Isolation of real roots of polynomial systems, complexity and condition number

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A general scheme

Algorithm (A generic subdivision algorithm)

INPUT: *An algebraic description of a semi-algebraic set.*
OUTPUT: *A topological description of the semi-algebraic set.*

Create a subdivision tree $\mathcal{T}$ and set its root to B_0.
Create a list of cells $\mathcal{C}$ and initialize it with $[B_0]$.

While $\mathcal{C} \neq \emptyset$

- $c = pop\ \mathcal{C}$
- **If regular**(c) $\mathcal{T} \leftarrow$ **process**(c) **else** $\mathcal{C} \leftarrow$ **subdivide**(c)

return assemble $(\mathcal{T})$

☞ **The problem:** *Given a system of polynomial equations with real (rational, integer) coefficients, isolate (approximate within a given precision ε) the real roots of the system in a domain $D \subset \mathbb{R}^n$.*

☞ **Regularity:** we will use

- an **exclusion** test to remove cells with no root;
- an **inclusion** test to check if the cell contains a unique root.

☞ **Analysis** will be performed in terms of

- d maximal degree of the equations;
- τ maximal size of the coefficients.
- intrinsic quantities of the system not necessarly computed by the algorithm.

How hard is the isolation problem?

Theorem (Separation bound)

$$\Delta = sep(A) = \min_{i \neq j} |\gamma_i - \gamma_j| \sim 2^{-\mathcal{O}(d^2 + d\tau)}$$

Example: Consider the Wilkinson polynomial

$$A = (x-1)(x-2)\cdots(x-20)$$

- Lower bound:

$$\Delta \geq 10^{-344}$$

- but actually

$$sep(A) = 1$$

Not all can be bad!

Theorem (Separation bound)

$$\Delta = sep(A) = \min_{i \neq j} |\gamma_i - \gamma_j| \sim 2^{-\mathcal{O}(d^2 + d\tau)}$$

$\Delta_j :=$ min dist(ζ_j, ζ_k) $k \neq j$.

Theorem (DMM_1)

$$\prod \Delta_j = \prod_j |\gamma_j - \gamma_{c_j}| \sim 2^{-\mathcal{O}(d^2 + d\tau)}$$

where γ_{c_j} is the closest root to γ_j [Davenport; 1985].

Not all can be bad, in dimension n

Theorem (Separation bound)

$$\Delta = sep(A) = \min_{i \neq j} |\gamma_i - \gamma_j| \sim 2^{-\mathcal{O}(nd^{2n-1}\tau)}$$

Theorem (DMM$_n$ [EMT'09])

$$\prod \Delta_j = \prod_j |\gamma_j - \gamma_{c_j}| \sim 2^{-\mathcal{O}(nd^{2n-1}\tau)}$$

where γ_{c_j} is the closest root to γ_j.

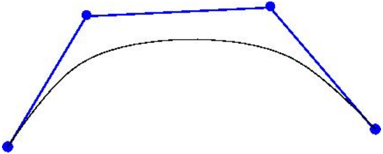
Univariate polynomials

Univariate Bernstein representation

For any $f(x) \in \mathbb{Q}[x]$ of degree d, with

$$f(x) = \sum_{i=0}^{d} c_i \binom{d}{i} (x-a)^i (b-x)^{d-i} (b-a)^{-d} = \sum_{i=0}^{d} c_i \, B_d^i(x; a, b),$$

The $\mathbf{c} = [c_i]_{i=0,\dots,d}$ are the *control coefficients* of f on $[a, b]$.



Properties:

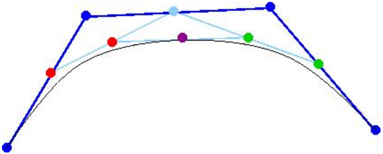
- $\sum_{i=0}^{d} B_d^i(x; a, b) = 1$; $\sum_{i=0}^{d} (a \frac{d-i}{d} + b \frac{i}{d}) \, B_d^i(x; a, b) = x$;
- $f(a) = c_0, f(b) = c_d$;
- $d\, f'(x) = \sum_{i=0}^{d-1} \Delta(\mathbf{c})_i \, B_{d-1}^i(x; a, b)$ where $\Delta(\mathbf{c})_i = c_{i+1} - c_i$;
- $(x, f(x))_{x \in [a,b]} \in$ convex hull of the points $\left(a \frac{d-i}{d} + b \frac{i}{d}, \, c_i\right)_{i=0..d}$
- $\#\{f(x) = 0; x \in [a, b]\} = V(\mathbf{c}) - 2p, \, p \in \mathbb{N}$.

