Fast computation of higher order derivatives of a black box function

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Abstract. Keywords: symbolic-numeric computing \cdot root finding \cdot polynomial algorithms \cdot computer algebra.

1 Background and Motivation

Let p(x) be a polynomial with roots $x_1,...,x_d \in \mathbb{C}$ so that

$$p(x) = \sum_{i=0}^{d} p_i x^i = p_d \prod_{i=1}^{d} (x - x_i), \ p_d \neq 0$$
 (1)

The reverse polynomial p_{rev} of p(x) is defined as

$$p_{\text{rev}}(x) := x^d p\left(\frac{1}{x}\right) = \sum_{i=0}^d p_i x^{d-i}, \ p_{\text{rev}}(x) = p_0 \prod_{j=1}^d \left(x - \frac{1}{x_j}\right) \text{ if } p_0 \neq 0.$$
 (2)

1.1 Root-squaring: DLG and FG root-finders

DLG root-squaring iterations (cf. [?]) are defined by

$$p_0(x) = \frac{1}{p_d} p(x), \ p_{k+1}(x^2) = (-1)^d p_k(x) p_k(-x), \ k = 0, 1, \dots \ell$$
 (3)

for a fixed positive integer ℓ .

TODO: description of the DLG root-finder, including the following key expressions:

Let the roots of equation p(x) = 0 satisfy

$$|x_1| \ge |x_2| \ge \dots \ge |x_{d-i+1}| > \max_{j > d-i+1} |x_j|.$$
 (4)

We use the fact

$$\frac{p'_k(0)}{p_k(0)} = \left(\frac{p'_{k-1}(x)}{p_{k-1}(x)}\right)'_{x=0} = \left(\frac{p'(x)}{p(x)}\right)^{(k)}_{x=0}, \ k = 1, 2, \dots$$
 (5)

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that

Notice an immediate extension:

$$\frac{p_{\ell}^{(k)}(0)}{p_{\ell}(0)} = \prod_{g=1}^{k} \left(\frac{p^{(g)}(x)}{p^{(g-1)}(x)}\right)_{x=0}^{(\ell)}, \ k = 1, 2, \dots$$
 (6)

FG iterations fixes a polynomial q(x) and computes

$$q_0(x) = q(x), \ q_{i+1}(x^2) = \dots$$
 (7)

TODO: description of the FG root-finder, including the following root radius assumption

$$|x_1| > |x_2| > \dots > |x_d|.$$
 (8)

The companion paper [] presents the root-finders in more detail.

1.2 DLG iterations for black box polynomials

Given the coefficients of $p_i(x)$ we can reduce the *i*th root-squaring iteration, that is, the computation of the coefficients of $p_{i+1}(x)$, to polynomial multiplication and perform it in $O(d \log(d))$ arithmetic operations. Unless the positive integer ℓ is small, the absolute values of the coefficients of $p_{\ell}(x)$ vary dramatically, and realistically one should either stop because of severe problems of numerical stability or apply the stable algorithm by Gregorio Malajovich and Jorge P. Zubelli [?], which performs a single root-squaring at arithmetic cost of order d^2 .

For a black box polynomial p(x), however, we apply DLG iterations without computing the coefficients, and the algorithm turns out to be quite efficient: for ℓ iterations evaluate p(x) at 2^{ℓ} equally spaced points on a circle and obtain the values of the polynomial $p_{\ell}(x) = \prod \left(x - x_j^{2^{\ell}}\right)$ at these 2^{ℓ} points.

1.3 Estimation of extremal root radii

If we do not know whether assumptions (??) and (??) hold, we can apply the following well-known bounds on the extremal root radii:

$$|x_d| \le d \left| \frac{p(0)}{p'(0)} \right| \text{ and } |x_1| \ge \left| \frac{p'_{\text{rev}}(0)}{d p_{\text{rev}}(0)} \right|. \tag{9}$$

We can deduce these bounds from the well-known expression

$$\frac{p'(x)}{p(x)} = \sum_{i=1}^{d} \frac{1}{x - x_j},\tag{10}$$

which we can obtain by differentiating the equation $p(x) = p_d \prod_{j=1}^d (x - x_j)$. By extending these bounds to the polynomial $p_k(x)$ of Eq. (??) we obtain

$$|x_d|^{2^k} \le d/\left|\left(\frac{p'(x)}{p(x)}\right)_{x=0}^{(k)}\right| \text{ and } |x_1|^{2^k} \ge \frac{1}{d}\left|\left(\frac{p'_{\text{rev}}(x)}{p_{\text{rev}}(x)}\right)_{x=0}^{(k)}\right|.$$
 (11)

Under the assumptions (??) for i = 2 for p(x) and for $p_{rev}(x)$, respectively, the latter two bounds become sharp as k increases, by virtue of (??), and next we argue informally that it tends to be sharp with a high probability under random root models. Indeed,

$$\frac{1}{|x_d|} \le \frac{1}{d} \left| \frac{p'(c)}{p(c)} \right| = \frac{1}{d} \left| \sum_{j=1}^d \frac{1}{c - x_j} \right| \tag{12}$$

by virtue of (??), and so the approximation to the root radius $|x_d|$ is poor if and only if severe cancellation occurs in the summation of the d roots, and similarly for the approximation of $r_1(c,p)$. Such a cancellation only occurs for a narrow class of polynomials p(x), with a low probability if we assume a random root model

Next we prove, however, that estimates (??) and (??) are extremely poor for worst case inputs.

Theorem 1. The ratios $|\frac{p(0)}{p'(0)}|$ and $|\frac{p_{\text{rev}}(0)}{p'_{\text{rev}}(0)}|$ are infinite for $p(x) = x^d - h^d$ and $h \neq 0$, while $|x_d| > |x_1| = |h|$.

Proof. Observe that the roots $x_j = h \exp(\frac{(j-1)\mathbf{i}}{2\pi d})$ of $p(x) = x^d - h^d$ for $j = 1, 2, \ldots, d$ are the dth roots of unity up to scaling by h.

