Polynomial root clustering and explicit deflation

Rémi Imbach1 * and Victor Y. Pan2 **

1 Courant Institute of Mathematical Sciences
New York University, USA
Email: remi.imbach@nyu.edu
https://cims.nyu.edu/~imbach/
2 City University of New York
Email: victor.pan@lehman.cuny.edu
http://comet.lehman.cuny.edu/vpan/

Abstract. We seek complex roots of a univariate polynomial $P$ with real or complex coefficients. We address this problem based on recent algorithms that use subdivision and have a nearly optimal complexity. They are particularly efficient when only roots in a given Region Of Interest (ROI) are sought. In this report we explore explicit deflation of $P$ to decrease its degree and the arithmetic cost of the subdivision.

1 Introduction

In this report we consider the problem of finding the complex roots of a univariate polynomial $P$ with real or complex coefficients. To address this problem, methods using simultaneous Newton-like iterations (e.g. Erhlich-Aberth iterations) have demonstrated their superiority, in practice, over other approaches. Beside the known fact that the convergence of such iterations to solutions is not shown, methods based on this idea are global in the sense that all the roots are found.

In contrast, recent approaches based on the subdivision of an initial box (the ROI for Region Of Interest) of the complex plane find only roots in this ROI, which is relevant in many areas of computational sciences. These methods have also a proved nearly optimal complexity, and the implementation described in [IPY18] have shown that they are a little more efficient for the local task of computing the roots in a ROI containing only a small number of roots (which is important in many computational areas) than the best algorithms for global task of approximation of all roots, based on Erhlich-Aberth iterations. These local methods compute clusters of roots, and are robust even in the case of multiple roots. To define the Local Clustering Problem (LCP), let us introduce some definitions. For any complex set $S$, $\text{Zero}(S, P)$ stands for the roots of $P$ in $S$, and $\#(S, P)$ for the number of roots, counted with multiplicity, of $P$ in $S$.

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We consider square complex boxes and complex discs. If $S$ is such a box (resp. disc) and $\delta$ is a positive real number, we denote by $\delta S$ the box (resp. disc) with the same center than $S$ but $\delta$ times its width (resp radius). A disc $\Delta$ is called an isolator if $\#(\Delta, P) > 0$ and it is natural if in addition $\#(\Delta, P) = \#(3\Delta, P)$. A set $\mathcal{R}$ of roots of $P$ for which there exist a natural isolator $\Delta$ with $\text{Zero}(\mathcal{R}, P) = \text{Zero}(\Delta, P)$ is called a natural cluster. The LCP is to compute natural isolators for natural clusters together with the sum of multiplicities of roots in the clusters:

**Local Clustering Problem (LCP):**

**Given:** a polynomial $P \in \mathbb{C}[z]$, a square complex box $B_0 \subset \mathbb{C}$, $\epsilon > 0$

**Output:** a set of pairs $\{(\Delta^1, m^1), \ldots, (\Delta^\ell, m^\ell)\}$ where:
- the $\Delta^j$s are pairwise disjoint discs of radius $\leq \epsilon$,
- each $m^j = \#(\Delta^j, P) = \#(3\Delta^j, P)$ and $m^j > 0$
- $\text{Zero}(B_0, P) \subseteq \bigcup_{j=1}^{\ell} \text{Zero}(\Delta^j, P) \subseteq \text{Zero}(2B_0, P)$

We present here a practical improvement obtained by successively deflating $P$. Once a set $S$ of $\#(S, P)$ roots of $P$ counted with multiplicities has been found, one can compute the factor $Q$ of $P$ that has exactly the roots $\text{Zero}(\mathbb{C}, P) \setminus \text{Zero}(S, P)$ with the same multiplicities, then compute clusters of roots of $Q$ that has a smaller degree than $P$.

**Previous works** Univariate polynomial root finding is a long standing quest that is still actual; it is intrinsically linked to polynomial factorization for which the theoretical record upper bound, which differs from an information lower bound by at most a polylogarithmic factor in the input size has been achieved in [Pan02]. Root-finder supporting such bit complexity bounds are said nearly optimal. User’s choice, however, has been for a while the package of subroutines MPsolve (see [BF00] and [BR14]), based on simultaneous Newton-like (i.e. Ehrlich-Aberth iterations). These iterations converge to all roots simultaneously with cubic convergence rate, but only locally, that is, near the roots, and empirically converge very fast globally, with no formal support known for this empirical behavior. Furthermore they compute a small number of roots in a ROI not much faster than all roots.