De Casteljau subdivision algorithm:

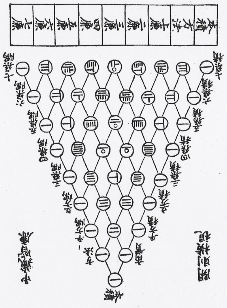
$$\begin{cases} c_i^0 = c_i, \quad i = 0, \ldots, d, \\ c_i^r(t) = (1-t)\, c_i^{r-1}(t) + t\, c_{i+1}^{r-1}(t), \quad i = 0, \ldots, d-r. \end{cases}$$

- $\mathbf{c}^-(t) = (c_0^0(t), c_0^1(t), \ldots, c_0^d(t))$ represents f on $[a, (1-t)\,a + t\,b]$.
- $\mathbf{c}^+(t) = (c_0^d(t), c_1^{d-1}(t), \ldots, c_d^0(t))$ represents f on $[(1-t)\,a + t\,b, b]$.

The geometric point of view.



The algebraic point of view.



Real root isolation for squarefree polynomials

- **Regularity:**
  - Count the number $V(\mathbf{c}; a, b)$ of coefficient sign changes.
  - $V(\mathbf{c}; a, b) = 0 \Rightarrow$ no root.
  - $V(\mathbf{c}; a, b) = 1 \Rightarrow$ a single root.
- **Subdivision:**

  If $V(\mathbf{c}) > 1$, split the interval in the middle using de Casteljau algorithm;

Continued Fraction solver [AC'76, ..., TE'08]

☞ Instead of changing the interval:

- Fix it: $]0, +\infty[$
- Change the fonction, by homography transformation:

$$\begin{array}{rcl} H :]0, +\infty[& \rightarrow &]\frac{a}{c}, \frac{b}{d}[\\ x & \mapsto & \dfrac{a + b\,x}{c + d\,x} \end{array}$$

- Work with $(f \circ H, H)$

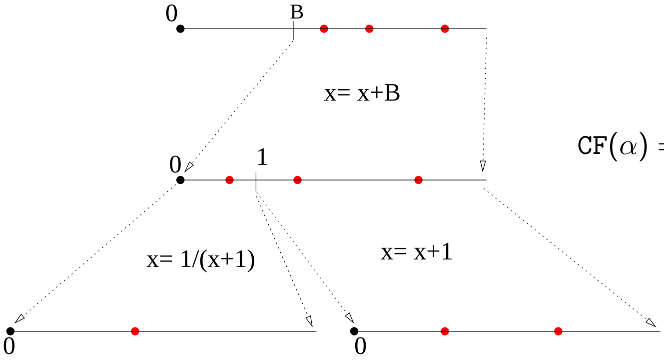
❒ **Regularity:**

- $V(f \circ H) = 0 \Rightarrow$ no root;
- $V(f \circ H) = 1 \Rightarrow$ a single root;

where $V(\cdot)$ is the number of sign changes of the coefficients in the monomial basis.

Subdivision:

- Compute a lower bound $b = L(f) \in \mathbb{N}$ of the roots of f in $\mathbb{R}_+$;
- Compute $f(x) := T_b(f) = f(x+n)$ and repeat until $L(f) = 0$;
- Split: $T_1(p) = p(x+1)$, $R(p) = (x+1)^d p(\frac{1}{x+1})$.



$$\mathtt{CF}(\alpha) = \lfloor \alpha \rfloor + \frac{1}{\mathtt{CF}\left(\frac{1}{\alpha - \lfloor \alpha \rfloor}\right)}$$

☞ Continued Fraction expansion of the roots:

$$\alpha = b_0 + \frac{1}{b_1 + \frac{1}{b_2 + \ldots}}$$

where b_i is the total shift between the i^{th} and $(i+1)^{\mathrm{th}}$ inversions.

