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Implementation of a Near-Optimal Complex Root Clustering Algorithm

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Abstract. We describe Ccluster, a software for computing natural ε-clusters of complex roots in a given box of the complex plane. This algorithm from Becker et al. (2016) is near-optimal when applied to the benchmark problem of isolating all complex roots of an integer polynomial. It is one of the first implementations of a near-optimal algorithm for complex roots. We describe some low level techniques for speeding up the algorithm. Its performance is compared with the well-known MPSolve library and Maple.

1 Introduction

The problem of root finding for a polynomial \( f(z) \) is a classical problem from antiquity, but remains the subject of active research to the present [6]. We consider a classic version of root finding:

Local root isolation problem:
Given: a polynomial \( f(z) \in \mathbb{C}[z] \), a box \( B_0 \subseteq \mathbb{C} \), \( \varepsilon > 0 \).
Output: a set \( \{\Delta_1, \ldots, \Delta_k\} \) of pairwise-disjoint discs of radius \( \leq \varepsilon \), each containing a unique root of \( f(z) \) in \( B_0 \).

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4 Irina Voiculescu informed us that her student Dan-Andrei Gheorghe has independently implemented the same algorithm in a Masters Thesis Project (May 18, 2017) at Oxford University. Sewon Park and Martin Ziegler at KAIST, Korea, have implemented a modified version of Becker et al. (2016) for polynomials having only real roots being the eigenvalues of symmetric square matrices with real coefficients. See the technical report CS-TR-2018-415 at https://cs.kaist.ac.kr/research/techReport.
It is local because we only look for roots in a locality, as specified by $B_0$. The local problem is useful in applications (especially in geometric computation) where we know where to look for the roots of interest. There are several variants of this problem: in the global version, we are not given $B_0$, signifying that we wish to find all the roots of $f$. The global version is easily reduced to the local one by specifying a $B_0$ that contains all roots of $f$. If we omit $\epsilon$, it amounts to setting $\epsilon = \infty$, representing the pure isolation problem.

Our main interest is a generalization of root isolation, to the lesser-studied problem of root clustering [10, 12, 8]. It is convenient to introduce two definitions: for any set $S \subseteq \mathbb{C}$, let $Z_f(S)$ denote the set of roots of $f$ in $S$, and let $\#_f(S)$ count the total multiplicity of the roots in $Z_f(S)$. Typically, $S$ is a disc or a box. For boxes and discs, we may write $kS$ (for any $k > 0$) to denote the dilation of $S$ by factor $k$, keeping the same center. The following problem was introduced in [16]:

**Local root clustering problem:**
Given: a polynomial $f(z)$, a box $B_0 \subseteq \mathbb{C}$, $\epsilon > 0$.
Output: a set of pairs $\{(\Delta_1, m_1), \ldots, (\Delta_k, m_k)\}$ where
- $\Delta_i$’s are pairwise-disjoint discs of radius $\leq \epsilon$,
- $m_i = \#_f(\Delta_i) = \#_f(3\Delta_i)$ for all $i$, and
- $Z_f(B_0) \subseteq \bigcup_{i=1}^{k} Z_f(\Delta_i)$.

This generalization of root isolation is necessary when we consider polynomials whose coefficients are non-algebraic (or when $f(z)$ is an analytic function, as in [16]). The requirement that $\#_f(\Delta_i) = \#_f(3\Delta_i)$ ensures that our output clusters are natural [1]; a polynomial of degree $d$ has at most $2d - 1$ natural clusters (see [16, Lemma 1]). The local root clustering algorithm for analytic functions of [16] has termination proof, but no complexity analysis. By restricting $f(z)$ to a polynomial, Becker et al. [2] succeeded in giving an algorithm and also its complexity analysis based on the geometry of the roots. When applied to the benchmark problem, where $f(z)$ is an integer polynomial of degree $d$ with $L$-bit coefficients, the algorithm can isolate all the roots of $f(z)$ with bit complexity $\tilde{O}(d^2(L + d))$. Pan [13] calls such bounds near-optimal (at least when $L \geq d$). The clustering algorithm studied in this paper comes from [1], which in turn is based on [2]. Previously, the Pan-Schönhage algorithm has achieved near-optimal bounds with divide-and-conquer methods [13], but [2, 1] was the first subdivision algorithm to achieve the near-optimal bound for complex roots. For real roots, Sagraloff-Mehlhorn [15] had earlier achieved near-optimal bound via subdivision.

