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Homotopies for solving polynomial systems within a bounded domain

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Abstract

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The problem considered in this paper is the computation of all solutions of a given polynomial system in a bounded domain. Proving Rouché's theorem by homotopy continuation concepts yields a new class of homotopy methods, the so-called regional homotopy methods. These methods rely on isolating a part of the system to be solved, which dominates the rest of the system on the border of the domain. As the dominant part has a sparser structure, it is easier to solve. It will be used as start system in the regional homotopy. The paper further describes practical homotopy construction methods by presenting estimators to obtain bounds for polynomials over a bounded domain. Applications illustrate the usefulness of the approach.

1. Introduction

In many practical applications a polynomial system $F(\mathbf{x})=\mathbf{0}$, with $F(f_1, f_2, \ldots, f_n)^{\mathrm{T}}$ and $\mathbf{x}=(x_1, x_2, \ldots, x_n)$, has to be solved. It occurs very often in practice that only solutions in a bounded domain are desired. This paper is an attempt to attack this problem by homotopy continuation methods. This introduction is further organized as follows. First some related work and background material on the problem will be mentioned. Second, basics about polynomial systems and recent research developments are explained. The third part introduces our approach.

From the theory of complex functions [7] it is well known that for a closed curve C in the complex plane and an analytical function $f(x)$, the number of roots of $f(x)$ in

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the interior of C can be computed as

$$\frac{1}{2\pi i} \oint_C \frac{f'(x)}{f(x)} \mathrm{d}x,$$

provided $f(x) \neq 0$, $\forall x \in C$. The generalization to the multivariate case can be found in [2, p. 102]. A review on quadrature methods for the determination of zeros of transcendental functions appeared in [9]. In [17], a homotopy continuation method has been presented for locating all zeros of an analytic function within a bounded domain. The problem of computing all real solutions of a system of nonlinear equations in some box has been considered in [11, 12]. For this purpose generalized bisection methods were developed, using interval arithmetic techniques. See [12, 13] for a comparison with continuation methods.

Homotopy continuation methods consist of two parts. First, the system to be solved is embedded in a family of systems $H(\mathbf{x}, t)$, the so-called homotopy. Methods to construct this embedding are known as homotopy methods. A homotopy frequently used for solving polynomial systems is the artificial parameter homotopy

$$H(\mathbf{x}, t) = \gamma(1-t)G(\mathbf{x}) + tF(\mathbf{x}), \quad \gamma \in \mathbb{C}_0 = \mathbb{C} \setminus \{0\}, \quad t: 0 \rightarrow 1.$$

The continuation parameter t connects the target system $F(\mathbf{x}) = \mathbf{0}$ to the start system $G(\mathbf{x}) = \mathbf{0}$, whose solutions are known. Second, continuation methods are applied to trace the solution paths starting at the known solutions of $G(\mathbf{x}) = \mathbf{0}$ which end at the desired solutions of $F(\mathbf{x}) = \mathbf{0}$. See [1] for an introduction to these methods. In [27], the solution of polynomial systems by continuation methods is treated. See [44] for a tutorial. Also software has been developed, see [27, 33, 45].

Earlier homotopies, like in [27, 44], relied on the total degree of the system, that is the product of all degrees of the individual polynomials in the system. For almost all practical applications, this leads to a lot of diverging paths, representing wasted computations. During the last decade, considerable research efforts have been spent in constructing homotopies which exploit the special structure of the polynomial system, in order to reduce the number of continuation paths to be computed. The use of a multihomogeneous Bézout number has been proposed in [28]. Coefficient-parameter polynomial continuation has been introduced in [30, 31] and put into practice in [32, 34, 42, 43]. In [19, 20] the random product homotopy has been presented. In [21], the cheater's homotopy has been developed. Nonlinear homotopies are defined in [22]. Solving real polynomial systems by real homotopies have been developed in [23], while applications can be found in [18, 24]. Homotopies based on generalized Bézout numbers have been constructed in [39, 40]. Symmetric homotopies are proposed in [37].