Theorem ([Vincent;1836], [Uspensky;1948], [Alesina,Galuzzi;1998])

Let $f \in \mathbb{Z}[x]$, and $b_0, b_1, \ldots, b_n \in \mathbb{Z}_+$, $\; n > \mathcal{O}(d\,\tau)$. The map

$$x \mapsto b_0 + \cfrac{1}{b_1 + \cfrac{1}{\ddots\, b_n + \cfrac{1}{x}}}$$

transforms $f(x)$ to $\tilde{f}(x)$ such that

1. $V(\tilde{f}) = 0 \Leftrightarrow f$ has no positive real roots.
2. $V(\tilde{f}) = 1 \Leftrightarrow f$ has one positive real root.

$\Rightarrow 2^{\mathcal{O}(d\tau)}$ [Vincent; 1836], [Uspensky;1948] ...,
$\mathcal{O}_B(d^5\tau^3)$ [Akritas;1980] ...

Termination & Complexity

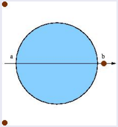
Proposition (Descartes' rule)

For $f := (\mathbf{c}, [a, b])$, $\#\{f(x) = 0; x \in [a, b]\} = V(\mathbf{c}) - 2p$, $p \in \mathbb{N}$.

Theorem

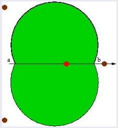
$V(\mathbf{c}^-) + V(\mathbf{c}^+) \leq V(\mathbf{c})$.

Theorem (Vincent)



If there is no complex root in the disc $D(m_{a,b}, \frac{|b-a|}{2}) \subset \mathbb{C}$, *then* $V(\mathbf{c}) = 0$.

Theorem (Two circles)



If there is no complex root in the union of the discs $D(T^+_{a,b}) \cup D(T^-_{a,b}) \subset \mathbb{C}$ *except a simple real root, then* $V(\mathbf{c}) = 1$.

Theorem (Mahler-Davenport-Mignotte)

Let $f \in \mathbb{Z}[x]$ (not necessarily square free),

$$\prod_{i=1}^{k} \Delta_k \geq \mathcal{M}(f)^{-d+1} d^{-\frac{d}{2}} (\frac{\sqrt{3}}{d})^k.$$

Proposition

Let $f \in \mathbb{Z}[x]$ of degree d and coefficients of bit size $\leq \tau$, with simple roots. Then, the number of subdivisions to isolate its real roots is $\mathcal{O}(d\tau + d \log d)$.

Theorem ([ESY'06], [EMT'06])

Let $f \in \mathbb{Z}[x]$ of degree d and coefficients of bit size $\leq \tau$. The binary cost of the subdivision solver is $\tilde{\mathcal{O}}_B(d^4\tau^2)$.

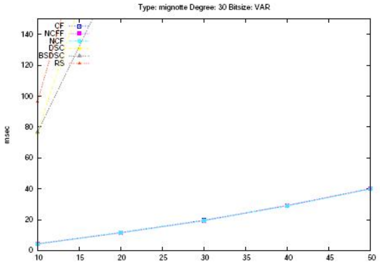
Average complexity [Tsigaridas, Emiris; 2008]

The expected complexity of **CF** is $\tilde{\mathcal{O}}_B(d^3\tau)$.

Mignotte polynomials

- Separation is not known a priori
- Difficult for subdivision solvers
- Approximate methods failed
- Only CF is efficient

Figure: Mignotte polynomials



Multivariate polynomials

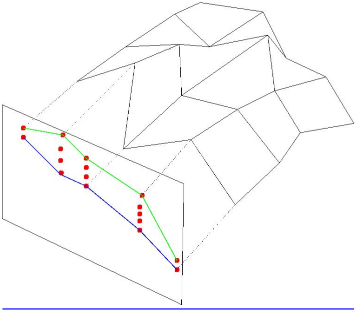
Multivariate Tensor product Bernstein representation

$$f(x_1, \dots, x_n) = \sum_{i_1=0}^{d_1} \cdots \sum_{i_n=0}^{d_n} c_{i_1,\dots,i_n} B_{d_1}^{i_1}(x_1; a_1, b_1) \cdots B_{d_n}^{j}(x_n; a_n, b_n)$$

associated with the box $\prod [a_i, b_i]$.

- **Subdivision** for each direction, similar to the univariate case.
- Arithmetic **complexity** of a subdivision bounded by $\mathcal{O}(d^{n+1})$ ($d = max(d_1, \dots, d_n)$), memory space $\mathcal{O}(d^n)$.