Why the emphasis on “subdivision”? It is because such algorithms are implementable and quite practical (e.g., [14]). Thus the near-optimal real subdivision algorithm of [15] was implemented shortly after its discovery, and reported in [11] with excellent results. In contrast, all the asymptotically efficient root algorithms (not necessarily near-optimal) based on divide-and-conquer methods of the last 30 years have never been implemented; a proof-of-concept implementation of Schönhage’s algorithm was reported in Gourdon’s thesis [9]). Computer algebra systems mainly rely on algorithms with a priori guarantees of correctness. But in practice, algorithms without such guarantees are widely used. For complex root isolation, one of
the most highly regarded multiprecision software is MPSolve [3]. The original algorithm in MPSolve was based on Erhlich-Aberth (EA) iteration; but since 2014, a “hybrid” algorithm [4] was introduced. It is based on the secular equation, and combines ideas from EA and eigensolve [7]. These algorithms are inherently global solvers (they must approximate all roots of a polynomial simultaneously). Another theoretical limitation is that the global convergence of these methods is not proven.

In this paper, we give a preliminary report about Ccluster, our implementation of the root clustering algorithm from [1].

![Graphical Output](image)

**Fig. 1.** Left: the connected components isolating all roots of the Bernoulli polynomial of degree 100. Right: the connected components isolating all roots of the Spiral polynomial of degree 64.

To illustrate the performance for the local versus global problem, consider the Bernoulli polynomials $\text{Bern}_d(z) := \sum_{k=0}^d \binom{d}{k} b_d - k z^k$ where $b_d$’s are the Bernoulli numbers. Figure 1(Left) shows the graphical output of Ccluster for $\text{Bern}_{100}(z)$. Table 1 has four timings $\tau_X$ (for $X = \ell, g, u, s$) in seconds: $\tau_\ell$ is the time for solving the local problem over a box $B_0 = [-1,1]^2$; $\tau_g$ is the time for the global problem over the box $B_0 = [-150,150]^2$ (which contains all the roots). The other two timings from MPSolve ($\tau_u$ for unisolve, $\tau_s$ for secsolve) will be explained later. For each instance, we also indicate the numbers of solutions (#Sols) and clusters (#Clus). When #Sols equals #Clus, we know the roots are isolated. Subdivision algorithms like ours naturally solve the local problem, but MPSolve can only solve the global problem. Table 1 shows that MPSolve remains unchallenged for the global problem. But in applications where locality can be exploited, local methods may win, as seen in the last two rows of the table. The corresponding time for Maple’s fsolve is also given; fsolve is not a guaranteed algorithm and may fail.

**Overview of Paper** In Section 2, we describe the experimental setup for Ccluster. Sections 3-5 describe some techniques for speeding up the basic algorithm. We conclude with Section 6.
2 Implementation and Experiments

The main implementation of Ccluster is in C language. We have an interface for Julia\(^5\). We based our big number computation on the arb\(^6\) library. The arb library implements ball arithmetic for real numbers, complex numbers and polynomials with complex coefficients. Each arithmetic operation is carried out with error bounds.

Test Suite We consider 7 families of polynomials, classic ones as well as some new ones constructed to have interesting clustering or multiple root structure.

(F1) The Bernoulli polynomial \(B_n(z)\) of degree \(d\) is described in Section 1.  
(F2) The Mignotte polynomial \(M_{n,a}(z) := z^d - 2(2^a z - 1)^2\) for a positive integer \(a\), has two roots whose separation is near the theoretical minimum separation bound.

