \\
&= \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3}-\frac{2\pi}{3n}\right)+1} + \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3}+\frac{\pi}{3n}\right)-\cos\left(\pi-\frac{\pi}{n}\right)} \\
&\quad + \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3}+\frac{\pi}{3n}\right)-\cos\left(\pi+\frac{\pi}{n}\right)} \\
&= \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3}-\frac{2\pi}{3n}\right)+1} + \frac{1}{\cos\left(\frac{\pi}{3}+\frac{\pi}{3n}\right)+\cos\left(\frac{\pi}{n}\right)} \\
&\le \frac{\frac{1}{2}}{\cos\left(\frac{\pi}{3}\right)+1} + \frac{1}{\cos\left(\frac{\pi}{3}+\frac{\pi}{15}\right)+\cos\left(\frac{\pi}{5}\right)} < \frac{4}{\pi}.
\end{aligned}$$

We used the fact that the first n with $n > 3$, and $n \bmod 3 = 2$, that comes into account is $n = 5$. The last inequality was determined by computation.

Summarizing, for all $n > 3$ we have shown that there is a set $S \subset L$ such

$$\frac{\pi}{4} \le M_2^S \le B_2^L .$$

7. Proof of (2.3) for $i = 1$ and $n > 2$. It suffices to find a subset $S \subset L$,

$$S \equiv \{\lambda_{m_1}, \lambda_{m_2}\}$$

such that

$$M_1^S \ge \frac{\pi}{4} .$$

Denote the central angle that form the vectors given by λ_{m_1} and λ_{m_2} as α_1. Then it can be easily shown that

$$M_1^S = \left(2 \frac{1}{2 \sin\left(\frac{\alpha_1}{2}\right)} \right)^{-1} = \sin\left(\frac{\alpha_1}{2}\right) . \tag{7.1}$$

As above we are going to choose the two points such that they are "maximally" uniformly distributed.

If n is even, we can find a set S of two uniformly distributed points such that $M_1^S = 1$, which proves our assertion.

For odd n we choose the indices m_1 and m_2 as

$$m_1 = 1, \quad m_2 = \frac{n+1}{2} + 1,$$

see Fig. 7.1.

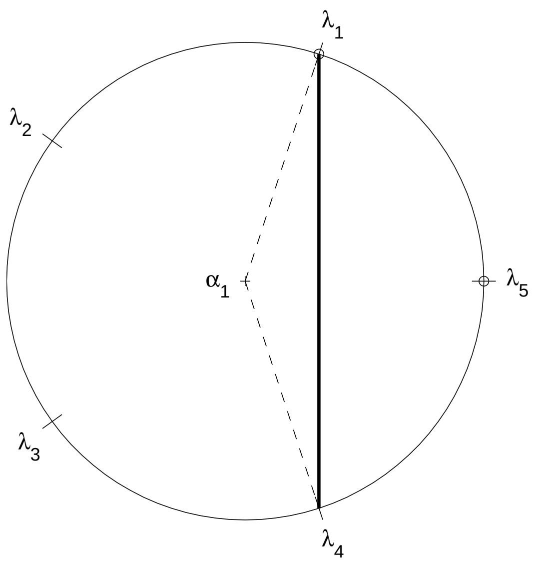

FIG. 7.1. *The choice of 2 points for odd n, $n = 5$.*

Then

$$\frac{\alpha_1}{2} = \frac{\frac{n+1}{2}\pi}{n} = \frac{\pi}{2} + \frac{\pi}{2n}\,,$$

and, using (7.1),

$$M_1^S = \sin\left(\frac{\pi}{2} + \frac{\pi}{2n}\right)\,.$$

Now realize that the first odd n with $n > 2$ that comes into account is $n = 3$. Therefore,

$$M_1^S \;=\; \sin\left(\frac{\pi}{2} + \frac{\pi}{2n}\right) \;\geq\; \sin\left(\frac{\pi}{2} + \frac{\pi}{6}\right) \;=\; \sin\left(\frac{\pi}{3}\right) \;=\; \frac{\sqrt{3}}{2} \;>\; \frac{\pi}{4}\,. \tag{7.2}$$

