



Numerical Evaluation and Comparison of Kalantari's Zero Bounds for Complex Polynomials

Matthias Dehmer^{1,2*}, Yury Robertovich Tsoy³

1 Department of Computer Science, Universität der Bundeswehr München, Neubiberg-München, Germany, **2** UMIT - The Health & Life Sciences University, Department for Biomedical Informatics and Mechatronics, Hall in Tyrol, Austria, **3** Image Mining Group, Institut Pasteur Korea, Bundang-gu, Seongnam-si, Gyeonggi-do, Republic of Korea

Abstract

In this paper, we investigate the performance of zero bounds due to Kalantari and Dehmer by using special classes of polynomials. Our findings are evidenced by numerical as well as analytical results.

Citation: Dehmer M, Tsoy YR (2014) Numerical Evaluation and Comparison of Kalantari's Zero Bounds for Complex Polynomials. PLoS ONE 9(10): e110540. doi:10.1371/journal.pone.0110540

Editor: Frank Emmert-Streib, Queen's University Belfast, United Kingdom

Received: July 17, 2014; **Accepted:** September 20, 2014; **Published:** October 28, 2014

Copyright: © 2014 Dehmer, Tsoy. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Data Availability: The authors confirm that all data underlying the findings are fully available without restriction. All relevant data are within the paper.

Funding: The authors have no funding or support to report.

Competing Interests: The authors confirm that co-author Matthias Dehmer is a PLOS ONE Editorial Board member. This does not alter the authors' adherence to PLOS ONE Editorial policies and criteria.

* Email: matthias.dehmer@umit.at

Introduction

The problem of calculating the zeros of polynomials has been at the core of various algorithmic problems in engineering, computer science, mathematics, and mathematical chemistry [1–5]. One the one hand, determining all zeros of a complex polynomial explicitly has been crucial for practical problems [6–7]. One the other hand, estimations (bounds) for the moduli of real and complex zeros have been important for many reasons. For example, sharp zero bounds can serve as starting values for numerical procedures to calculate the zeros explicitly as already mentioned above. Also, zero bounds have been proven useful when estimating eigenvalues of matrices [8,9].

We emphasize that numerous papers and books have been contributed dealing with the problem of locating the zeros of complex polynomials, see, e.g., [1–5,10,11]. Many papers thereof discuss the problem of determining disks in the complex plane where all zeros of a complex polynomial are situated. In view of the vast amount of existing zero bounds, their optimality has only been little investigated. In fact, many of the bounds which have been used extensively in practice do not give the precise annulus containing all zeros of a given polynomial. Also, sharpness results do not exist for all bounds which are practically to use.

In this paper, we deal with the problem of evaluating the quality of zero bounds numerically. A successor of this paper is [12]. In [12], we have put the emphasis on evaluating the quality of known bounds such as the ones due to Joyal, Mohammad, Kojima and Kalantari, see [12–16]. Another paper dealing with evaluating the quality of zero bounds numerically is due to McNamee and Olhovskiy [17] who also evaluated classical and Kalantari's bounds on a set of polynomials with random real or complex roots. More precisely, they implemented 45 zero bounds for estimating the zeros with maximal modulus. These bounds have been evaluated on 1200 polynomials with random real or complex roots [17].

The main contribution of this paper is as follows: We focus on evaluating zero bounds developed by Kalantari [16] and Dehmer [1,18] solely. In [17], it was claimed that some of the Kalantari's

bounds are optimal on the mentioned set of polynomials. We show that some of the proposed bounds outperform Kalantari's bounds on special classes of polynomials. That proves it can be worthwhile to consider special classes of polynomials and special bounds which have been developed to operate on these classes. Examples for such bounds can be found in [18]. Also, we derive some analytical conditions to compare bounds due to Dehmer and Kalantari by means of inequalities, see, section 'Numerical Results and Interpretation'.

Methods

In the following, we state the zero bounds for locating the zeros of complex polynomials as theorems we will explore in this paper. The numerical results will be presented in the section 'Results'.

Kalantari and Dehmer Bounds

Theorem 1 (Kalantari [16]). Let $m \geq 2$ and let $r_m \in [\frac{1}{2}, 1)$ be the positive root of the polynomial

$$q(t) := t^{m-1} + t - 1. \tag{1}$$

For $m = 2$ and $r_2 = \frac{1}{2}$, all zeros of the complex polynomial

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0, \quad a_n a_{n-1} \neq 0,$$

lie in the closed disk

$$K \left(0, 2 \cdot \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} \right). \tag{2}$$