Reduction



$$m_j(f;x_j) = \sum_{i_j=0}^{d_j} \min_{\{0\le i_k\le d_k, k\ne j\}} b_{i_1,\ldots,i_n} B_{d_j}^{i_j}(x_j;a_j,b_j)$$

$$M_j(f;x_j) = \sum_{i_j=0}^{d_j} \max_{\{0\le i_k\le d_k, k\ne j\}} b_{i_1,\ldots,i_n} B_{d_j}^{i_j}(x_j;a_j,b_j).$$

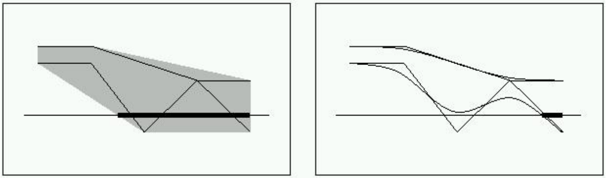
Proposition (PS93)

The intersection of the convex hull of the control polygon with the axis contains the projection of the zeroes of $\mathbf{f}(\mathbf{u}) = 0$.

Proposition

For any $\mathbf{u} = (u_1, \ldots, u_n) \in \mathcal{D}$, *and any* $j = 1, \ldots, n$, *we have*

$$m_j(f; u_j) \leq f(\mathbf{u}) \leq M_j(f; u_j).$$



Use the roots of $m_j(f, u_j) = 0$**,** $M_j(f, u_j) = 0$ **to reduce the domain of search.**

Multivariate Monomial Tensor Representation

Homography (or Möbius transformation)

Bijective projective transformation $\mathcal{H} = (\mathcal{H}_1, \ldots, \mathcal{H}_n)$ over $\mathbb{P}^1 \times \cdots \times \mathbb{P}^1$,

$$x_k \mapsto \mathcal{H}_k(x_k) = \frac{\alpha_k x_k + \beta_k}{\gamma_k x_k + \delta_k}, \quad \alpha_k, \beta_k, \gamma_k, \delta_k \in \mathbb{Z}, \;\; \alpha_k \delta_k - \beta_k \gamma_k \neq 0$$

$$H(f) := \prod_{k=1}^{n} (\gamma_k x_k + \delta_k)^{d_k} \cdot (f \circ \mathcal{H})(x)$$

Base homographies:

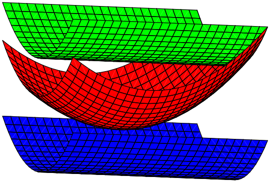
- translation by $c \in \mathbb{Z}$: $\quad T_k^c(f) = f|_{x_k = x_k + c}$
- contraction by $c \in \mathbb{Z}$: $\quad C_k^c(f) = f|_{x_k = c x_k}$
- reciprocal polynomial: $R_k(f) = x_k^{d_k} f|_{x_k = 1/x_k}$

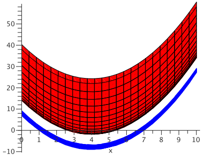
Lemma

The group of homographies is generated by R_k, C_k^c, T_k^c, $k = 1, \ldots, n$.

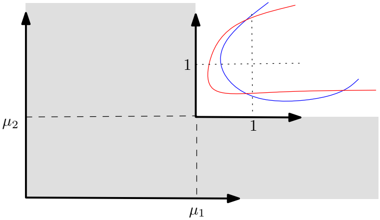
Reduction step

- Bounding the graph of f_i by cylinders in $\mathbb{R}^{n+1}$:





- Reducing the domain using univariate lower bounds:



$$m_k(f;x_k) = \sum_{i_k=0}^{d_k} \min_{i_1,\ldots,\widehat{i_k},\ldots,i_n} c_{i_1\ldots i_n}\, x_k^{i_k} \quad , \quad M_k(f;x_k) = \sum_{i_k=0}^{d_k} \max_{i_1,\ldots,\widehat{i_k},\ldots,i_n} c_{i_1\ldots i_n}\, x_k^{i_k}$$

Lemma

$$m_k(f;x_k) \le \frac{f(x)}{\prod_{s\neq k} \sum_{i_s=0}^{d_s} x_s^{i_s}} \le M_k(f;x_k) \quad , \quad k = 1,\ldots,n$$