The problem persists for the root radius $r_d(w, p)$ where p'(w) and $p'_{rev}(w)$ vanish; rotation of the variable $p(x) \leftarrow t(x) = p(ax)$ for |a| = 1 does not fix it but shifts $p(x) \leftarrow t(x) = p(x - c)$ for $c \neq 0$ can fix it, thus enhancing the power of estimates (??) and (??).

1.4 Classical estimates for extremal root radii

Next we recall some non-costly estimates known for the extremal root radii $r_1 = r_1(0, p)$ and $r_d = r_d(0, p)$ in terms of the coefficients of p (cf. [?], and [?]) and the two parameters

$$\tilde{r}_{-} := \min_{i \ge 1} \left| \frac{p_0}{p_i} \right|^{\frac{1}{i}}, \tilde{r}_{+} := \max_{i \ge 1} \left| \frac{p_{d-i}}{p_d} \right|^{\frac{1}{i}}$$
 (13)

These bounds on r_1 and r_d hold in dual pairs since $r_1(0,p)r_d(0,p_{\text{rev}})=1$. Furthermore, we have that

$$\frac{1}{d}\tilde{r}_{+} \le r_{1} < 2\tilde{r}_{+}, \frac{1}{2}\tilde{r}_{-} \le r_{d} \le d\tilde{r}_{-}, \tag{14}$$

$$\tilde{r}_{+}\sqrt{\frac{2}{d}} \le r_{1} \le \frac{1+\sqrt{5}}{2}\tilde{r}_{+} < 1.62\tilde{r}_{+} \text{ if } p_{d-1} = 0,$$
 (15)

$$0.618\tilde{r}_{-} < \frac{2}{1+\sqrt{5}}\tilde{r}_{-} \le r_{d} \le \sqrt{\frac{d}{2}}\tilde{r}_{-} \text{ if } p_{1} = 0, \tag{16}$$

$$r_1 \le 1 + \sum_{i=0}^{d-1} \left| \frac{p_i}{p_d} \right|, \frac{1}{r_d} \le 1 + \sum_{i=1}^d \left| \frac{p_i}{p_0} \right|.$$
 (17)

 $M(p):=|p_d|\max_{j=1}^d \{1,|x_j|\}$ is said to be the Mahler measure of p, and so $M\left(p_{\mathrm{rev}}\right):=|p_0|\max_{j=1}^d \left\{1,\frac{1}{|x_j|}\right\}$. It holds that

$$r_1^2 \le \frac{M(p)^2}{|p_d|} \le \max_{i=0}^{d-1} \left| \frac{p_i}{p_d} \right|^2, \frac{1}{r_d^2} \le \frac{M(p_{\text{rev}})^2}{|p_0|^2} \le \max_{i=1}^d \left| \frac{p_i}{p_0} \right|^2$$
 (18)

It is shown in [?] that we can get a very fast approximation of all root radii of p at the origin at a very low cost, which complements the estimates ??, ??, ??, ??, and ??.

One can extend all these bounds to the estimates for the root radii $r_j(c,p)$ for any fixed complex c and all j by observing that $r_j(c,p) = r_j(0,t)$ for the polynomial t(x) = p(x-c) and applying Taylor's shift; i.e., applying the mapping $S_{c,\rho}: p(x) \mapsto p\left(\frac{x-c}{\rho}\right)$.

The algorithms in Sec. ?? closely approximate root radii $r_j(c,p)$ for a black box polynomial p and a complex point c at reasonably low cost, but the next well-known upper bounds on r_d and lower bounds on r_1 (cf. [?],[?],[?],[?], and [?]) are computed at even a lower cost, defined by a single fraction $\frac{p_0}{p_i}$ or $\frac{p_{d-i}}{p_d}$ for any i, albeit these bounds are excessively large for the worst case input. Finally,

we have that $r_d \leq \rho_{i,-} := \left(\binom{d}{i} \left| \frac{p_0}{p_i} \right| \right)^{\frac{1}{i}}, \frac{1}{r_1} \leq \frac{1}{\rho_{i,+}} := \left(\binom{d}{i} \left| \frac{p_d}{p_{d-i}} \right| \right)^{\frac{1}{i}}$ and therefore, since $p^{(i)}(0) = i! p_i$ for all i > 0, that

$$r_{d} \le \rho_{i,-} = \left(i! \begin{pmatrix} d \\ i \end{pmatrix} \left| \frac{p(0)}{p^{(i)}(0)} \right| \right)^{\frac{1}{i}}, \frac{1}{r_{1}} \le \frac{1}{\rho_{i,+}} = \left(i! \begin{pmatrix} d \\ i \end{pmatrix} \left| \frac{p_{\text{rev}}(0)}{p_{\text{rev}}^{(i)}(0)} \right| \right)^{\frac{1}{i}}$$
(19)

for all i; from which we obtain relations ?? for i = 1.

1.5 Higher order derivatives of $\frac{p'(0)}{p(0)}$

Recall that the ratios $\frac{p'(0)}{p(0)}$ and $\frac{xp'(0)}{p(0)}$ play a key role in the root-finders and root-radii computations. We evaluate the ratio $p'(x)/p(x) = p'_0(x)/p_0(x)$ by applying the recurrence

$$\frac{p'_{i+1}(x)}{p_{i+1}(x)} = \frac{1}{2\sqrt{x}} \left(\frac{p'_{i}(\sqrt{x})}{p_{i}(\sqrt{x})} - \frac{p'_{i}(-\sqrt{x})}{p_{i}(-\sqrt{x})} \right), \ i = 0, 1, \dots$$
 (20)

Recurrences (??) and (??) reduce the evaluation of $p_{\ell}(c)$ to the evaluation of p(c) at $q=2^{\ell}$ points $c^{1/q}$ and for $c\neq 0$ reduce the evaluation of the ratio

 $p'_{\ell}(x)/p_{\ell}(x)$ at x=c to the evaluation of the ratio p'(x)/p(x) at the latter $q=2^{\ell}$ points $x=c^{1/q}$. We will see that we can apply recurrence (??) to support fast convergence to the convex hull of the roots.