Summarizing, for all $n > 2$ there is a set S such that

$$\frac{\pi}{4} \;<\; M_1^S \;\leq\; B_1^L.$$

8. General approach for proving (2.3). A general proof of (2.3) for the nth roots of unity and all $i = 1, \ldots, n-1$ might be based on the following approach: Let n and $i < n$ be given. We look for a subset set $S \subseteq L$, $|S| = i+1$ such that

$$M_i^S \;\geq\; \frac{\pi}{4}\,. \tag{8.1}$$

Choose $i+1$ points from L such that they are "maximally" uniformly distributed. One possibility for such a set S is the one that contains points from L with indices

$$m_j \;=\; \mathrm{round}\left(\frac{(j-1)\,n}{i+1}\right) + 1, \qquad j = 1, \ldots, i+1\,. \tag{8.2}$$

For every i one may then try to prove the inequality

$$(M_i^S)^{-1} \;=\; 2^{-i} \sum_{j=1}^{i+1} \left[\prod_{\substack{k=1\\k\neq j}}^{i+1} \sin\left(\frac{|m_j - m_k|\,\pi}{n}\right)\right]^{-1} \;\leq\; \frac{4}{\pi}\,, \tag{8.3}$$

as in previous sections. The numerical experiments in Section 9 clearly demonstrate that the inequality (8.3) holds for the sets S with indices (8.2). Still, it is unclear how to formally describe the proof of (8.3) using this idea.

Note that B_i^L represents a certain functional defined on a subset of the roots of unity. Our idea for a proof then is to find a subset that is "maximally" uniformly distributed to maximize this functional. Inversely, a maximizer of the functional leads to a distribution of points that may be called "maximally" uniformly distributed with respect to the given functional. Similar problems have been studied in analytic geometry, but we do not know an approach from this field that could be applied to our specific problem.

9. Numerical experiments. For a given n and $i < n$, we define S, $|S| = i+1$, as a set of $i+1$ points from L with indices m_j computed according to (8.2). Using (8.3) we compute the value M_i^S and compare it with the constant $\pi/4$.

Fig. 9.1 demonstrates clearly that the value M_i^S (solid line) is always greater than $\pi/4$ (dashed line). When n is a prime number (right part of the Fig. 9.1: $n = 7$, $n = 13$, $n = 73$, $n = 137$), M_i^S decreases monotonically to the value $\pi/4$. In other cases ($n = 8$, $n = 12$, $n = 64$, $n = 133 = 7 \cdot 19$) there always exist $i \geq 1$ such that $n \bmod (i+1) = 0$, i.e. there exist subsets S of L containing exactly the $(i+1)$st roots of unity. In such cases we obtain

$$M_i^S = 1,$$

which can be seen well in left part of the Fig. 9.1. Although $M_i^S = 1$ for some i, the curve of M_i^S has decreasing tendency and approaches $\pi/4$ for i close to n.

Conclusions. Our numerical experiments support our conjecture that

$$M_i^L \;\leq\; \frac{4}{\pi}\, B_i^L\,, \qquad i = 1, \ldots, n-1\,, \tag{9.1}$$

where L contains the nth roots of unity. We proved this inequality for $i = 1, 2, n-3, n-2$ (it is trivial for $i = n-1$). We also showed that the constant $4/\pi$ is the smallest possible one, since the inequality is sharp for $i = n-2$. We believe that the min-max problem on roots of unity is an extremal case for which the ratio of M_i^L and its lower approximation B_i^L tends to be maximal. In other words, we expect (9.1) to hold for *any* set of n distinct complex numbers L.

REFERENCES

[1] R. A. DeVore and G. G. Lorentz, *Constructive approximation*, vol. 303 of Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences], Springer-Verlag, Berlin, 1993.

[2] J. Liesen and P. Tichý, *The worst-case GMRES for normal matrices*, submitted to BIT, (2003).

[3] Y. Saad and M. H. Schultz, *GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM Journal on Scientific and Statistical Computing, 7 (1986), pp. 856–869.