In contrast, recent approaches based on subdivision compute the roots in a fixed ROI at the cost that decrease at least proportionally to the number of roots. In the case where only the real roots are sought, subdivision can be mixed with the Descartes rule of signs and Newton iterations ([SM16]) to achieve a near optimal complexity. The implementation described in [KRS16] demonstrated the practical efficiency of this approach.

In the complex case, a subdivision method with a nearly optimal complexity have also been proposed in [BSS+16]. This method computes natural clusters and is robust in the case of multiple roots; its implementation ([IPY18]) is a little more efficient than MPsolve for ROI’s containing only several roots; when all the roots are sought, MPsolve remains the user’s choice.

A recent study of polynomial deflation can be found in [Pan18].
2 Root clustering with explicit deflation

The base root clustering algorithm We rely here on a procedure

\[ \text{clusterPol}(Q, D, \epsilon, C, n) \]

based on the reduction of a research domain \( D \) taking as input:

- a polynomial \( Q \) satisfying \( \text{Zero}(C, Q) \subseteq \text{Zero}(C, P) \) given as an oracle,
- the search domain \( D \),
- an \( \epsilon > 0 \),
- a list \( C \) of pairwise disjoint \( \epsilon \)-clusters of roots of \( P \) in \( \mathbb{C} \setminus D \) and
- an integer \( n \).

It finds at most \( n \) \( \epsilon \)-clusters of roots of \( Q \) in \( D \) and reduces the search domain. More precisely, it returns a list \( C^* \) of \( \ell \) pairwise disjoint \( \epsilon \)-clusters of roots of \( Q \) and a domain \( D^* \subset D \) so that:

(i) \( \text{Zero}(D, Q) \subseteq \text{Zero}(C^* \cup D^*, Q) \),
(ii) \( \text{Zero}(C^*, Q) \subseteq \text{Zero}(D, Q) \),
(iii) either \( \ell = n \), or \( D^* \) is empty,
(iv) elements in \( C^* \cup C \) are pairwise disjoints.

Such a procedure can be implemented for instance with an algorithm based on box quadri-section, in which case the search domain will be a queue of boxes that are leaves in the subdivision tree of \( B_0 \).

Remark 1 Let \( C^*, D^* \) be the result of \( \text{clusterPol}(Q, D, \epsilon, C, n) \) where \( Q \) is such that \( \text{Zero}(C, Q) \subseteq \text{Zero}(C, P) \). If \( D_0 \) is such that \( D \subset D_0 \) and \( C \) contains all the roots of \( P \) in \( D_0 \setminus D \), then \( C \cup C^* \) contains all the roots of \( P \) in \( D_0 \setminus D^* \); if in addition \( D^* \) is empty, \( C \cup C^* \) is a solution for the LCP for \( P, D_0, \epsilon \).

We also rely on a procedure

\[ \text{refine}(C, L) \]

taking as an input a list \( C \) of pairwise disjoints natural \( \epsilon \)-clusters of roots of \( P \) and an integer \( L > 1 \), and returning a list \( C^* \) of pairwise disjoints natural \( 2^{-L} \)-clusters of roots of \( P \) so that \( \text{Zero}(C, P) = \text{Zero}(C^*, P) \); \( \text{refine}(C, L) \) possibly splits clusters in \( C \).

Root clustering with explicit deflation We present in Algo. 1 our main procedure for computing clusters of roots of \( P \) with explicit deflation. At each re-entrance in the \textbf{while} loop in step 2, \( C \) contains natural \( \epsilon \)-clusters of roots of \( P \) that are in \( D_0 \setminus D \), and all the roots of \( P \) in \( D_0 \setminus D \) are in \( C \). Let \( Q \) be the unique monic polynomial that has exactly the roots of \( P \) that are not in \( C \), with the same multiplicities as in \( P \). An oracle for \( Q \) is obtained in step 3 by specializing for arguments \( P, C \) the procedure \text{OracleForQ} defined in Algo. 2.