Equations (??) and (??) enable us to strengthen upper estimates in Eq. ?? and more generally Eq. ?? for root radii $r_j(0,p)$ at the origin because $r_j(0,p_\ell) = r_j(0,p)^{2^\ell}$ for $j=1,\ldots,d$ (see Eq. ??); we can approximate the higher order derivatives $\left(\frac{p^{(g)}(x)}{p^{(g-1)}(x)}\right)^{(\ell)}$ at x=0 by using a divided difference (See Alg. 5 of [companion papper]). Besides the listed applications of root-squaring, one can apply DLG iterations to randomized exclusion tests for sparse polynomials. One can apply root-squaring $p(x) \mapsto p_\ell(x)$ to improve the error bound for the approximation of the power sums of the roots of p(x) in the unit disc D(0,1) by Cauchy sums, but the improvement is about as much as the additional cost incurred by increasing the number q of points of evaluation of the ratio $\frac{p'}{p}$.

Remark 1. One can approximate the leading coefficient p_d of a black box polynomial p(x). This coefficient is not involved in recurrence (??), and one can apply recurrence (??) by using a crude approximation to p_d and if needed can scale polynomials $p_i(x)$ for some i.

We can treat $\frac{p'(x)}{p(x)}$ as another blackbox that runs the same order of cost since the same blackbox oracle that evaluates p(x) can be used to evaluate p'(x) as well, based on the following theorem:

Theorem 2. Given an algorithm that evaluates a black box polynomial p(x) at a point x over a field K of constants by using A additions and subtractions, S scalar multiplications (that is, multiplications by elements of the field K), and M other multiplications and divisions, one can extend this algorithm to the evaluation at x of both p(x) and p'(x) by using 2A + M additions and subtractions, 2S scalar multiplications, and 3M other multiplications and divisions.

Proof. [?] and [?] prove the theorem for any function $f(x_1, \ldots, x_s)$ that has partial derivatives in all its s variables x_1, \ldots, x_s .

2 Our Algorithm for Evaluating $\left(\frac{p'(x)}{p(x)}\right)^{(\ell)}$

In this section we present the design of the general algorithm for approximating the root radius given by Eq. ??. There are two main steps: 1) going down the rational root tree, *i.e.*, performing Alg. ??, and 2) going up the rational root tree, *i.e.*, performing Alg. ??. The going-down is depicted in Fig. ?? and the going-up is depicted in Fig. ??. The other procedures are simple bookkeeping/preprocessing steps in between the two main going-down/going-up steps. In particular we 1) first convert a complex number x into polar coordinates r, θ where $\theta \approx \frac{p}{q} = \frac{p}{2\epsilon}$, *i.e.*, perform Alg. ??, 2) perform the first going-down pass which gives the rational angles for the roots of x in fraction form, *i.e.*, perform

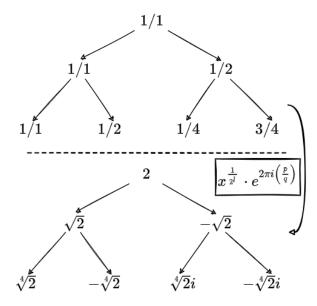


Fig. 1. The upper tree depicts the steps of Circle_Roots_Rational_Form(p,q,l) in Alg.?? for $l=2,\,p=1,$ and q=1. The lower tree depicts the steps of Roots(r,t,u,l) in Alg.?? for $r=2,\,l=2,\,p=1,$ and q=1

Fig. 2.

Alg. ??, 3) perform the second pass of the going-down algorithm where we compute the values $|x|^{\frac{1}{2^m}} \exp(2\pi i \frac{p}{q})$ at the m^{th} level, and 4) finally compute the values given by Eq. ?? going back up the rational root tree.

The intuition behind Alg. ?? is that the square root operation satisfies

$$p\%q \neq 0 \implies \sqrt{\exp\left(2\pi i \frac{p}{q}\right)} = \exp\left(2\pi i \frac{p}{2q}\right)$$
 (21)

and

$$p\%q = 0 \implies \sqrt{\exp\left(2\pi i \frac{1}{1}\right)} = \exp\left(2\pi i \frac{1}{1}\right) = 1,$$
 (22)

and the negation operation satisfies

$$p\%q \neq 0 \implies -\exp\left(2\pi i \frac{r}{s}\right) = \exp\left(2\pi i \frac{2r+s}{2s}\right)$$
 (23)

and

$$p\%q = 0 \implies \sqrt{\exp\left(2\pi i \frac{1}{1}\right)} = \exp\left(2\pi i \frac{1}{2}\right) = -1;$$
 (24)

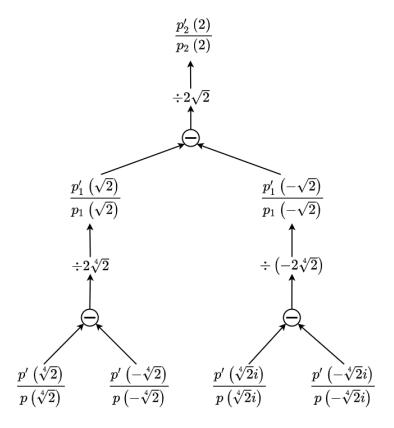


Fig. 3. The steps of DLG_RATIONAL_FORM(p, p', r, t, u, l) in Alg.?? for r = 2, l = 2, t = 1, and u = 1.

Fig. 4.

therefore, the first four lines of Alg. ?? compute the (angle of the) positive square root, \sqrt{x} , of complex number on the unit circle and the next four lines Alg. ?? computes the (angle of the) negative square root, $-\sqrt{x}$. Therefore, we have:

Theorem 3. For a complex number x with a rational angle $\frac{p}{q}$, i.e., $x = |x| \exp\left(2\pi i \frac{p}{q}\right)$, Alg. ?? correctly computes the roots in Eq. ??. In particular, for a rational angle in fractional form, it does so with exact precision.