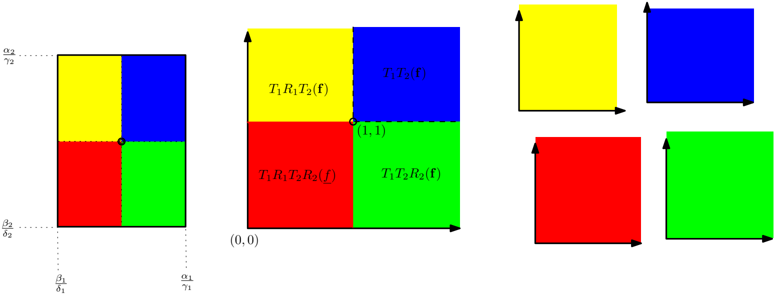
Corollary (lower bounds on the coordinates of the zeros)

$$\mu_k := \begin{cases} \text{min. pos. root of } M_k(f,x_k) & \text{if } M_k(f;0) < 0 \\ \text{min. pos. root of } m_k(f,x_k) & \text{if } m_k(f;0) > 0 \\ 0 & \text{otherwise} \end{cases}$$

All positive roots of f lie in $\mathbb{R}_{>\mu_1} \times \cdots \times \mathbb{R}_{>\mu_n}$.

☞ **Use the lowest root of $m_k(f_j, x_k)$ or $M_k(f_j, x_k)$ to reduce the domain.**

Subdivision



Keep in memory:

- Transformed polynomials: $H(f_1), \ldots, H(f_s)$ as coefficient *tensors*.
- $4n$ integers: $\alpha_k, \beta_k, \gamma_k, \delta_k$, $k = 1, \ldots, n$ to keep track of the domain.

Exclusion criterion

- No sign variation of the coefficients in the Bernstein/monomial basis $\Rightarrow$ no real root in the domain $\mathcal{D}$.

  or

- $|\mathbf{f}(\mathbf{m})| > |K_1(\mathbf{f})|\,|\mathcal{D}| \Rightarrow$ no root in $\mathcal{D}$,
  where $\mathbf{m}$ is the center of $\mathcal{D}$ and $K_1(\mathbf{f})$ is a bound on the Lipschitz constant of $\mathbf{f}$ on $\mathcal{D}$.

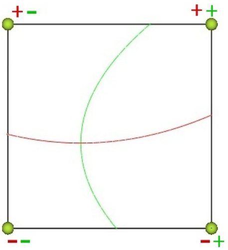
Inclusion criterion

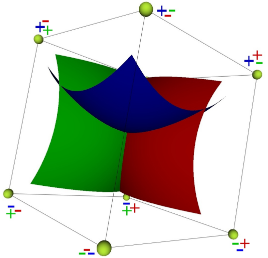
Miranda Theorem

If for every pair of parallel faces there exists f_i that attains opposite signs on the faces, then $f_1, \ldots, f_n$ have at least one root inside the box.

Lemma

If the Jacobian has a constant sign in the box, then there is at most one root of $f_1, \ldots, f_n$ inside the box.





☞ or use α-theory [BCSS98]:

- $\beta := \beta(\mathbf{f};\mathbf{x}) = ||D\mathbf{f}(\mathbf{x})^{-1}\mathbf{f}(\mathbf{x})||$
- $\gamma := \gamma(\mathbf{f};\mathbf{x}) = sup_{k\geq 2}\left(\frac{1}{k!}||D\mathbf{f}(\mathbf{x})^{-1}D^k\mathbf{f}(x,y)||\right)^{1/(k-1)}$
- $\alpha := \alpha(\mathbf{f};\mathbf{x}) = \beta\gamma$.

Theorem

If $\alpha(\mathbf{f};\mathbf{x}) < \alpha_0$ then

- $\mathbf{x}$ is an approximate zero of $\mathbf{f}$;
- Its associated zero ζ is in $B(\mathbf{x};\frac{u_0}{\gamma(\mathbf{f};\mathbf{x})})$;
- For any point $\mathbf{z} \in B(\mathbf{x};\frac{u_0}{\gamma(\mathbf{f};\mathbf{x})})$, Newton interation converges quadratically from $\mathbf{z}$ to ζ.