This procedure uses power sums of roots of \( P \). Provided that \text{OracleForQ} is correct, the correctness of Algo. 1 is a direct consequence of rem. 1.
Algorithm 1 ClusterWithDeflation\( (P, D_0, \epsilon, n) \)

**Input:** An oracle for a polynomial \( P \), a ROI \( D_0 \), \( \epsilon > 0 \), \( n \geq 1 \).

**Output:** Natural \( \epsilon \)-clusters of \( P \) in \( D_0 \).

1. \( C, D \leftarrow \text{clusterPol}(P, D_0, \emptyset, \epsilon, n) \)
2. **while** \( D \) is not empty **do**
   3. \( Q \leftarrow \text{OracleForQ}(P, C, .) \)
   4. \( C^*, D \leftarrow \text{clusterPol}(Q, D, \epsilon, C, n) \)
   5. \( C \leftarrow C \cup C^* \)
3. **return** \( C \)

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**Power sums of roots** For a polynomial \( P \) and a set \( S \) of roots (given with multiplicities) of \( P \), the first \( n \) power sums of the roots in \( S \) are the \( n \)-dimensional vector \( (a_1, \ldots, a_n) \) where \( a_i = \sum_{\alpha \in S} \#(\alpha, P) \times \alpha^i \). In the case where \( P \) is given by its coefficients, one can compute the first \( n \) power sums of all its roots for \( n \leq d_P \) (where \( d_P \) is the degree of \( P \)), with Newton identities. Here we will assume the existence of a procedure

\[
\text{CoeffsToPS}(P, n, L)
\]

taking as an input an oracle for a polynomial \( P \), a precision \( L \geq 1 \) and an integer \( n \geq 1 \) and returning \( L \)-bit approximations for the first \( n \) power sums of all the roots of \( P \).

Conversely, given an \( n \)-dimensional vector \( (a_1, \ldots, a_n) \) whose \( i \)-th component is the \( i \)-th power sum of \( d \) complex numbers \( (a_1, \ldots, a_d) \) with \( d \leq n \), one can compute the unique monic polynomial \( Q \) of degree \( d \) having the \( a_i \)’s as its roots. Then again, one can apply Newton identities. Here we assume the existence of a procedure

\[
\text{PSToCoeffs}((\tilde{a}_1, \ldots, \tilde{a}_n), L, d)
\]

taking in input \( L \)-bit approximations \( (\tilde{a}_1, \ldots, \tilde{a}_n) \) for the first \( n \) power sums of \( d \) complex numbers \( (a_1, \ldots, a_d) \) and returning a pair \( (\tilde{Q}, L') \) where \( \tilde{Q} \) is an \( L' \)-bit approximation for the unique monic polynomial \( Q \) of degree \( d \) having \( (a_1, \ldots, a_d) \) as roots.

**Polynomial deflation with power sums** Given a set \( C \) of clusters of roots of \( P \), we use power sums to compute an oracle for the unique monic polynomial \( Q \) whose set of roots is exactly \( \text{Zero}(C, P) \setminus \text{Zero}(C, P) \) with the same multiplicities than in \( P \). First, the degree \( d \) of \( Q \) is \( d_P - \#(C, P) \). Now if \( (a_1, \ldots, a_d) \) are the first \( d \) power sums of the roots of \( P \) and \( (b_1, \ldots, b_d) \) are the first \( d \) power sums of the roots of \( P \) in \( C \), then \( (a_1 - b_1, \ldots, a_d - b_d) \) are the \( d \) first power sums of the roots of \( Q \) and the coefficients for \( Q \) can be computed from these power sums. The procedure \( \text{OracleForQ}(P, C, L) \) described in Algo. 2 turns this reasoning into an oracle for \( Q \). The power sums of the roots of \( P \) and the roots of \( P \) in \( C \) are only known as oracles; one can increase the precision asked from those oracles until the computed polynomial \( Q \) has the precision \( L \) asked from an input.
In step 8, we suppose that error bounds are computed while carrying out the arithmetic operations that return the pair \((\tilde{c}_s, L_s)\) meaning that \(\tilde{c}_s\) is an \(L_s\)-bit approximation of the result.

**Algorithm 2** OracleForQ\((P, \mathcal{C}, L)\)

**Input:** An oracle for a polynomial \(P\), a set \(\mathcal{C}\) of clusters of roots of \(P\), a precision \(L \geq 1\).

**Output:** An \(L\)-bit approximation for the unique monic polynomial \(Q\) of degree \(d_P - \#(\mathcal{C}, P)\) whose set of roots is exactly \(\text{Zero}(\mathcal{C}, P) \setminus \text{Zero}(\mathcal{C}', P)\) with the same multiplicities as in \(P\).