Proof. Equations ??, ??, and ?? give the base case and the theorem follows by a straightforward induction.

Alg. ?? and Alg. ?? are both straightforward, so for the rest of this section we focus on the intuition behind Alg. ??.

Alg. ?? is a dynamic programming on Equation ??. Therefore, by Thm. ??, we have that Alg. ?? correctly computes Eq. ??. Specifically, Alg. ?? does the

Algorithm 1 Circle Roots Rational Form(p,q,l)

```
if p\%q == 0 then
  r,s:=(1,1)
else
  r,s:=(p,2q)
end if
if r\%s == 0 then
  t, u := (1,2)
else
  t, u := (2r + s, 2s)
end if
if l == 1 then
  return [(r,s),(t,u)]
else if l != 0 then
  left := Circle Roots Rational Form(r, s, l - 1)
  right := CIRCLE\_ROOTS\_RATIONAL\_FORM(t, u, l - 1)
  return left \cup right
else
  return [(p,q)]
end if
```

Algorithm 2 Roots(r, t, u, l)

```
root_tree = Circle_Roots_Rational_Form(p, q, l)
circ_root = [exp (2 \cdot \pi \cdot i \cdot \frac{r}{s}) for r, s in root_tree]
roots = [\sqrt[2^l]{r}-root for root in circ_root]
return roots
```

Algorithm 3 DLG RATIONAL FORM(p, p', r, t, u, l)

```
\begin{aligned} & \operatorname{root} := \operatorname{Roots}(r,t,u,l) \\ & \operatorname{for} \ r_i \in \operatorname{root} \ \operatorname{\mathbf{do}} \\ & \operatorname{base\_step}[i] := \frac{p'(r_i)}{p(r_i)} \\ & \operatorname{\mathbf{end}} \ \operatorname{\mathbf{for}} \\ & \operatorname{diff}[0] := \operatorname{base\_step} \\ & \operatorname{\mathbf{for}} \ i \leq l \ \operatorname{\mathbf{do}} \\ & \operatorname{\mathbf{for}} \ j \leq 2^{l-i-1} \ \operatorname{\mathbf{do}} \\ & \operatorname{diff}[i+1][j] := \frac{1}{2} \frac{\operatorname{diff}[i][2j] - \operatorname{diff}[i][2j+1]}{\operatorname{root}[2j]} \\ & \operatorname{root} = \operatorname{roots}(r,t,u,l-1-i) \\ & \operatorname{\mathbf{end}} \ \operatorname{\mathbf{for}} \\ & \operatorname{\mathbf{end}} \ \operatorname{\mathbf{for}} \\ & \operatorname{\mathbf{red}} \ \operatorname{\mathbf{for}} \\ & \operatorname{\mathbf{for}} \\ & \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \\ & \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \\ & \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \\ & \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}} \ \operatorname{\mathbf{red}}
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following: 1) it computes the last layer of the recursion Eq. ?? (i.e., it computes $p'(x^{\frac{1}{2^l}})/p(x^{\frac{1}{2^l}})$) and then 2) it recursively applies Eq. ?? via dynamic programming until it finally computes $\frac{p'_{\ell}(x)}{p_{\ell}(x)}$ which is the desired quantity. The former is given by the line "base_step[i] := $\frac{p'(r_i)}{p(r_i)}$ " and the latter is given by the line "diff[i+1][j]:= $\frac{1}{2}\frac{\text{diff}[i][2j]-\text{diff}[i][2j+1]}{\text{root}[2j]}$ " in Alg. ??; the desired output (i.e., $p'(x^{\frac{1}{2^l}})/p(x^{\frac{1}{2^l}})$) is given by the line "diff[l][0]".

Algorithm 4 DLG (p, p', l, x, ϵ)

```
angle := \frac{1}{2\pi i} \log(x)
u := 2^{\epsilon}
t := (angle \cdot u)\%1
r := |x|
return DLG_RATIONAL_FORM(p, p', r, t, u, l)
```

The final step in the algorithm is to use Alg. ?? to compute root radius approximations r_d and r_1 . The procedure is given by Alg. ??. The rationale for

Algorithm 5 DLG_ROOT_RADIUS $(p, p', p_{rev}, p'_{rev}, l, \epsilon, \delta)$