Theorem 2 (Kalantari [16]). Let $m \geq 2$ and let $r_m \in [\frac{1}{2}, 1)$ be the positive root of the polynomial

$$q(t) := t^{m-1} + t - 1.$$

For $m=3$ and $r_3 = \frac{2}{\sqrt{5}+1}$, all zeros of the complex polynomial

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0, \quad a_n a_{n-1} \neq 0,$$

lie in the closed disk

$$K\left(0, \frac{\sqrt{5}+1}{2} \cdot \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1} a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} \right), \quad (3)$$

$$a_{-1} := 0.$$

Theorem 3 (Dehmer [18]). Let

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0, \quad a_n a_{n-1} \neq 0,$$

be a complex polynomial. All zeros of $f(z)$ lie in the closed disk

$$K\left(0, \frac{1+\phi_2}{2} + \frac{\sqrt{(\phi_2-1)^2 + 4M_1}}{2}\right), \quad (4)$$

where

$$\phi_2 := \left| \frac{a_{n-1}}{a_n} \right| \quad \text{and} \quad M_2 := \max_{0 \leq j \leq n-2} \left| \frac{a_j}{a_n} \right|. \quad (5)$$

The next theorem gives a bound for polynomials with restrictions on the coefficients. Dehmer [1] has shown that such bounds can be more precise and often lead to better results when locating the zeros of polynomials. See also Table 3.

Theorem 4 (Dehmer [18]). Let

$$M_3 := \max_{2 \leq j \leq n} \left| \frac{a_{n-1} a_{n-j} - a_n a_{n-j-1}}{a_n^2} \right|, \quad a_{-1} := 0, \quad (6)$$

and

$$\phi_1 := \frac{|a_{n-1}^2 - a_n a_{n-2}|}{|a_n|^2}. \quad (7)$$

In addition, let

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0, \quad a_n a_{n-1} \neq 0,$$

be a complex polynomial. All zeros of $f(z)$ lie in the closed disk $K(0, \delta)$ where $\delta > 1$ is the largest positive root of the equation

$$z^3 - z^2 - (M_3 + \phi_1)z + \phi_1 = 0. \quad (8)$$

Moreover,

$$1 < \delta < 1 + \sqrt{M_3 + \phi_1}. \quad (9)$$

Theorem 5 (Dehmer [18]). Let

$$f(z) = z^n - a_1 z + a_0, \quad a_1 a_0 \neq 0, \quad n > 2,$$

be a complex polynomial. All zeros of $f(z)$ lie in $K(0, \max(1, \delta))$, where δ is the unique positive root of the equation

$$z^n - |a_1|z - |a_0| = 0. \quad (10)$$

Theorem 6 (Dehmer [18]). Let $M_4 := \max(|a_1|, |a_0|)$ and let

$$f(z) = z^n - a_1 z + a_0, \quad a_1 a_0 \neq 0, \quad n > 2,$$

be a polynomial with arbitrary coefficients. All zeros of $f(z)$ lie in $K(0, \max(1, \delta))$, where δ is the unique positive root of the equation

$$z^n - M_4 z - M_4 = 0. \quad (11)$$

In [18], the following upper bound for these lacunary polynomials (see Theorem 6) has been stated without proof. Next, we here prove this result by assuming that the coefficients are positive and real-valued.

Theorem 7. If the polynomial $f(z) = z^n - a_1 z + a_0$, $a_1, a_0 > 0, n > 2$, has two positive zeros, its largest positive zero δ satisfies

$$\delta < \frac{1}{2} + \frac{\sqrt{4a_1 + 1}}{2}. \quad (12)$$

Proof. Since $a_1, a_0 > 0$ we infer by using the Descartes' rule of signs [10] that $f(z)$ has either 2 or no positive zeros. We see that $f(0) = a_0 > 0, f(1) = 1 - a_1 + a_0$ and $\lim_{z \rightarrow +\infty} f(z) = +\infty$. If $f(1) \geq 0$, it follows that $f(z)$ must have two positive zeros. The largest one is denoted as δ and we obtain $\delta > 1$. In order to get an estimation for δ , we consider

$$f(\delta) = \delta^n - a_1 \delta + a_0 = 0. \quad (13)$$

By using the finite geometric series, we obtain

$$\frac{\delta^{n+1} - \delta^n}{\delta - 1} - a_1\delta + a_0 = 0, \tag{14}$$

and

$$\frac{\delta^{n+1} - \delta^n}{\delta - 1} - a_1\delta < 0. \tag{15}$$

This inequality leads to

$$\delta(\delta^n - \delta^{n-1} - a_1\delta + a_1) < 0, \tag{16}$$

and finally to

$$\delta(\delta^{n-1} - \delta^{n-2} - a_1) < -a_1. \tag{17}$$

However, this yields

$$\delta^{n-1} - \delta^{n-2} - a_1 < 0. \tag{18}$$

In order to get an inequality for δ , we set $n=3$. We get

$$\delta^2 - \delta - a_1 < 0. \tag{19}$$

Determining the zeros of the latter function gives

$$\delta_{1,2} = \frac{1}{2} \pm \frac{\sqrt{1+4a_1}}{2}. \tag{20}$$

As

$$\delta_1 = \delta = \frac{1}{2} + \frac{\sqrt{1+4a_1}}{2} > 1, \tag{21}$$

we only consider the largest positive zero of the two. Now we define

$$f_1(\delta) := \delta^{n-1} - \delta^{n-2} - a_1, \tag{22}$$

$$f_2(\delta) := \delta^2 - \delta - a_1. \tag{23}$$

If we can prove that the positive zero of $f_1(\delta)$ does not fall outside the interval $[0, \frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}]$, we obtain Inequality 12. For this, we must prove that f_1 is strictly monotonically increasing in a certain interval.