1: \(d_Q \leftarrow d_P - \#(\mathcal{C}, P)\)
2: \(L_{\text{temp}} \leftarrow L\), \(L_{\text{res}} \leftarrow 0\)
3: while \(L_{\text{res}} < L\) do
4: \(L_{\text{temp}} \leftarrow 2L_{\text{temp}}\)
5: \(\{(\Delta_j, m_j)| 1 \leq j \leq \ell\} \leftarrow \text{refine}(\mathcal{C}, L_{\text{temp}})\) // the \(c(\Delta_j)\)'s are \(L_{\text{temp}}\)-bit approx. for the roots of \(P\) in \(\mathcal{C}\)
6: \((\tilde{a}_1, \ldots, \tilde{a}_{d_Q}) \leftarrow \text{CoeffsToPS}(P, d_Q, L_{\text{temp}})\) // \(L_{\text{temp}}\)-bit approx. for the \(d_Q\) first PS of all the roots of \(P\)
7: for \(s\) in 1, \ldots, \(d_Q\) do
8: \((\tilde{c}_s, L_s) \leftarrow \tilde{a}_s - \sum_{j=1}^{\ell} m_j \times (c(\Delta_j))^s\) // \(L_s\)-bit approx. for the \(s\)-th PS of \(Q\), with \(L_s < L_{\text{temp}}\)
9: \((\tilde{Q}, L_{\text{res}}) \leftarrow \text{PSToCoeffs}((\tilde{c}_1, \ldots, \tilde{c}_{d_Q}), \text{min}, L_s, d_Q)\)
10: return \(\tilde{Q}\)

**Implementation** We implemented the procedures ClusterWithDeflation and OracleForQ in Julia. For the procedure clusterPol, we used a modified version of Ccluster, implementing a depth first search in the subdivision tree. For the procedure refine, we used Ccluster. We will denote by CclusterD our prototype implementation of ClusterWithDeflation. We also incorporated improvements described in previous section: for polynomials in \(\mathbb{R}[z]\), Ccluster is CclusterR.

**Numerical results** We compare running times of Ccluster and CclusterD for finding \(\epsilon\)-clusters of polynomials in \(\mathbb{R}[z]\) and \(\mathbb{C}[z]\). We used three families of polynomials:
- Bernoulli polynomials \(\text{Bern}_d(z) = \sum_{k=0}^{d} \binom{d}{k} b_{d-k} z^k\) where \(b_i\)'s are the Bernoulli numbers,
- Mandelbrot polynomials (see [BF00]): let \(P_0(z) = 1\) and consider the sequence of polynomials
  \[ P_k(z) = zP_{k-1}(z)P_{k-1}(z) + 1 \]  

We define \(\text{Mand}_d(z)\) as \(P_{\lfloor \log_{2}(d+1) \rfloor}(z)\),
Fig. 1. Clusters of roots, all containing one root, for the Bernoulli polynomial of degree 64.

Fig. 2. Left: Clusters of roots, all containing one root, for the Mandelbrot polynomial of degree 63. Right: Clusters of roots, all containing one root, for the Spiral polynomial of degree 64.
Table 1. Comparison of running times of Ccluster (without deflation) and CclusterD (with deflations) for polynomials with increasing degree $d$.

| Polynomial | $d$ | $t_1$  | $t_2$  | $t_3/t_2$ | $t_4$  | $t_5$  | maxprec |
|------------|-----|--------|--------|-----------|--------|--------|---------|
| Bernoulli  | 128 | 5.44   | 4.05   | 1.34      | 0.18   | 0.05   | 0.05    | 424     |
| Bernoulli  | 256 | 33.7   | 25.0   | 1.38      | 1.18   | 0.05   | 0.36    | 848     |
| Bernoulli  | 512 | 192    | 144    | 1.33      | 10.7   | 0.07   | 0.04    | 1696    |
| Mandelbrot | 127 | 5.97   | 4.11   | 1.45      | 0.18   | 0.04   | 0.11    | 424     |
| Mandelbrot | 255 | 32.3   | 23.3   | 1.38      | 1.18   | 0.05   | 0.36    | 848     |
| Mandelbrot | 511 | 212    | 149    | 1.42      | 10.7   | 0.07   | 0.04    | 1696    |
| Spiral     | 128 | 15.5   | 9.13   | 1.70      | 0.52   | 0.06   | 0.09    | 424     |
| Spiral     | 256 | 93.0   | 63.3   | 1.47      | 1.18   | 0.07   | 0.40    | 848     |
| Spiral     | 512 | 560    | 423    | 1.32      | 85.1   | 0.20   | 0.27    | 3392    |

The roots of Bernoulli polynomial of degree 64 are drawn in fig. 1 Mandelbrot and Spiral polynomials of degrees 63 and 64 are drawn in fig. 2.

In the next section, we will discuss future works and potential improvements to our current approach.
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