```
Uniformly Randomly Generate x in the unit circle d := \deg(p) r_{\min} := d/\mathrm{DLG}(p, p', l, x \cdot 2^{-\delta}, \epsilon) r_{\max} := \mathrm{DLG}(p_{\mathrm{rev}}, p'_{\mathrm{rev}}, l, x \cdot 2^{-\delta}, \epsilon)/d
```

generating a random x is that there may be roots close to 0 and thus, by taking the limit in certain directions, we avoid these possible poles; in particular, we have that

$$\lim_{\delta, \epsilon \to \infty} \mathrm{DLG}(p, p', l, x \cdot 2^{-\delta}, \epsilon) = \frac{p'_{\ell}(0)}{p_{\ell}(0)} = \left(\frac{p'_{\ell-1}(x)}{p_{\ell-1}(x)}\right)'_{x=0} = \left(\frac{p'(x)}{p(x)}\right)^{(\ell)}_{x=0}, \quad (25)$$

for any x, if $p(0) \neq 0$ (See Thm ??).

3 Theoretical Analysis

We now give some theoretical guarantees: Thm. ?? proves the correctness of Alg. ??, and Thm. ?? and Thm. ?? give computational complexity bounds.

3.1 Correctness of the output

Theorem 4. If $p(0) \neq 0$, then Alg. ?? computes the bounds given by Eq. ?? with probability 1.

Proof. By Lem. ?? we have that the limit in Eq. ?? is well defined. Since there are at most finitely many roots for p_{ℓ} with a high probability Alg. ?? computes the correct approximation to the bounds in Eq. ??.

3.2 Complexity

Theorem 5. Alg. ?? performs q floating point subtractions, divisions, and multiplications and q applications of \sin and \cos , where $q=2^l$; furthermore, Alg. ?? performs at most Cq integer additions, "multiplications-by-2", and $\%2^{\epsilon}$ (i.e., $mod\ 2^{\epsilon}$) operations, where C=1,3,2 respectively.

Proof. Looking at Fig. ?? and Fig. ??, we can see that the computational tree for the Alg. ?? is a binary tree with $2^l = q$ nodes; the proof for the constants C = 1, 3, 2 follows similarly follows from the inspection of the operations performed in Alg. ??.

Theorem 6. The Cq integer additions, "multiplications-by-2", and $\%2^{\epsilon}$ (i.e., $mod\ 2^{\epsilon}$) operations in Alg. ?? have negligible overhead. More precisely, integer additions are always additions of $2 \epsilon \log \ell$ -bit integers and "multiplications-by-2" and $\%2^{\epsilon}$ (i.e., $mod\ 2^{\epsilon}$) operations have constant time overhead.

Proof. Since Alg. ?? always passes in a denominator which is a power of two all of the integer % and \cdot operations are in fact "multiplications-by-2", and %2 $^{\epsilon}$ (i.e., mod 2 $^{\epsilon}$) operations by a straightforward proof similar to the one in Alg. ??. Thus these operation are essentially constant overhead bit shift operations on a computing machine with binary words. Since p%r always reduces $p\mapsto 1$, we have that whenever an overflow of more than $\log r$ -bits happens in Alg. ?? it gets converted to an $\log r$ -bit integer; therefore, it suffices to prove that $\log r$ is bounded by $\epsilon \log \ell$. However, this once again follows by induction on the binary computation tree: since this tree has depth ℓ we see that any denominator is bounded by $\epsilon \log \ell$ by a simple induction.

In order to prove Thm. ?? we must first prove Lem. ??.

Lemma 1. If $p(0) \neq 0$, then the limit $\lim_{x\to 0} \frac{p'_{\ell}(x)}{p_{\ell}(x)}$ is always well-defined.

Proof. By applying induction on Eq. ??, we have that $p_l(0) \neq 0$ if $p(0) \neq 0$, and thus it suffices to consider the behavior of the numerator in Eq. ??. The case $\ell = 1$ follows from an application of L'Hopital's rule. For $\ell \neq 1$, there are two cases: either \sqrt{x} divides the numerator of $\frac{p'_\ell(\sqrt{x})}{p_\ell(\sqrt{x})}$ or it does not. If it does, then we are done since we can once again apply L'Hopital's rule. Otherwise, we get that $p'_\ell(\sqrt{x}) = c_0 + c_1\sqrt{x} + ... + c_k(\sqrt{x})^k$ for some c_i with $c_0 \neq 0$. But then we

have

$$\begin{split} \frac{p'_{\ell+1}(\sqrt{x}\)}{p_{\ell+1}(\sqrt{x}\)} &= \frac{1}{2\sqrt{x}} \Big(\frac{p'_{\ell}(\sqrt{x}\)}{p_{\ell}(\sqrt{x}\)} - \frac{p'_{\ell}(-\sqrt{x}\)}{p_{\ell}(-\sqrt{x}\)} \Big) \\ &= \frac{1}{2\sqrt{x}} \frac{b_0c_0 + \sqrt{x} \cdot N_1(\sqrt{x}) - b_0c_0 - \sqrt{x} \cdot N_2(\sqrt{x})}{p'_{\ell}(\sqrt{x}\)p'_{\ell}(-\sqrt{x}\)} \\ &= \frac{1}{2} \frac{N_1(\sqrt{x}) - N_2(\sqrt{x})}{p'_{\ell}(\sqrt{x}\)p'_{\ell}(-\sqrt{x}\)}, \end{split}$$

for some polynomials N_1 and N_2 with $b_0 = p'_{\ell}(0)$. Therefore the limit at zero is once again well-defined.

3.3 Stability

Lemma 2. The (relative) condition number operator κ satisfies the following properties:

1.
$$\kappa\{f\}(x) = |x \log'(f(x))|$$

2. $\kappa\left\{\frac{f}{g}\right\}(x) = ||\kappa\{f\}(x)| - |\kappa\{g\}(x)||$
3. $\kappa\{x^d\}(x) = d$