Applying the Descartes' rule of signs to $f_1(\delta)$ yields that its positive zero is unique. Also, $f_1(0) = f_1(1) = -a_1$ and $\lim_{\delta \rightarrow +\infty} f_1(\delta) = +\infty$. To prove the monotonicity, we consider

$$f'_1(\delta) = (n-1)\delta^{n-2} - (n-2)\delta^{n-3} > 0, \tag{24}$$

that leads to

$$\delta > \frac{n-1}{n-2}. \tag{25}$$

As we here assume $\delta > 1$, we see $f_1(\delta)$ is strictly monotonically increasing for $\delta > 1$. Finally we now prove that

$$0 = f_2\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right) < f_1\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right), \tag{26}$$

hence,

$$f_1\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right) > 0. \tag{27}$$

Together with the monotonicity, that means that the positive zero of $f_1(\delta)$ does not fall outside the $[0, \frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}]$. We start with the inequality

$$\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)^{n-1} - \left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)^{n-2} - a_1 > 0. \tag{28}$$

By performing elementary calculations, we get

$$\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2} > \frac{a_1}{\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)^{n-2}} + 1. \tag{29}$$

From this inequality, we also infer

$$n > \frac{\log\left(\frac{a_1}{\frac{\sqrt{1+4a_1}}{2} - \frac{1}{2}}\right)}{\log\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)} + 2. \tag{30}$$

We finally show that the right hand side of this inequality is less than 4. That means claiming

$$\frac{\log\left(\frac{a_1}{\frac{\sqrt{1+4a_1}}{2} - \frac{1}{2}}\right)}{\log\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)} + 2 < 4, \tag{31}$$

Yields

$$\left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)^3 - \left(\frac{1}{2} + \frac{\sqrt{1+4a_1}}{2}\right)^2 - a_1 > 0. \tag{32}$$

But by performing elementary calculations we find that this inequality is valid for $a_1 > 0$. \square

Results

Data: Classes of Complex Polynomials

As in [12], we define the classes of polynomials used in this study as follows. Note that the abbreviation ‘GD’ in the below stated definitions stands for *Gaussian Distribution*.

Definition 1

$$C_1 := \{f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0 | a_i \in \mathbb{C} \text{ sampled from GD.}\} \tag{33}$$

Definition 2

$$C_2 := \{f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0 | a_i \in \mathbb{C} \text{ uniformly distributed and } |a_i| < 1, i=0, 1, \dots, n.\} \tag{34}$$

Definition 3

$$C_3 := \{f(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_0 | a_i \in \mathbb{C} \text{ sampled from GD and } \frac{|a_i|}{|a_n|} < 1, i=0, 1, \dots, n-1.\} \tag{35}$$

Definition 4

$$C_4 := \{f(z) := f_1(z)f_2(z) | f_1(z) := a_{n_1} z^{n_1} + a_{n_1-1} z^{n_1-1} + \dots + a_1 z + a_0, f_2(z) := b_{n_2} z^{n_2} + b_{n_2-1} z^{n_2-1} + \dots + b_1 z + b_0, a_i, b_i \in \mathbb{C} \text{ sampled from GD and } |a_{n_1}| > |a_i|, i=0, 1, \dots, n_1-1, |b_{n_2}| > |b_i|, i=0, 1, \dots, n_2-1.\} \tag{36}$$

Definition 5

$$C_5 := \{f(z) := f_1(z)f_2(z) | f_1(z) := a_{n_1} z^{n_1} + a_{n_1-1} z^{n_1-1} + \dots + a_1 z + a_0, f_2(z) := b_{n_2} z^{n_2} + b_{n_2-1} z^{n_2-1} + \dots + b_1 z + b_0, a_i \in \mathbb{C}, i=0, 1, \dots, n_1, b_i \in \mathbb{C}, i=0, 1, \dots, n_2, \text{ sampled from GD.}\} \tag{37}$$

Definition 6

$$C_6 := \{f(z) := z^n - a_1 z + a_0, a_1, a_0 \in \mathbb{C}, a_1 a_0 \neq 0 \text{ sampled from GD.}\} \tag{38}$$

These polynomials are called lacunary polynomials [4,5].