Very recently, it has been (re)discovered that, when exploiting Newton polytopes to model the structure of the system, accurate upper bounds for the number of solutions can be computed. In [4], it has been proven that the mixed volume of the Newton polytopes of the system coincides with the number of isolated solutions of a system with the same structure but with randomly chosen coefficients. The mixed volume of

a polynomial system is also called the BKK bound, named after the three principal investigators, see also [16, 14]. Recently, algorithms based on this bound have been implemented in [8, 41] to solve sparse polynomial systems. Estimates for the number of real roots are presented in [15, 35], where the proofs are algorithmic. One of the conclusions of this research is that the complexity of solving a polynomial system depends on the number of terms of each individual equation. The sparser the system, the easier it will be solved. This is of great importance for the following.

The key idea of this paper is the application of the theorem of Rouché, which will be described in the next section. It is sufficient to isolate a dominant part of the system on the border of the domain, to solve it and use it as start system in the homotopy. The idea of considering only a part of a system in order to estimate the number of solutions in a certain domain, was already presented in the theory of fewnomials, see the work of Khovanskiĭ [15]. In [15, p. 82], the notion of estimating spectrum is introduced, where a spectrum of a polynomial stands for its set of exponents. Estimating means that only part of the spectrum is considered.

The third section presents the practical realization of this idea, by the description of techniques for the construction of a regional homotopy for solving polynomial systems in a bounded domain. The domains considered are product domains where each component domain consists of a band in the complex plane. When slices are taken out of the band, real domains are obtained, which help to compute only the real solutions of a polynomial system. The construction techniques use arithmetics in complex space which can be considered as analogues to interval methods. Applications are considered in the fourth section. The last section contains our conclusion.

2. The Theorem of Rouché

The theorem of Rouché can be found in many classical books on complex analysis, see e.g. [46, p. 322; 7, p. 206; 3, p. 30]. Note that analytic functions are considered, which is more general than working with polynomials. See [29] for the application of continuation to analytic systems. Before we can prove Rouché's theorem by using concepts of homotopy continuation, we first need to recall some definitions.

Definition 2.1. Let $\mathbf{x}^*$ be a solution of a system of analytic functions $F(\mathbf{x}) = \mathbf{0}$. Then $\mathbf{x}^*$ is said to be an *isolated* solution, if there exists a neighborhood of $\mathbf{x}^*$ containing no other solution of F than $\mathbf{x}^*$.

Definition 2.2. A solution $\mathbf{x}^*$ is a *nonsingular* or *regular* solution of a system of analytic functions F if the Jacobian matrix of F at $\mathbf{x}^*$ has full rank. Otherwise $\mathbf{x}^*$ is called a *singular* or *nonregular* solution of F.

A nonsingular solution is always isolated, but the opposite is not true.

Definition 2.3. Consider an isolated and singular solution $\mathbf{x}^*$ of a system $F(\mathbf{x})=\mathbf{0}$ of analytic functions. Then $\mathbf{x}^*$ has a *multiplicity equal to m*, if for a random perturbation of the system F (e.g. by adding random constants), m nonsingular solutions lie in the neighborhood of $\mathbf{x}^*$.

The multivariate theorem of Rouché can be stated as follows.

Theorem 2.1. *If*

(1) $\mathbf{D}$ *is a multidimensional bounded domain in* $\mathbb{C}^n$, $\partial\mathbf{D}$ *its border;*

(2) $F=(f_1,f_2,\ldots,f_n)^{\mathrm{T}}$ *and* $G=(g_1,g_2,\ldots,g_n)^{\mathrm{T}}$ *are systems of analytical functions in* $\mathbf{x}$ *in the closure of* $\mathbf{D}$;

(3) $\forall\mathbf{x}\in\partial\mathbf{D}$: $\|G(\mathbf{x})\|<\|F(\mathbf{x})\|$, *for some norm* $\|\cdot\|$ *on* $\mathbb{C}^n$;

then $F+G$ *and* F *have the same number of isolated solutions in* $\mathbf{D}$, *counted with multiplicity.*

Its proof follows immediately from

Theorem 2.2. *Let* F, G, *and* $\mathbf{D}$ *be defined as in Theorem* 2.1. *Assume all isolated solutions of* F *in* $\mathbf{D}$ *are regular. Consider the homotopy*

$$H(\mathbf{x},t)=F(\mathbf{x})+tG(\mathbf{x}),\quad t\in\mathbb{C},\quad |t|\leqslant 1.$$

For each isolated solution $\mathbf{x}^*$: $(F+G)(\mathbf{x}^*)=\mathbf{0}$, $\mathbf{x}^*\in\mathbf{D}$, *with multiplicity equal to m, m paths originating at isolated solutions of* $F(\mathbf{x})=\mathbf{0}$ *in* $\mathbf{D}$ *and converging to* $\mathbf{x}^*$ *exist. Furthermore, these paths are smooth, nonintersecting and strictly increasing in t, i.e. no path turns back to a solution of F as t is incremented towards* 1.