(F3) The Wilkinson polynomials \(W_{n,k}(z) := \prod_{i=1}^{d} (z - k)\).  
(F4) The Spiral Polynomial \(S_{n,k}(z) := \prod_{i=1}^{d} \left( z - \frac{1}{3} e^{2\pi i k/n} \right) \). See Figure 1(Right) for \(S_{n,k}(z)\).

(F5) Wilkinson Multiple: \(W_{n,k,1}(z) := \prod_{i=1}^{d} (z - k)^k\). Wilkinson\(n,1)(z)\) has degree \(d = D(D+1)/2\) where the root \(z = k\) has multiplicity \(k\) (for \(k = 1, \ldots, D\)).

(F6) Mignotte Cluster: \(M_{n,a,k}(z) := x^d - 2(2^a z - 1)^k(2^a z + 1)^k\). This polynomial has degree \(d\) (assuming \(d \geq 2k\)) and has a cluster of \(k\) roots near \(2^{-a}\) and a cluster of \(k\) roots near \(-2^{-a}\).

(F7) Nested Cluster: \(NestC_{n,d}(z)\) has degree \(d = 3^D\) and is defined by induction on \(D\): \(NestC_{1,1}(z) := z^3 - 1\) with roots \(\omega, \omega^2, \omega^3 = 1\) where \(\omega = e^{2\pi i/3}\). Inductively, if the roots of \(NestC_{n,D}(z)\) are \(\{r_j: j = 1, \ldots, 3^D\}\), then we define \(NestC_{n+1,1}(z) := \prod_{j=1}^{3^D} \left( z - r_j + \frac{\omega^j}{10^p} \right) \left( z - r_j - \frac{\omega^j}{10^p} \right) \left( z - r_j - \frac{1}{10^p} \right) \). See Figure 2 for the natural \(\varepsilon\)-clusters of \(NestC_{n,3}(z)\).

Timing Running times are sequential times on a Intel(R) Core(TM) i3 CPU 530 @ 2.93GHz machine with linux. Ccluster implements the algorithm described in [1] with differences coming from the improvements described in Sections 3-5 below. Unless explicitly specified, the value of \(\varepsilon\) for Ccluster is set to \(2^{-53}\); roughly speaking, it falls back to asking for 15 guaranteed decimal digits.

\(^5\) https://julialang.org/. Download our code in https://github.com/rimbach/Ccluster.  
\(^6\) http://arblib.org/. Download our code in https://github.com/rimbach/Ccluster.jl.
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Fig. 2. Left: 3 clusters of \texttt{NestClu}_3 found with $\varepsilon = 1$. Right: Zoomed view of 9 clusters of \texttt{NestClu}_3 found with $\varepsilon = \frac{1}{10}$. Note: The initial box is in thick lines; the thin lines show the subdivisions tree.

\texttt{MPSolve} For external comparison, we use \texttt{MPSolve}. It was shown to be superior to major software such as Maple or Mathematica [3]. There are two root solvers in \texttt{MPSolve}: the original \texttt{unisolve} [3] which is based on the Ehrlich-Aberth iteration and the new hybrid algorithm called \texttt{secsolve} [4]. These are called with the commands \texttt{mpsolve -au -G1 -o γ -j1} and \texttt{mpsolve -as -G1 -o γ -j1} (respectively). \texttt{-G1} means that \texttt{MPSolve} tries to find for each root a unique complex disc containing it, such that Newton iteration is guaranteed to converge quadratically toward the root starting from the center of the disc. \texttt{-o γ} means that \texttt{MPSolve} stops when the complex disc containing the root has radius less that $10^{-γ}$, regardless of whether it is isolating or not. Unless explicitly specified, we set $γ = 16$. \texttt{-j1} means that the process is not parallelized. Although \texttt{MPSolve} does not do general local search, it has an option to search only within the unit disc. This option does not seem to lead to much improvement.