Statistical Analysis

In order to perform a statistical analysis, we have generated 1000 complex polynomials for each of the Definitions 1–6 and $n = 2, \dots, 9$. For each polynomial $f(z)$, different bounds have been computed according to the Theorems 1–6. The following entity

has been calculated:

$$\rho_{Th.i} = B_{Th.i} / r_M, \tag{39}$$

where $B_{Th.i}$ - bound value due to Theorem i , $r_M = \max\{|r_i|, i=1, \dots, n\}$ - maximal modulus among the roots $\{r_i\}_{i=1, \dots, n}$ for the polynomial $f(z)$. This entity reflects tightness of the bound, and its properties are:

1. $\rho \geq 1$.
2. If $\rho_{Th.i_1} < \rho_{Th.i_2}$, then the bound of Theorem i_1 is tighter than the bound of Theorem i_2 .

To compare different bounds averaged values of ρ were calculated for a fixed n (Tables 1–6). The figures 1–3 illustrate the averaged bounds with 95% confidence intervals (dashed lines). The confidence intervals have been obtained by using two-sided t -test for 999 degrees of freedom:

$$E[\rho] - t_{5,999} * \sigma_\rho / \sqrt{n} \leq \rho \leq E[\rho] + t_{5,999} * \sigma_\rho / \sqrt{n},$$

where $E[\rho]$ and σ_ρ - are average and standard deviation for ρ ; $t_{5,999}$ - t -distribution value for 95% two-sided critical regions with 999 degrees of freedom.

The pairwise comparison of the averaged values ρ has been performed by using paired t -test. As a result we see that in the majority of cases, the values of ρ for the Theorems 1–6 are statistically different.

Numerical Results and Interpretation

We restrict our analysis to evaluate the performance of the bounds due to Kalantari and Dehmer only, see, section ‘Methods’. In order to do so, we employ the classes of polynomials represented by Definitions 1–6.

General polynomials. We start by interpreting the Tables 1–5 and see that Kalantari’s bound given by Theorem 1 is often worse than the zero bounds due to Dehmer, except the bound given by Theorem 4. Lets consider the polynomials of Definition 1 as this class is quite general. Except Theorem 4, the mean ratios of the bounds due to Dehmer are smaller than the ones by using Kalantari’s bound given by Theorem 1. In particular this holds for Theorem 3 as well. Also, we observe that Theorem 2 due to Kalantari is optimal for $n > 4$ when using the Definitions 1–3; by using the Definitions 4–5, we obtain the optimality for $n > 3$. We emphasize that the results for Definition 6 (lacunary polynomials) will be discussed separately. In summary, this does not mean that no special polynomials exist whose evaluation may give the opposite result.

The analytical comparison of the bounds has been intricate. That means it might be difficult to compare bounds which rely on different concepts (e.g., explicit vs. implicit bounds, see [18]). Zero bounds are explicit if their values represent functions of the polynomial coefficients [18]. In contrast, a zero bound is called implicit if the value of the bound is a positive zero of a concomitant polynomial [18]. For instance, Theorem 1 and Theorem 3 are explicit but the Theorems 4–6 are implicit.

In case of using the explicit zero bounds Theorem 1 and Theorem 3, it is straightforward to derive an analytical expression (condition) to compare the bounds by means of inequalities. If we start with the inequality (i.e., we assume that Theorem 1 is better than Theorem 3),

$$2 \cdot \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} > \frac{1 + \phi_2}{2} + \frac{\sqrt{(\phi_2 - 1)^2 + 4M_1}}{2}, \quad (40)$$

we derive

$$\begin{aligned} \phi_2 \cdot \left(4 - 8 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} \right) &> 4M_1 + 8 \cdot \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} \\ &- 16 \left(\max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} \right)^2. \end{aligned} \quad (41)$$

If $4 - 8 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} > 0$, then we finally get the condition

$$\phi_2 = \left| \frac{a_{n-1}}{a_n} \right| > \frac{M_1 + 2 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} - 4 \cdot \left(\max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} \right)^2}{1 - 2 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}}}. \quad (42)$$

Otherwise, we yield

$$\phi_2 = \left| \frac{a_{n-1}}{a_n} \right| < \frac{M_1 + 2 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} - 4 \cdot \left(\max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} \right)^2}{1 - 2 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}}}, \quad (43)$$

with $4 - 8 \max_{1 \leq k \leq n} \left(\left| \frac{a_{n-k}}{a_n} \right| \right)^{\frac{1}{k}} < 0$. These inequalities can be used to compare Theorem 1 and Theorem 3 by means of inequalities assuming that Theorem 1 is worse than Theorem 3. Such a condition seems to be useful as we see by Tables 1–5 that the mean ratios of Theorem 3 are less than the ones by using Theorem 1.