Proof. This follows from the definition of the condition number.

Theorem 7. If $p_{\ell}(0) \neq 0$, then $\frac{p'_{\ell}(x)}{p_{\ell}(x)}$ is well-conditioned at any point sufficiently close to 0.

Proof. The proof of Lem. ?? gives us that $\frac{p'_{\ell}(x)}{p_{\ell}(x)}$ is a well behaved rational function at any point close to zero and thus the condition number $\kappa\{\frac{p'_{\ell}}{p_{\ell}}\}(x)$ is well defined at this point since the condition number of arithmetic operations of functions are themselves arithmetic operations in those same functions and the conditions number for a polynomial of degree $d \in \mathbb{R}$ is exactly d; therefore, $\kappa\{\frac{p'_{\ell}}{p_{\ell}}\}(x)$ has a well defined/bounded condition number in the limit to zero.

Remark 2. Even though Thm. ?? states that $\frac{p'_{\ell}(x)}{p_{\ell}(x)}$ is highly stable, in practice, computating this function requires the use of trigonometric functions (i.e., the roots in Alg. ??); therefore, our added precision in Alg. ?? helps with the instability associated with Alg. ??. Intuitively this helps the instability because the trigonometric functions are the only subroutines in the algorithm that have a non constant condition number and thus, special care must be taken with them.

4 Experimental Results

4.1 Setup

We now present the results of our experiments in which we compute the bounds on the extremal root radii $|x_1|$ and $|x_d|$ given by ?? for the polynomials in the

test suite of MPSolve. The test suite covers a number of univariate polynomial families over a range of degrees. (A fuller description of the test suite can be found in https://numpi.dm.unipi.it/mpsolve-2.2/mpsolve.pdf.)

Given a polynomial p(x) of degree d, we use an implementation of DLG iterations that incorporates our algorithm from Section ?? for computing $(p'(x)/p(x))^{(\ell)}$ and in turn compute bounds, or estimates for root radii, r_1 and r_d given by ?? on extremal root radii $|x_1|$ and $|x_d|$, respectively. The performance of these bounds are evaluated on the relative error in comparison to the corresponding root radius computed by MPSolve. That is,

relative error
$$(r_i) = \frac{\left|r_i - |x_i|\right|}{|x_i|}, \ i = 1, d,$$

where $|x_i|$ is the root radius found using MPSolve and r_i is our estimate for the root radii.

All experiments were run using Python 3.7.7 and MPSolve 3.2.1 on MacOS 11.6.1 with 2.8 GHz Dual-Core Intel Core i5 with 8 GB memory.

4.2 Tables

The columns of the tables, in order, are

- -d =degree of the input polynomial
- $\ell =$ number of iterations
- $-e = -\log(|x|)$
- mp.dps: the mpmath precision level used
- the relative errors for the minimum and maximum root radii
- total runtime,
- the extremal root radii as computed by MPsolve for the particular given polynomial.

The entries '-' in the tables indicate the test was terminated before completion.

Table 1. Experimental Data for chebyshev

			мР	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
20	4	616	332	0.155	0.0939	0.27	[0.0785, 0.997]
40	5	616	332	0.0981	0.0589	1.13	[0.0393, 0.999]
80	6	617	334	0.0593	0.0353		[0.0196, 1.0]
			334	2.71			[0.00982, 1.0]
320	8	617	334	37.6	0.465	88.4	[0.00491, 1.0]

 ${\bf Table~2.~Experimental~Data~for~chrma}$

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	${\rm DPS}$	Error r_d	ERROR r_1	TIME	ROOT RADIUS
21	4	616	332	0.215	0.139	0.22	[1.0, 3.17]
	-	-					[1.0, 3.25]
341	8	617	334	0.717	0.547	105.48	[0.884, 3.41]

Table 3. Experimental Data for chrma_d

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
20	4	616	332	0.16	0.175	0.26	[1.3, 3.01]
							[1.1, 3.06]
340	8	617	334	0.658	0.699	93.82	[0.741, 3.11]

Table 4. Experimental Data for chrmc

\overline{d}	ℓ	e			MPSOLVE ROOT RADIUS
	_		 0.211 0.718		[1.0, 3.03] [0.897, 4.13]

Table 5. Experimental Data for chrmc_d

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
11	3	616	332	0.251	0.242	0.05	[1.27, 2.8]
43	5	616	332	0.101	0.0996	1.23	[1.02, 2.97]
171	7	617	334	0.268	1.13	22.05	[0.715, 3.07]
683	3 9	619	338	0.164	0.257	374.69	[0.519, 3.1]

Table 6. Experimental Data for curz

	_						
			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	${\bf TIME}$	ROOT RADIUS
20	4	616	332	0.156	0.854	0.21	[0.452, 1.15]
40	5	616	332	0.199	0.776	1.13	[0.379, 1.26]
80	6	617	334	0.086	0.227	5.49	[0.318, 1.34]
160	7	617	334	0.0385	0.509	20.79	[0.271, 1.38]

Table 7. Experimental Data for easy

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
100	6	617	334	0.12	0.0809	6.35	[0.949, 0.98]
200	7	617	334	0.068	0.047		[0.971, 0.99]
400	8	617	334	0.0381	0.0265		[0.983, 0.995]