3 Improved Soft Pellet Test

The key predicate in [1] is a form of Pellet test denoted $\tilde{T}_G^k(\Delta,k)$ (with implicit $f(z)$). This is modified in Figure 3 by adding an outer while-loop to control the number of Graeffe-Dandelin iterations. We try to get a definite decision (i.e., anything other than a \texttt{unresolved}) from the soft comparison for the current Graeffe iteration. This is done by increasing the precision $L$ for approximating the coefficients of $\tilde{f}$ in the innermost while-loop. Thus we have two versions of our algorithm: (V1) uses the original $\tilde{T}_k^G(\Delta,k)$ in [1], and (V2) uses the modified form in Figure 3. Let $τV1$ and $τV2$ be timings for the 2 versions. Table 2 shows the time $τV1$ (in seconds) and the ratio $τV1/τV2$. We see that (V2) achieves a consistent 2.3 to 3-fold speed up.

In (V2), as in [1], we use $\tilde{T}_0^G(\Delta)$ (defined as $\tilde{T}_k^G(\Delta,0)$) to prove that a box $B$ has no root. We propose a new version (V3) that uses $\tilde{T}_k^G(\Delta)$ (defined as $\tilde{T}_k^G(\Delta,d)$, where $d$ is the degree of $f$) instead of $\tilde{T}_0^G(\Delta)$ to achieve this goal: instead of just
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\[ f(z) \text{ is implicit argument} \]

Output: \( r \in \{-1.0, \ldots, k\} \)

\[
\text{ASSERT: if } r \geq 0, \text{ then } \# f(\Delta) = r
\]

\[
L \leftarrow 53, \quad d \leftarrow \deg(f), \quad N \leftarrow 4 + \lfloor \log_2(1 + \log_2(d)) \rfloor, \quad i \leftarrow 0
\]

\[
f \leftarrow \text{getApproximation}(f, L)
\]

\[
\bar{f} \leftarrow \text{TaylorShift}(f, \Delta)
\]

While \( i \leq N \)

Let \( \bar{f} \) be the \( i \)-th Graeffe iteration of \( \bar{f} \)

\[
r \leftarrow 0
\]

While \( r \leq k \)

\[
\begin{align*}
\bar{f} & \leftarrow \text{IntCompare}( |\bar{f}|_r, \sum_{k \neq r} |\bar{f}|_k 2^{-L}) \\
\text{While } \bar{f} & = \text{unresolved}
\end{align*}
\]

\[
\begin{align*}
L & \leftarrow 2L \\
\bar{f} & \leftarrow \text{getApproximation}(f, L) \\
\bar{f} & \leftarrow \text{TaylorShift}(\bar{f}, \Delta)
\end{align*}
\]

If \( \bar{f} \) be \( i \)-th Graeffe iteration of \( \bar{f} \)

\[
j \leftarrow \text{IntCompare}( |\bar{f}|_r, \sum_{k \neq r} |\bar{f}|_k 2^{-L})
\]

If \( j = \text{true} \) then Return \( r \)

\[
r \leftarrow r + 1
\]

\[ i \leftarrow i + 1 \]

Return \(-1\)

\[ 2 \text{ IntCompare}(a, b, 2^{-L}) \text{ compares } L \text{-bit approximations of real numbers } a \text{ and } b. \text{ It returns true (resp. false) only if } a > b \text{ (resp. } a < b). \text{ It returns unresolved when } L \text{ is too small to conclude.} \]

\[ \bar{T}_k^G(\Delta, k) \]

Fig. 3. \( \bar{T}_k^G(\Delta, k) \) is the absolute value of the coefficient of the monomial of degree \( i \) of \( \bar{f} \), for \( 0 \leq i \leq d \).