To get an inequality for the assumption that Kalantari’s bound given by Theorem 2 is better than Dehmer’s bound given by Theorem 3, we start with assuming

$$\frac{\sqrt{5} + 1}{2} \cdot \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} < \frac{1 + \phi_2}{2} + \frac{\sqrt{(\phi_2 - 1)^2 + 4M_1}}{2} \quad (44)$$

We yield

$$\begin{aligned} \phi_2 \cdot \left(4 - 2 \cdot (\sqrt{5} + 1) \cdot \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} \right) \\ < 4M_1 + 2 \cdot (\sqrt{5} + 1) \cdot \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} \\ - (\sqrt{5} + 1)^2 \cdot \left(\max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} \right)^2. \end{aligned} \quad (45)$$

If $4 - 2 \cdot (\sqrt{5} + 1) \cdot \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} > 0$, we obtain

$$\phi_2 = \left| \frac{a_{n-1}}{a_n} \right| < \frac{4M_1 + 2 \cdot (\sqrt{5} + 1) \cdot Y - (\sqrt{5} + 1)^2 \cdot Y^2}{4 - 2 \cdot (\sqrt{5} + 1) Y}, \quad (46)$$

with

$$Y := \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}}. \quad (47)$$

Otherwise, we infer

$$\phi_2 = \left| \frac{a_{n-1}}{a_n} \right| > \frac{4M_1 + 2 \cdot (\sqrt{5} + 1) \cdot Y - (\sqrt{5} + 1)^2 \cdot Y^2}{4 - 2 \cdot (\sqrt{5} + 1) Y}, \quad (48)$$

with

$$4 - 2 \cdot (\sqrt{5} + 1) \cdot \max_{2 \leq k \leq n+1} \left(\left| \frac{a_{n-1}a_{n-k+1} - a_n a_{n-k}}{a_n^2} \right| \right)^{\frac{1}{k}} < 0.$$

We note that all these inequalities can be evaluated explicitly and, hence, the corresponding conditions (inequalities) may be useful in practice.

Lacunary polynomials. The results of the evaluation for lacunary polynomials (see Definition 6) can be seen in Table 6. Dehmer’s bounds given by Theorem 5 and Theorem 6 which have been designed for lacunary polynomials outperform both Kalantari bounds. For example, if we evaluate Theorem 1 and Theorem 2 for the polynomials of Definition 6), we obtain

$$B_{Th.1} := 2 \cdot \max \left(|a_1|^{\frac{1}{|n-1|}}, |a_0|^{\frac{1}{|h|}} \right), \quad (49)$$

and

$$B_{Th.2} := \frac{\sqrt{5} + 1}{2} \cdot \max \left(|a_1|^{\frac{1}{|n-1|}}, |a_0|^{\frac{1}{|h|}} \right). \quad (50)$$

Note that $a_n = 1, a_{n-k} = 0, 1 \leq k \leq n - 2$. So, we see that these bounds differ by a constant factor only. The bound of Theorem 5 becomes to

$$B_{Th.5} := \max(1, \delta), \delta > 1. \quad (51)$$

According to Theorem 7, an upper bound for δ is $\delta < \frac{1}{2} + \frac{\sqrt{4a_1 + 1}}{2}$ if $a_0, a_1 > 0$. Note that this bound does not depend on a_0 . If $a_1 < 1$, we infer $\delta < 1.618034$. We observe that we always obtain $B_{Th.1} > 2$ if $|a_1| > 1$ or $|a_0| > 1$. When considering Theorem 2, we always get $B_{Th.2} > 1.618034$ if $|a_1| > 1$ or $|a_0| > 1$. Even if $|a_0|, |a_1| < 1$, but the degree of the polynomials tends to be very large, the bounds of Theorem 1 and Theorem 2 tend to 2 and 1.618034, respectively. In summary, we see that the bound for lacunary polynomials due to Dehmer (see Theorem 6) gives often tighter bounds; in particular when $a_1 < 1$. Similar arguments can be applied when considering Theorem 6.

Table 1. Ratios for the polynomials by using Definition 1; $2 \leq n \leq 9$.

	2	3	4	5	6	7	8	9
Kalantari, Th. (1)	1.740618	1.674687	1.640986	1.615829	1.622275	1.62177	1.615899	1.625303
Kalantari, Th. (2)	1.444768	1.39455	1.36902	1.352937	1.354811	1.353599	1.349038	1.354005
Dehmer, Th. (3)	1.500152	1.436359	1.420059	1.411527	1.42618	1.432393	1.445271	1.45789
Dehmer, Th. (4)	1.449222	1.566359	1.634031	1.673176	1.732903	1.770081	1.807097	1.831334

doi:10.1371/journal.pone.0110540.t001

Table 2. Ratios for the polynomials by using Definition 2; $2 \leq n \leq 9$.