1600	10	619	338	0.01	0.00	2228.22	[0.995, 0.999]
3200	11	619	338	0.00	-	-	[0.997, 0.999]

Table 8. Experimental Data for exp

			мР	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
50	5	616	332	3.76	0.126	1.48	[14.9, 39.4]
100	6 (617	334	0.367	0.0598	7.37	[28.9, 83.9]
200	7	617	334	0.714	0.839	28.22	[56.8, 176.0]
400	8 (617	334	0.965	0.985	107.96	[113.0, 365.0]

Table 9. Experimental Data for geom1

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
10	3	616	332	0.334	0.25	0.05	[1.0, 1.0 E + 18]
15	3	616	332	0.403	1.0	0.08	$[1.0, 1.0\mathrm{E}{+28}]$
20	4	616	332	0.206	1.0	0.28	$[1.0, 1.0\mathrm{E}{+38}]$
40	5	616	332	0.122	1.0	1.18	[1.0, 1.0E+78]

Table 10. Experimental Data for geom2

d ℓ e					MPSOLVE ROOT RADIUS
15 3 616 20 4 616	332 332	$2.63\mathrm{e}{+26}$	$0.287 \\ 0.171$	$0.06 \\ 0.23$	[1.0E-18, 1.0] [1.0E-28, 1.0] [1.0E-38, 1.0] [1.0E-78, 1.0]

Table 11. Experimental Data for geom3

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	${\rm DPS}$	error r_d	Error r_1	TIME	ROOT RADIUS
10	3	616	332	0.334	0.25	0.05	[9.54E-7, 0.25]
20	4	616	332	2.41	0.171		$[9.09 \mathrm{e}\text{-}13, 0.25]$
40	5	616	332	$1.95\mathrm{e}{+18}$	0.109	1.15	$[8.27 \mathrm{e}\text{-}25, 0.25]$
80	6	617	334	$1.83\mathrm{e}{+45}$	0.0662	5.73	$[6.84 \mathrm{E}\text{-}49, 0.25]$

Table 12. Experimental Data for geom4

d	o	0		RELATIVE			MPSOLVE ROOT RADIUS
<u>u</u>	·	C	Dra	Ention 1 _d	EITHOR / I	TIME	TOOT RADIUS
10	3	616	332	0.334	0.25	0.05	[4.0, 1.05 E + 6]
20	4	616	332	0.206	0.707	0.27	$[4.0, 1.1\text{E}{+}12]$
40	5	616	332	0.122	1.0	1.15	$[4.0, 1.21\mathrm{E}{+24}]$
80	6	617	334	0.0709	1.0	5.28	$[4.0, 1.46 \mathrm{e}{+48}]$

Table 13. Experimental Data for hermite

			мР	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
20	4	616	332	0.155	0.129	0.28	[0.245, 5.39]
40	5	616	332	0.0981			[0.175, 8.1]
80	6	617	334	0.0593	0.0555	5.97	[0.124, 11.9]
160	7	617	334	0.0348	0.0335	23.56	[0.0877, 17.2]
320	8	617	334	2.08	0.785	88.88	[0.062, 24.7]

Table 14. Experimental Data for kam1

		MP	RELATIVE	RELATIV	E RUN-	MPSOLVE
$d \ell$	e	DPS	error r_d	ERROR 1	r_1 TIME	ROOT RADIUS
7 2 6	15	331	0.368	1.0	0.01	
726	15	331	0.368	1.0		[3.0E-40, 1.0E+4]
7 2 6	15	331	$2.37\mathrm{E}{+93}$	1.0	0.01	$[3.0\mathrm{E}\text{-}140, 1.0\mathrm{E}\text{+}14]$

Table 15. Experimental Data for kam2

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	error r_d	Error r_1	TIME	ROOT RADIUS
9	3	616	332	0.107	1.0	0.03	[1.73E-6, 251.0]
9	3	616	332	0.107	1.0		[1.73E-20, 1.0E+8]
9	3	616	332	4.23 E + 46	1.0	0.03	[1.73 E-70, 1.0 E+28]

Table 16. Experimental Data for kam3

		MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d ℓ	e	DPS	error r_d	ERROR r_1	TIME	ROOT RADIUS
9 3	616	332	0.107	1.0	0.03	[1.73E-6, 251.0]
93	616	332	0.107	1.0		[1.73E-20, 1.0E+8]
93	616	332	4.23 E + 46	1.0	0.03	$[1.73 \mathrm{e}\text{-}70, 1.0 \mathrm{e}\text{+}28]$

Table 17. Experimental Data for kir1

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
44	5	616	332	4.41 E-5	0.000443	1.28	[0.5, 0.5]
84	6	617	334	2.29e- 5	0.000464	2.9	[0.5, 0.5]
164	7	617	334	1.16e-5	0.000476	9.79	[0.5, 0.5]
8	3	616	332	0.000244	0.000244	0.02	[0.5, 0.5]

Table 18. Experimental Data for kir1_mod

							MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
44	5	616	332	0.000983	0.00095	1.26	[0.5, 0.5]
							[0.498, 0.502]
164	7	617	334	0.00734	0.00749	10.35	[0.496, 0.504]

 ${\bf Table\ 19.\ Experimental\ Data\ for\ lagurerre}$

J	0				RELATIVE		MPSOLVE
a	Ł	e	DPS	ERROR r_d	ERROR r_1	TIME	ROOT RADIUS
20	4	616	332	0.206	0.167	0.22	[0.0705, 66.5]
40	5	616	332	0.122	0.108	1.28	[0.0357, 142.0]
80	6	617	334	0.0709	0.0659	5.63	[0.018, 297.0]
160	7	617	334	3.09	0.954	22.21	[0.00901, 610.0]
320	8 (617	334	41.4	0.996	89.64	$[0.00451, 1.24\mathrm{E}{+3}]$

 ${\bf Table~20.~Experimental~Data~for~lar1}$

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	error r_d	Error r_1	TIME	ROOT RADIUS
20	4	616	332	7.06 E + 9	1.0	0.1	[3.73E-22, 1.0E+50]
200	7	617	334	$9.69 \text{E}{+}19$	0.311	0.83	[3.73E-22, 41.0]

Table 21. Experimental Data for legendre

			мР	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
20	4	616	332	0.155	0.0969	0.25	[0.0765, 0.993]
40	5	616	332	0.0981	0.0604	1.15	[0.0388, 0.998]
80	6	617	334	0.0593			[0.0195, 1.0]
160	7	617	334	2.72	0.0637	19.97	[0.00979, 1.0]
320	8	617	334	37.7	0.456	81.12	[0.0049, 1.0]

Table 22. Experimental Data for 1sr

			мР	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
24	4	616	332	2.88E + 8	1.0	0.29	[1.0e-20, 1.0e+20]
52	5	616	332	$1.81\mathrm{E}{+14}$	1.0	0.25	$[1.0\mathrm{E}\text{-}20, 1.0\mathrm{E}\!+\!10]$
52	5	616	332	$1.81\mathrm{E}{+34}$	1.0	0.22	[1.0E-40, 1.0E+20]