|         | V1     | V2     | V1/V2 | V3     | V1/V3 |
|---------|--------|--------|--------|--------|--------|
| Bern96()          | (2308, 686, 20223) | (19.6) | (2308, 686, 6025) | 2.84 | (2308, 6, 2201) | 7.06 |
| Mign4();14       | (2060, 622, 18018) | 17.3  | (2060, 622, 5326) | 1.03 | (2060, 20, 2080) | 7.66 |
| Wilk4()          | (2148, 674, 18053) | 23.1  | (2148, 674, 5692) | 2.74 | (2148, 0, 2140) | 7.23 |
| Spiri4()         | (2512, 728, 22176) | 22.7  | (2512, 728, 8595) | 2.39 | (2512, 15, 2670) | 4.46 |
| WilkMul4();11    | (2512, 728, 22176) | 22.7  | (2512, 728, 8595) | 2.39 | (2512, 15, 2670) | 4.46 |
| MignClu4();14;3  | (2092, 618, 18515) | 20.0  | (2092, 618, 5600) | 3.00 | (2092, 12, 2481) | 6.57 |
| NestClu4();4     | (3532, 1001, 30961) | 90.2  | (3532, 1001, 9654) | 3.09 | (3532, 24, 4584) | 6.81 |

Table 2. Solving within the initial box \([-50, 50]^2\) with \( \varepsilon = 2^{-53} \) with versions (V1), (V2) and (V3) of Ccluster. n1: number of discarding tests, n2: number of discarding tests returning -1 (inconclusive), n3: total number of Graeffe iterations. \( \tau \text{V1} \) (resp. \( \tau \text{V2}, \tau \text{V3} \)): sequential time for V1 (resp. V2, V3) in seconds.

showing that \( B \) has no root, it upper bounds \( \# f(B) \). Although counter-intuitive, this yields a substantial improvement because it led to fewer Graeffe iterations overall. The timing for (V3) is \( \tau \text{V3} \), but we display only the ratio \( \tau \text{V1}/\tau \text{V3} \) in the last column of Table 2. This ratio shows that (V3) enjoys a 3.3-7.7 fold speedup. Comparing \( n3 \) for (V2) and (V3) explains this speedup.
4 Filtering

A technique for speeding up the evaluation of predicates is the idea of filters (e.g., [5]). The various Pellet tests can be viewed as a box predicate $C$ that maps a box $B \subseteq C$ to a value\footnote{We treat two-valued predicates for simplicity; the discussion could be extended to predicates (like $T_4^G$) which returns a finite set of values.} in \{true, false\}. If $C^-$ is another box predicate with property that $C^-(B) = \text{false}$ implies $C(B) = \text{false}$, we call $C^-$ a falsehood filter. If $C^-$ is efficient relatively to $C$, and “efficacious” (informally, $C(B) = \text{false}$ is likely to yield $C^-(B) = \text{false}$), then it is useful to first compute $C^-(B)$. If $C^-(B) = \text{false}$, we do not need to compute $C(B)$. The predicate $C_0$ used in Ccluster is defined as follows: $C_0(B)$ is true if $T_4^G(\Delta_B)$ returns 0 (then $B$ contains no root of $f$) and is false if $T_4^G(\Delta_B)$ returns $-1$ or $k > 0$ (then $B$ may contain some roots of $f$). We next present the falsehood filter $C_0^-(B)$ for $C_0$.

Let $f_A$ denote the Taylor shift of $f$ in $\Delta$, $f_A^{[i]}$ its $i$-th Graeffe iterate, $(f_A^{[i]})_j$ the $j$-th coefficient of $f_A^{[i]}$, and $|f_A^{[i]}|$ its absolute value of the $j$-th coefficient. Let $d$ be the degree of $f$. The assertion below is a direct consequence of the classical test of Pellet (see [2][p. 12]) and justify the correctness of our filters:

(A) if $|f_A^{[N]}| \leq |f_A^{[N]}|_0 + |f_A^{[N]}|_d$ then $T_4^G(\Delta)$ returns $-1$ or $k > 0$.