	2	3	4	5	6	7	8	9
Kalantari, Th. (1)	1.704931	1.625397	1.582924	1.572831	1.554937	1.556792	1.553397	1.566236
Kalantari, Th. (2)	1.429949	1.37537	1.357003	1.342865	1.340357	1.335035	1.330336	1.33636
Dehmer, Th. (3)	1.483377	1.432982	1.398882	1.39568	1.381683	1.390759	1.400006	1.413897
Dehmer, Th. (4)	1.369496	1.483964	1.517359	1.548124	1.551111	1.563088	1.596057	1.609

doi:10.1371/journal.pone.0110540.t002

Table 3. Ratios for the polynomials by using Definition 3; $2 \leq n \leq 9$.

	2	3	4	5	6	7	8	9
Kalantari, Th. (1)	1.739731	1.676344	1.633205	1.613733	1.618263	1.616748	1.623021	1.620896
Kalantari, Th. (2)	1.44096	1.392649	1.365094	1.348481	1.351714	1.354525	1.350528	1.351485
Dehmer, Th. (3)	1.627128	1.463874	1.424159	1.411194	1.418361	1.425269	1.441339	1.446148
Dehmer, Th. (4)	1.394486	1.495732	1.571549	1.630066	1.665533	1.696626	1.739386	1.777438

doi:10.1371/journal.pone.0110540.t003

Table 4. Ratios for the polynomials by using Definition 4; $2 \leq n \leq 9$.

	2	3	4	5	6	7	8	9
Kalantari, Th. (1)	1.750715	2.012142	1.837759	1.838256	1.823758	1.820873	1.810426	1.83248
Kalantari, Th. (2)	1.45379	1.572551	1.459837	1.460034	1.454432	1.461645	1.445665	1.457515
Dehmer, Th. (3)	1.609873	1.749532	1.566365	1.562589	1.56622	1.581601	1.58269	1.629539
Dehmer, Th. (4)	1.388793	1.773258	1.722926	1.783884	1.859031	1.979154	2.005109	2.168481

doi:10.1371/journal.pone.0110540.t004

Table 5. Ratios for the polynomials by using Definition 5; $2 \leq n \leq 9$.

	2	3	4	5	6	7	8	9
Kalantari, Th. (1)	1.776129	2.05439	2.000812	1.953628	1.926602	1.908316	1.900434	1.911558
Kalantari, Th. (2)	1.455061	1.592503	1.533934	1.528648	1.508396	1.499813	1.500933	1.500791
Dehmer, Th. (3)	1.519732	1.646073	1.614704	1.609604	1.625371	1.633324	1.677303	1.703949
Dehmer, Th. (4)	1.449809	1.841836	1.90772	2.015138	2.123091	2.222602	2.429363	2.520859

doi:10.1371/journal.pone.0110540.t005

Table 6. Ratios for the polynomials by using Definition 6 (lacunary polynomials); $2 \leq n \leq 9$.

	2	3	4	5	6	7	8	9
Kalantari, Th. (1)	1.779496	1.730165	1.782391	1.822496	1.853114	1.872392	1.889178	1.902321
Kalantari, Th. (2)	1.467053	1.399733	1.441984	1.47443	1.499201	1.514797	1.528377	1.53901
Dehmer, Th. (5)	1.185785	1.03211	1.011294	1.00614	1.004918	1.002322	1.002466	1.001667
Dehmer, Th. (6)	1.429314	1.146872	1.088454	1.064075	1.052297	1.041634	1.037083	1.032652

doi:10.1371/journal.pone.0110540.t006

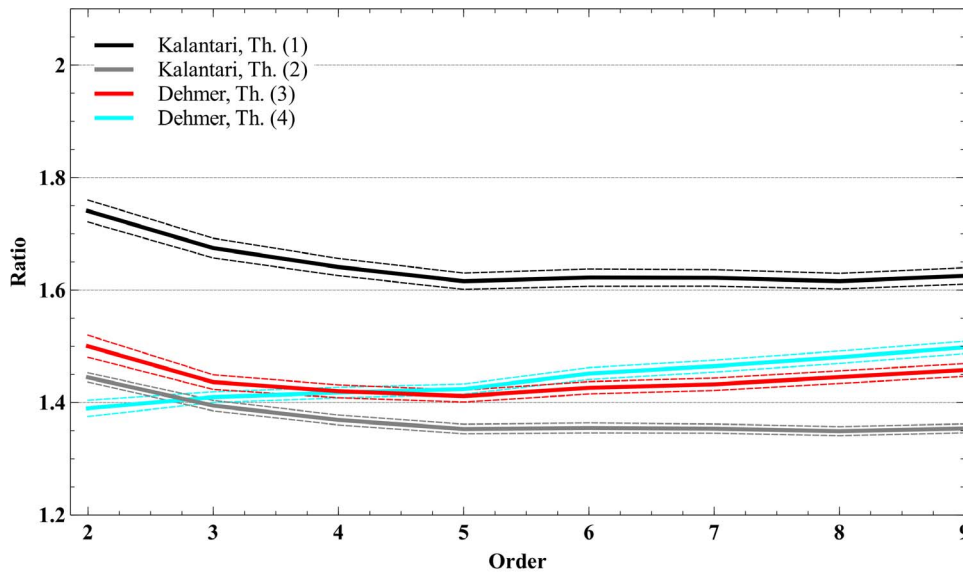


Figure 1. Bound ratios vs. polynomial order for Definition 1.
doi:10.1371/journal.pone.0110540.g001