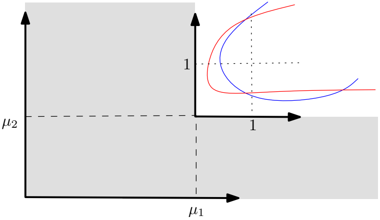
$\Rightarrow$ Same root for all the points in a connected components of $\cup_{\alpha(\mathbf{f};\mathbf{m})<\alpha_0} B(\mathbf{m};\frac{u_0}{\gamma(\mathbf{f};\mathbf{m})})$.

Subdivision speed

$\Delta_i(\zeta)$: local separation bound of ζ_i,
$k_i(\zeta)$: # of steps that isolate ζ_i

- Continued fraction expansion:

$$\zeta_1 = b_0^{(1)} + \cfrac{1}{b_1^{(1)} + \cfrac{1}{b_2^{(1)} + \cdots}} = \frac{P_{k_i(\zeta)}^{(1)}}{Q_{k_i(\zeta)}^{(1)}}$$



$$\left| \frac{P_{k_i(\zeta)}^{(1)}}{Q_{k_i(\zeta)}^{(1)}} - \zeta_j \right| < \phi^{-2k_i(\zeta)+1} \leq \Delta_i(\zeta),$$

- Bernstein binary subdivision:

$$\left| m_{k_i(\zeta)} - \zeta_i \right| < \sqrt{n}\, 2^{-k_i(\zeta)} |\mathcal{D}_0| \leq \Delta_i(\zeta),$$

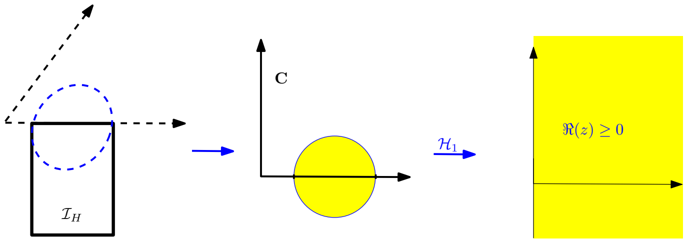
Complexity analysis

Vincent Theorem in several variables

Let $f(\mathbf{x}) = \sum_{\mathbf{i} i=0}^{\mathbf{d}} c_{\mathbf{i}} \mathbf{x}^{\mathbf{i}}$ with $c_{\mathbf{i}} \in \mathbb{R}$, without (complex) solutions s.t. $\Re(z_k) \geq 0$ for some k. Then all its coefficients $c_{\mathbf{i}}$ are of the same sign.

Corollary

If the complex multidisk associated to a domain $\mathcal{I}_H$ does not intersect $\{z \in (\mathbb{P}^1)^n : f_i(z) = 0\}$ then the coeffs. of $H(f_i)$ have no sign changes.



Definition (ε-tubular neighborhood & "entropy")

- $\tau_\varepsilon(f) = \{x \in \mathbb{R}^n \ : \ \exists z \in \mathbb{C}^n,\ f(z) = 0, \text{ s.t. } \|z - x\|_\infty < \varepsilon\}$.
- $\tau_\varepsilon(\mathbf{f}) := \cap_{i=1}^{s} \tau_\varepsilon(f_i)$ for $\mathbf{f} = (f_1, \ldots, f_s)$.
- $N_\varepsilon(\mathbf{f}) :=$ minimal number of boxes of size $< \varepsilon$ covering $\tau_\varepsilon(\mathbf{f})$ in a complete binary subdivision of D_0.

Proposition

The number of boxes of size ε not excluded is less that $N_\varepsilon(\mathbf{f})$.

Remark:

- $N_\varepsilon(\mathbf{f}) \leq \varepsilon^{-n}\mathrm{Vol}(\tau_{2\,\varepsilon}(\mathbf{f}))$.
- $N_\varepsilon(\mathbf{f})$ bounded for $\varepsilon > 0$: $N_*(\mathbf{f}) := \max_{\varepsilon > 0} N_\varepsilon(\mathbf{f})$.
- For a square system ($s = n$) with simple roots

$$\lim_{\varepsilon \to 0} N_\varepsilon(\mathbf{f}) \leq \lim_{\varepsilon \to 0} \varepsilon^{-n}\mathrm{Vol}(\tau_{2\varepsilon}(\mathbf{f})) \leq c(n) \sum_{\zeta \in \mathcal{D}_0} \frac{\prod_i ||\nabla f_i(\zeta)||}{|J_{\mathbf{f}}(\zeta)|}.$$

- By preconditionning $\mathbf{f}' := J_{\mathbf{f}}(\mathbf{m})^{-1}\mathbf{f}$, limit $= c(n) \sum_{\zeta \in \mathcal{D}} 1$.