Our $C_0^-$ filter computes $|f_A^{[N]}|_0$, $|f_A^{[N]}|_1$ and $|f_A^{[N]}|_d$ and checks hypothesis of (A) using IntCompare. $|f_A^{[N]}|_0$ and $|f_A^{[N]}|_d$ can respectively be computed as $(|f_A|_0)^{2N}$ and $(|f_A|_d)^{2N}$. $|f_A^{[N]}|_1$ can be computed with the following well known formula:

\[
(f_A^{[i+1]})_k = (-1)^k((f_A^{[i]})_k)^2 + 2\sum_{j=1}^{k-1}(-1)^j(f_A^{[i]})_j(f_A^{[i]})_{2k-j}
\]  \hspace{1cm} (1)

Obtaining $|f_A^{[N]}|_1$ with eq. (1) requires to know $2^{N-1}+1$ coefficients of $f_A^{[i]}$, $2^{N-2}+1$ coefficients of $f_A^{[i]}$, ..., and finally $3 = 2^1+1$ coefficients of $f_A^{[N-1]}$. In particular, it requires to compute entirely the iterations $f_A^{[i]}$ such that $2^{N-i} \leq d$, and it is possible to do it more efficiently that with eq. (1) (for instance with the formula given in definition 2 of [2]).

Our $C_0^-$ filter takes as input a precision $L$, the Taylor shift $f_A$ of the $L$ bit approximation of $f$ and its $i$-th Graeffe iteration $f_A^{[i]}$ such that $2^{N-i} \leq \frac{L}{4}$ and $2^{N-(i+1)} > \frac{L}{2}$. It computes $|f_A^{[N]}|_0$, $|f_A^{[N]}|_d$ and the $2^{N-i}+1$ first coefficients of $f_A^{[i]}$ for $i < j \leq N$ with eq. (1). Then it checks the hypothesis of (A) using IntCompare, and returns false if it is verified, and true otherwise. In practice, it is implemented within the procedure implementing $T_4^G(\Delta_B)$.

Incorporating $C_0^-$ into Version (V3), we obtain (V4) and the speed up can be seen in Table 3. Filtering with $C_0^-$ becomes more effective as degree grows and this is because one has $2^{N-i} \leq \frac{L}{4}$ for smaller $i$ (recall that $N = 4 + \lfloor \log_2(1 + \log_2(d)) \rfloor$).
Table 3. Solving within the initial box $[-50, 50]^2$ with $\epsilon = 2^{-53}$ with versions (V3), (V4) of Ccluster. n3: number of Graeffe iterations. $\tau$V3 and $\tau$V4: sequential time in seconds.

|     | V3 | V4 |
|-----|----|----|
|     | n3 | n3 | (V3)/(V4) |
| (V3) |    |    |          |
| $d = 64$ | 2291 | 2684 | 1.08 |
| $d = 128$ | 4496 | 3983 | 1.13 |
| $d = 256$ | 8847 | 9545 | 1.19 |
| $d = 512$ | 15963 | 6200 | 1.42 |
| $d = 767$ | 19804 | 1832 | 1.53 |
| (V4) |    |    |          |
| $d = 64$ | 2080 | 2418 | 1.22 |
| $d = 128$ | 3899 | 1216 | 1.21 |
| $d = 256$ | 7605 | 8333 | 1.33 |
| $d = 512$ | 15227 | 6740 | 1.57 |

Table 4. Solving within the box $[-50, 50]^2$ with versions (V4) and (V4) of Ccluster with three values of $\epsilon$. $\tau$53 (resp. $\tau$530, $\tau$5300): sequential time for (V4) and (V4) in seconds.
6 Conclusion

Implementing subdivision algorithms is relatively easy but achieving state-of-art performance requires much optimization and low-level development. This paper explores several such techniques. We do well compared to fsolve in Maple, but the performance of MPSolve is superior to the global version of Ccluster. But Ccluster can still shine when looking for local roots or when ε is large.

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