Summary and Conclusion

In this paper, we explored the performance of zero bounds due to Kalantari and Dehmer. In earlier contributions, it has been claimed [17] that Kalantari’s bounds are often better than classical zero bounds. A similar study has been performed by Dehmer and Tsoy [12] who evaluated classical and more recent zero bounds for complex and real polynomials as well.

The main result of this paper is that some of the bounds due to Dehmer outperform the bounds due to Kalantari for special classes of polynomials. In particular when using lacunary polynomials (i.e., many coefficients equal zero) Dehmer’s bounds showed excellent performance. We have underpinned our discussion to interpret the numerical results by analytical results. In particular, we have proved an upper bound for lacunary

polynomials (see Theorem 7) and obtained conditions for some special cases to check whether one bound is better (or worse) than another by means of inequalities.

Another interesting line of research is to study the zeros of graph polynomials. Some recent related work dealing with applications on graph polynomials are [19–21]. In these contributions, graph polynomials have been used to encode special graphs, e.g., chemical graphs and also exhaustively generated networks. Consequently their zeros could be studied in terms of investigating structural properties of networks, see [22]. Zero bounds may play an important role to estimate the moduli of the underlying polynomials efficiently and to use these quantities for discriminating networks or to explore structural properties such as branching [20,23,24].

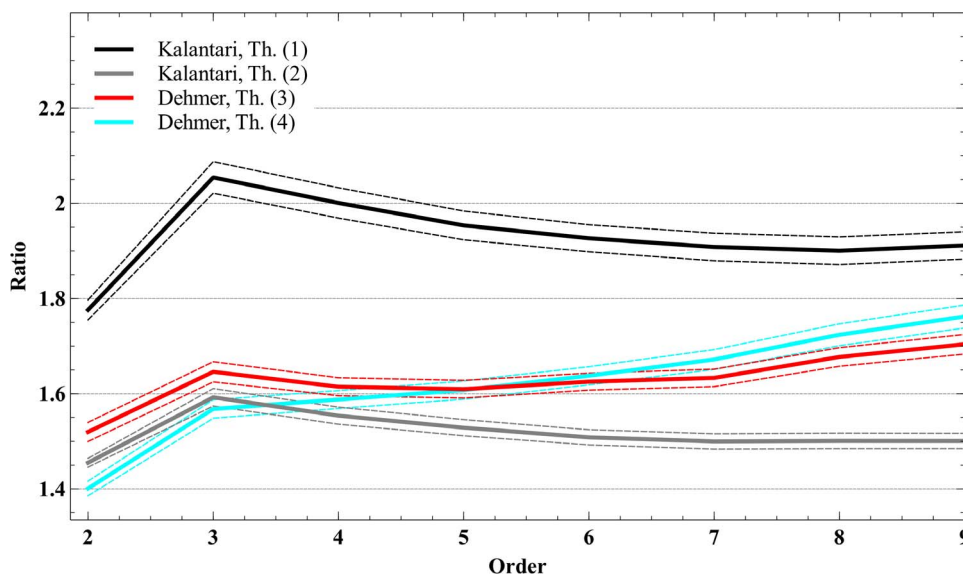


Figure 2. Bound ratios vs. polynomial order for Definition 5.
doi:10.1371/journal.pone.0110540.g002