In case F has isolated singular solutions in $\mathbf{D}$, perturb F into F', of which the isolated solutions in $\mathbf{D}$ are all regular. As the perturbations are small, $\|F'(\mathbf{x})\|>\|G(\mathbf{x})\|$, $\forall\mathbf{x}\in\partial\mathbf{D}$. Theorem 2.2 can then be applied for F' instead of F. Afterwards, the paths starting at isolated solutions of $F'(\mathbf{x})=\mathbf{0}$ in $\mathbf{D}$ can naturally be extended to the isolated solutions of $F(\mathbf{x})=\mathbf{0}$ in $\mathbf{D}$.

Proof of Theorem 2.2. There are two parts in the proof. First the singularities of the solution paths will be investigated. The second part proves the boundedness of the paths.

The solution paths start at $t=0$ at regular solutions and remain regular until some singularity is encountered. Singular solution paths are solutions of the system $H(\mathbf{x},t)=\mathbf{0}$, augmented with the determinant of the Jacobian matrix.

$$S(\mathbf{x},t)=\begin{cases}H(\mathbf{x},t)=\mathbf{0},\\ \det(H_x(\mathbf{x},t))=\mathbf{0}.\end{cases}$$

The solution set to $S(\mathbf{x},t)=\mathbf{0}$ defines an analytic variety V in $(n+1)$-dimensional complex space. By elimination theory for analytic varieties, see [46, Lemma 4F, p. 48], its projection on the last component $W=\pi_{n+1}(V)$ is an analytic variety, provided

$S(\mathbf{x}, t) \neq \mathbf{0}$, $\forall \mathbf{x} \in \partial\mathbf{D}$, $\forall t \in \mathbb{C}$, $|t| \leqslant 1$. This condition is satisfied, as will become clear in the second part of the proof.

W is a one-dimensional complex variety, i.e. the solution set of an analytic function. It consists of all points t for which the solution of $H(\mathbf{x}, t) = \mathbf{0}$ is singular. As F has only regular solutions, $W \neq \mathbb{C}$, as $0 \notin W$. By [10, Theorem 43, p. 93], W is a set of isolated points. W is bounded, so $\# W < \infty$. Hence, when encountering a singularity during continuation, it is always isolated and can be circumvented by a procedure similar to the one proposed in [6], i.e. by moving in complex space around the singularity. So, the solution paths remain regular for $|t| < 1$. When $F + G$ has an isolated singularity with multiplicity m, m regular solutions of a perturbed system lie in its neighborhood. Thus, m paths converge to it. As this proves the regularity of the solution paths, the first part is finished.

In this second part of the proof, it will be proved that solution paths starting at solutions of $F(\mathbf{x}) = \mathbf{0}$ which lie in the domain $\mathbf{D}$, remain in $\mathbf{D}$, as the continuation parameter t changes from 0 to 1. Furthermore, no new solutions enter the domain during continuation.

Consider a solution leaving or entering the domain, during continuation. This solution crosses the border of the domain, which can be expressed by

$$\exists t_0 \in \mathbb{C}, |t_0| \leqslant 1, \exists \mathbf{x}_0 \in \partial\mathbf{D}: \quad H(\mathbf{x}_0, t_0) = F(\mathbf{x}_0) + t_0 G(\mathbf{x}_0) = 0.$$

Consequently,

$$F(\mathbf{x}_0) = -t_0 G(\mathbf{x}_0) \Rightarrow \|F(\mathbf{x}_0)\| = |t_0| \cdot \|G(\mathbf{x}_0)\| \text{ and } |t_0| \leqslant 1,$$

whence $\|F(\mathbf{x}_0)\| \leqslant \|G(\mathbf{x}_0)\|$, which contradicts the third assumption of Theorem 2.1.