52	5	616	332	$1.81\mathrm{E}{+74}$	1.0	0.2	$[1.0\mathrm{E}\text{-}80, 1.0\mathrm{E}\text{+}40]$
224	7	617	334	$3.62\mathrm{e}{+18}$	1.0	9.8	$[1.0\mathrm{E}\text{-}20, 1.0\mathrm{E}\text{+}20]$
500	8	617	334	1.92 E + 3	1.0	6.79	$[0.0001, 2.0\mathrm{E}{+4}]$
500	8	617	334	5.77 E + 3	0.995	3.27	[3.33E-5, 1.0E+3]
500	8	617	334	1.05	1.0	3.05	$[0.0916, 1.0\mathrm{E}{+200}]$

Table 23. Experimental Data for mand

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
31	4	616	332	0.295	0.144	0.4	[0.445, 2.0]
63	5	616	332	0.127	0.0854	2.16	[0.403, 2.0]
127	6	617	334	0.0898	0.0488	8.58	[0.373, 2.0]
255	7	617	334	0.0609	0.701	37.41	[0.351, 2.0]
511	8	617	334	0.0234	1.63	174.71	[0.334, 2.0]
1023	9	619	338	0.357	0.142	569.08	[0.321, 2.0]
2047	10	619	338	1.12	0.241	2372.57	[0.311, 2.0]
4095	11	619	338	1.68	0.38	9209.19	[0.303, 2.0]

Table 24. Experimental Data for mig1

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
20	4	616	332	0.126	1.0	0.08	[0.01, 2.26]
50	5	616	332	0.0157	0.987	1.8	$[0.00999, 1.83 \mathrm{E}{+}3]$
100	6	617	334	0.0563	1.0	0.5	[0.01, 1.15]
100	6	617	334	0.0183	1.0	4.05	[0.01, 7.92]
200	7	617	334	2.66	1.0	0.8	[0.01, 1.07]
200	7	617	334	2.59	0.999	9.37	[0.01, 2.33]
500	8	617	334	18.2	0.99	1.59	[0.01, 1.03]
500	8	617	334	18.0	0.984	15.65	[0.01, 1.36]

Table 25. Experimental Data for mult

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
15	3	616	332	0.29	0.189	0.12	[0.869, 1.07]
20	4	616	332	0.0782			[0.01, 2.68]
				0.213			[1.0, 20.0]
68	6	617	334	0.0566	0.0556	4.59	[0.25, 2.24]

Table 26. Experimental Data for nroots

d	l.	e	MP	RELATIVE ERROR r_d			MPSOLVE ROOT RADIUS
	_						
50				5.18E+13	1.0	0.12	[1.0, 1.0]
100	6	617	334	$7.06 \mathrm{E}{+6}$	1.0	0.19	[1.0, 1.0]
200	7	617	334	2.69E + 3	1.0	0.39	[1.0, 1.0]
400	8	617	334	50.5	0.981	0.79	[1.0, 1.0]
800	9	619	338	6.34	0.864	1.73	[1.0, 1.0]
1600	10	619	338	1.71	0.631	3.19	[1.0, 1.0]
3200	11	619	338	0.645	0.392	6.79	[1.0, 1.0]
6400	12	623	346	0.289	0.224	14.55	[1.0, 1.0]

 ${\bf Table~27.~Experimental~Data~for~nrooti}$

d	l			RELATIVE			
\overline{a}	Ł	e	DPS	ERROR T _d	ERROR T ₁	TIME	ROOT RADIUS
50	5	616	332	$4.94 {\rm E}\!+\!13$	1.0	0.1	[1.0, 1.0]
100	6	617	334	7.07E+6	1.0	0.32	[1.0, 1.0]
200	7	617	334	$2.69\mathrm{e}{+3}$	1.0	0.46	[1.0, 1.0]
400	8	617	334	50.5	0.981	0.85	[1.0, 1.0]
800	9	619	338	6.34	0.864	1.85	[1.0, 1.0]
1600	10	619	338	1.71	0.631	3.23	[1.0, 1.0]
3200	11	619	338	0.645	0.392	7.02	[1.0, 1.0]
6400	12	623	346	0.289	0.224	13.31	[1.0, 1.0]

Table 28. Experimental Data for sendra

\overline{d}	l	e			RELATIVE		MPSOLVE ROOT RADIUS
	_		334	$\frac{0.658}{}$		24.34	
	_		332 334	0.283 0.809	0.158		[0.9, 2.05]
	_		332	0.809 0.159	$\frac{1.64}{0.101}$	88.08 1.25	[0.994, 2.0] [0.95, 2.02]
80	6	617	334	0.287	0.573	5.2	[0.975, 2.01]

 ${\bf Table\ 29.\ Experimental\ Data\ for\ sparse}$

			MP	RELATIVE	RELATIVE	RUN-	MPSOLVE
d	ℓ	e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
100	6	617	334	0.11	1.0	0.26	[0.968, 1.01]
200	7	617	334	0.0361	0.995	1.16	[0.969, 1.0]
400	8	617	334	0.0211	0.929	2.19	[0.969, 1.0]
800	9	619	338	0.0118	0.739	6.56	[0.969, 1.0]
6400	12	623	346	0.00202	0.158	72.81	[0.969, 1.0]

 ${\bf Table~30.}~{\bf Experimental~Data~for~spiral}$

	мР	RELATIVE	RELATIVE	RUN-	MPSOLVE
d ℓ e	DPS	Error r_d	Error r_1	TIME	ROOT RADIUS
		5.1 E- 7			
$15\ 3\ 616$	332	3.49e-7	1.15e-6	0.07	[1.0, 1.0]
$20\ 4\ 616$	332	4.55E- 7	1.3E-6	0.23	[1.0, 1.0]
$25\ 4\ 616$	332	3.67 E-7	1.25 E-6	0.29	[1.0, 1.0]
30 4 616	332	3.08e-7	1.21e-6	0.41	[1.0, 1.0]

Table 31. Experimental Data for toep

							MPSOLVE
d	ℓ	e	DPS	Error r_d	ERROR r_1	TIME	ROOT RADIUS
128	7	617	334	0.0386	0.562	18.71	[1.31, 64.4]
256	8	617	334	0.0219	0.918	73.35	[1.34, 64.4]
128	7	617	334	0.0386	0.0272	17.68	[0.4, 13.2]
256	8	617	334	0.0225	0.599	72.66	[0.383, 13.2]

MP.- RELATIVE RELATIVE RUN-MPSOLVE DPS ERROR r_d ERROR r_1 TIME ROOT RADIUS 20 4 616 332 0.206 0.141[1.0, 20.0]0.2246163320.2370.08590.33 [1.0, 319.0]40 5 616 332 0.1220.09271.27 [1.0, 40.0] $6\ 617\ 334$ 0.07090.1215.59[1.0, 80.0]160 7 617 334 0.0404 0.82421.82 [1.0, 160.0]320 8 617 334 0.0228 0.98389.77 [1.0, 320.0]

Table 32. Experimental Data for wilk

4.3 Observations

The results overall verify our theoretical analysis that our root radii approximations perform well when p(x) has no roots extremely close to zero whereas the estimates are poor otherwise. Remarkably, despite the fact $x^n - a^n$ being the worst family of input, as follows from Sec. 3, our implementation performs well for the **nroots** and **nrooti** families of polynomials.

5 Conclusion

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