For some $\rho > 0$, $\tau_\rho(\mathbf{f}) \subset \cup_{\zeta \in \mathcal{D}} B(\zeta, \frac{u_0}{\gamma(\mathbf{f},\zeta)})$.

Definition (Lipshitz constant)

$$K_1(\mathbf{f}, \mathcal{D}) := \max(1, \frac{Lipschitz\ \ constant(\mathbf{f})}{||\mathbf{f}||}).$$

Definition (CKMW)

- $\kappa(\mathbf{f}, \mathbf{x}) := \frac{||\mathbf{f}||}{(||\mathbf{f}||\mu_\mathbf{f}(\mathbf{x})^{-2} + ||\mathbf{f}(\mathbf{x})||_\infty)^{1/2}}$ where $\mu_\mathbf{f}(\mathbf{x}) = ||J_\mathbf{f}(\mathbf{x})||$.
- $\kappa(\mathbf{f}) := \max_{\zeta \in \mathcal{D}; \mathbf{f}(\zeta)=0} \kappa(\mathbf{f}, \zeta)$.

Proposition

For $\varepsilon < \frac{cst(d)}{K_1(\mathbf{f},\mathcal{D})^2 \kappa(\mathbf{f})^2}$, a retained box of size $\leq \varepsilon$ satifies the inclusion test.

Proposition

The arithmetic complexity is $\tilde{\mathcal{O}}(N_*(\mathbf{f})\, d^{n+1}(\log \kappa(\mathbf{f}) + \log K_1(\mathbf{f})))$.

Complexity analysis for exact input over $\mathbb{Z}$

☞ **To simplify the complexity analysis, we assume that `exclude()` and `include()` test always give a correct answer.**

- Generalization of DMM bound [EMT'09]:

$$\prod_{\zeta \in V} \Delta_i(\zeta) \geq 2^{-2n\tau d^{2n-1} - d^{2n}/2} \left(nd^n\right)^{-nd^{2n}}$$

- Overall

$$\begin{aligned} \#\text{STEPS} \leq \quad & n \sum_{\zeta \in V} k_i(\zeta) \leq n^2 \frac{1}{2} R - n^2 \frac{1}{2} \sum_{\zeta \in V} \lg \Delta_i(\zeta) \\ \leq \quad & 2n^2 \tau d^{2n-1} + 2n^2 d^n \lg(nd^{2n}) \end{aligned}$$

Lemma

The number of reduction/subdivision steps is $\tilde{\mathcal{O}}(n^2\tau d^{2n-1})$.

- Complexity of shifting $(\mathbf{x} = \mathbf{x} + \mathbf{u})$ [Gathen,Gerhard;1997]: $\tilde{\mathcal{O}}_B(n^2 d^n \tau + d^{n+1} n^3 \sigma)$, obtained as nd^{n-1} univariate shifts
- σ is bounding the bit size of partial quotients in the CF expansion of the roots: $E[\log b_i] = \mathcal{O}(\log \mathcal{K}) = \mathcal{O}(1)$.
- Bound computation with cost $\mathcal{C}_1$,
  Tests evaluation with cost $\mathcal{C}_2$.

Theorem

The total complexity is $\tilde{\mathcal{O}}_B(2^n n^7 d^{5n-1} \tau^2 \sigma + (\mathcal{C}_1 + \mathcal{C}_2) n^2 \tau d^{n-1})$.

- Best rational approximation of the (coords. of the) real roots.
- Improvement by initial scaling: apply $C_k^{1/2^\ell}$ to the input.
  - The real roots are multiplied by 2^ℓ and their distance increases.
  - Total complexity improves by an order of $d^{2n}\tau$.
- $n = 1$: matches average complexity of [TE'08].
- **mCF** is implemented in MATHEMAGIX, in the C++ module `realroot`.
  - Uses GMP arithmetic to work with large integer coefficients.
  - Polynomials based on dense tensor (higher dimensional matrix) representation.
  - Univariate solving by classic CF algorithm, special case of **mCF**. DFS traversal of the subdivision tree returns only the (floor of the) first positive root.

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