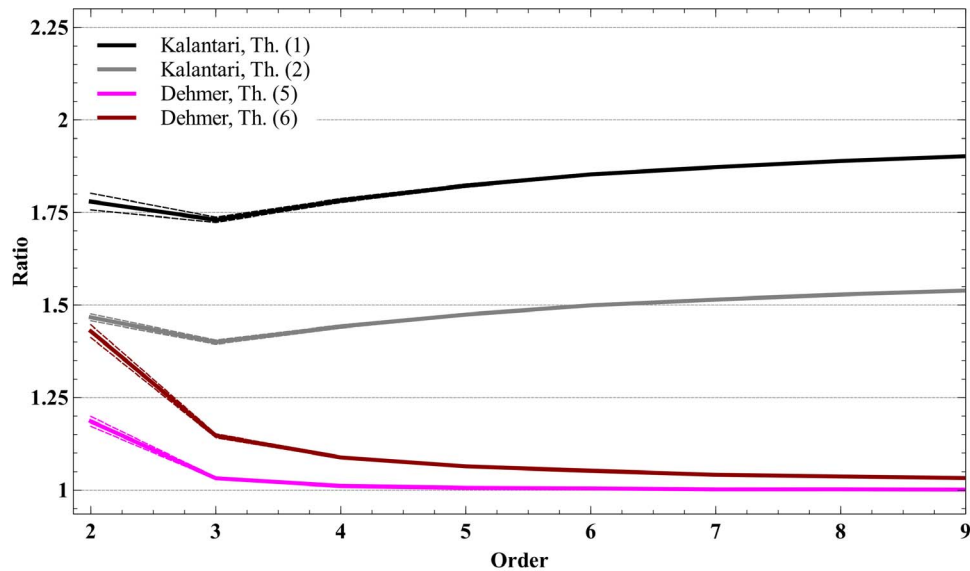


Figure 3. Bound ratios vs. polynomial order for Definition 6.
doi:10.1371/journal.pone.0110540.g003

Author Contributions

Analyzed the data: YT. Wrote the paper: MD YT.

References

- Dehmer M (2006) On the location of zeros of complex polynomials. *Journal of Inequalities in Pure and Applied Mathematics*, Vol 7 (1).
- Heitzinger W, Troch WI, Valentin G (1985) *Praxis nichtlinearer Gleichungen*. Carl Hanser Verlag. München, Wien, Germany, Austria.
- Mignotte M, Stefanescu D (1999) *Polynomials: An Algorithmic Approach*. Discrete Mathematics and Theoretical Computer Science. Springer. Singapore.
- Prasolov VV (2004) *Polynomials*. Springer.
- Rahman QI, Schmeisser G (2002) *Analytic Theory of Polynomials. Critical Points, Zeros and Extremal Properties*. Clarendon Press. Oxford, UK.
- Householder AS (1970) *The Numerical Treatment of a single Nonlinear Equation*. McGraw-Hill. New York, NY, USA.
- Obreschkoff N (1963) *Verteilung und Berechnung der Nullstellen reeller Polynome*. Hochschulbücher für Mathematik, Vol. 55. VEB Deutscher Verlag der Wissenschaften. Berlin, Germany.
- Cvetković DM, Doob M, Sachs H (1980) *Spectra of Graphs. Theory and Application*. Deutscher Verlag der Wissenschaften. Berlin, Germany.
- Sagan H (1989) *Boundary and Eigenvalue Problems in Mathematical Physics*. Dover Publications.
- Marden M (1966) *Geometry of polynomials*. Mathematical Surveys of the American Mathematical Society, Vol. 3. Rhode Island, USA.
- Mohammad QG (1965) On the zeros of polynomials. *American Mathematical Monthly* 72: 35–38.
- Dehmer M, Tsoy YR (2012) The quality of zero bounds for complex polynomials. *PLoS ONE* 7: e39537.
- Joyal A, Labelle G, Rahman QI (1967) On the location of polynomials. *Canadian Mathematical Bulletin* 10: 53–63.
- Kuniyeda M (1916) Note on the roots of algebraic equations. *Tōhoku Math J* 8: 167–173.
- Kojima J (1914) On a theorem of Hadamard and its applications. *Tōhoku Mathematical Journal* 5: 54–60.
- Kalantari B (2005) An infinite family of bounds on zeros of analytic functions and relationship to smale's bound. *Mathematics of Computation* 74: 841–852.
- McNamee JM, Olhovskiy M (2005) A comparison of a priori bounds on (real or complex) roots of polynomials. In: *Proceedings of 17th IMACS World Congress*, Paris, France.
- Dehmer M, Mowshowitz A (2011) Bounds on the moduli of polynomial zeros. *Applied Mathematics and Computation* 218: 4128–4137.
- Chou CP, Witek HA (2014) Zzdecomposer: A graphical toolkit for analyzing the zhang-zhang polynomials of benzenoid structures. *MATCH Communications in Mathematical and in Computer Chemistry* 71: 741–764.
- Dehmer M, Shi Y, Emmert-Streib F (2014) Structural differentiation of graphs using hosoya-based indices. *PLoS ONE* 9: e102459.
- Lou Z, Huang Q, Yiu D (2014) On the characteristic polynomial and the spectrum of a hexagonal system. *MATCH Communications in Mathematical and in Computer Chemistry* 72: 153–164.
- Dehmer M, Ilić A (2012) Location of zeros of wiener and distance polynomials. *PLoS ONE* 7: e28328.
- Bonchev D (1995) Topological order in molecules 1. Molecular branching revisited. *Journal of Molecular Structure: THEOCHEM* 336: 137–156.
- Schutte M, Dehmer M (2013) Large-scale analysis of structural branching measures. *Journal of Mathematical Chemistry* 52: 805–819.