[4] I. Zavorin, D. O'Leary, and H. Elman, *Complete stagnation of GMRES*, Linear Algebra and its Applications, 367 (2003), pp. 165–183.

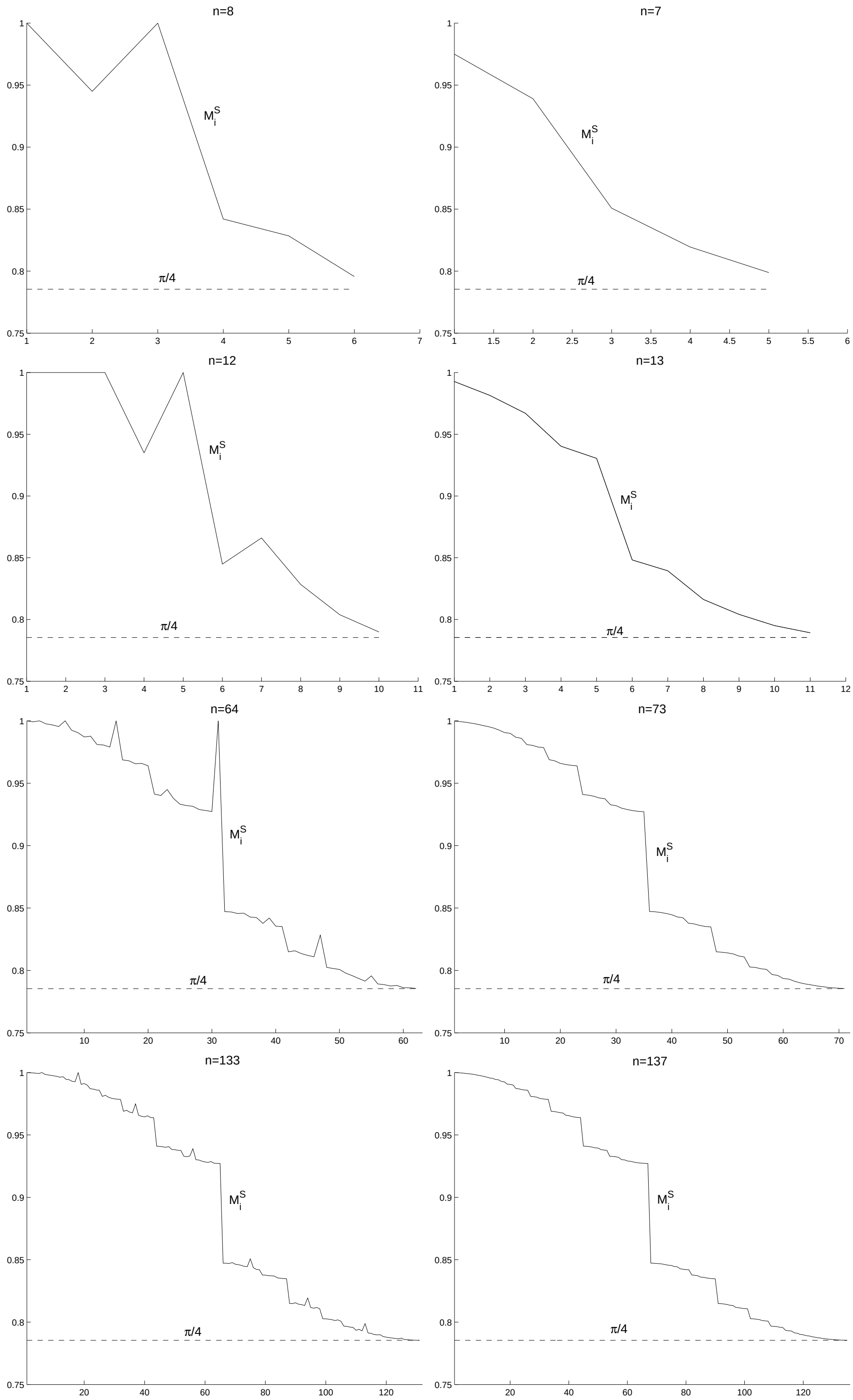

FIG. 9.1. *The value M_i^S (solid line) is always greater than $\pi/4$ (dashed line).*