Each isolated solution of $F(\mathbf{x}) = \mathbf{0}$ in $\mathbf{D}$ is connected to an isolated solution of $(F + G)(\mathbf{x}) = \mathbf{0}$ in $\mathbf{D}$. Assume the reverse does not hold. Then, a path originating at an isolated solution of $(F + G)(\mathbf{x})$ in $\mathbf{D}$, defined by the homotopy $H(\mathbf{x}, t) = \mathbf{0}$, for $t: 1 \to 0$, should leave $\mathbf{D}$, which is impossible. □

The third assumption of Theorem 2.1 prevents a solution from leaving or entering the domain $\mathbf{D}$. Hence, to compute all solutions to the system $(F + G)(\mathbf{x}) = \mathbf{0}$ in the domain $\mathbf{D}$, the homotopy $H(\mathbf{x}, t) = F(\mathbf{x}) + tG(\mathbf{x})$ can be used. Note that Theorem 2.2 delivers also a homotopy for computing solutions outside a bounded domain, providing F and G are also analytic outside the domain.

3. Regional homotopy construction

This section is concerned with the practical realization of Rouchés theorem for computing all solutions to a Laurent polynomial system $F(\mathbf{x}) = \mathbf{0}$ in a bounded domain.

A regional homotopy continuation method can in general be described as:

(1) Search for a dominant part $F_{\partial\mathbf{D}}$ of F, so that the following holds:

$$\forall \mathbf{x} \in \partial\mathbf{D}: \quad \|F_{\partial\mathbf{D}}(\mathbf{x})\| > \|(F - F_{\partial\mathbf{D}})(\mathbf{x})\|.$$

This is the most crucial part of the method. Its effectiveness mainly relies on the estimators for finding lower and upper bounds for polynomials over some bounded domain. In the following subsections some product domains will be considered.

(2) Solve $F_{\partial \mathbf{D}}(\mathbf{x})=\mathbf{0}$.

As $F_{\partial \mathbf{D}}$ is only a part of F, its structure will be more sparse which makes it easier to solve.

(3) Follow the continuation paths defined by the homotopy

$$H(\mathbf{x},t)=F_{\partial \mathbf{D}}(\mathbf{x})+t(F-F_{\partial \mathbf{D}})(\mathbf{x}), \quad t\in\mathbb{C} \text{ for } t:0\rightarrow 1.$$

Classical continuation methods can be applied. Theorem 2.2 assures that only those solution curves starting at the solutions of $F_{\partial \mathbf{D}}(\mathbf{x})=\mathbf{0}$ in the domain $\partial\mathbf{D}$ need to be followed. It is important to note that the solutions of $F_{\partial \mathbf{D}}$ in $\mathbf{D}$ should be well conditioned in order to start the continuation without numerical difficulties. To establish the condition of the homotopy, one should tear the system apart in a random way, by leaving for some terms a small portion of them to the rest of the system. For a constant term c, this can be realized as follows: $c=c_{\partial \mathbf{D}}+(c-c_{\partial \mathbf{D}})$. One has some freedom in choosing the constant $c_{\partial \mathbf{D}}$ that will belong to the dominant part of the system.

As the method will be applied for systems of Laurent polynomial systems, some notation is needed. A multivariate (Laurent) polynomial can be described as

$$f(x)=\sum_{k=0}^{N} c_k \mathbf{x}^{q_k}, \quad c_k\in\mathbb{C},\ q_k\in\mathbb{Z}^n, \text{ where } \mathbf{x}^{q_k}=x_1^{q_{k1}}x_2^{q_{k2}}\cdots x_n^{q_{kn}},$$

using a multiindex notation. As also negative exponents are allowed, more general polynomials are considered, the so-called Laurent polynomials.

The following subsections propose a simple computational model which supports the automatic construction of a regional homotopy. Product domains will be considered: $\mathbf{D}=D_1\times D_2\times\cdots\times D_n$ with ∂D_k as border for the kth domain D_k. Then

$$\partial\mathbf{D}=\{\mathbf{x}=(x_1,x_2,\ldots,x_n) \mid \exists k: x_k\in\partial D_k\}.$$

3.1. Estimators based on radius

The first domain considered is a band centered around the origin of the complex plane. Fig. 1 pictures the domain for one component. For $\mathbf{x}\in\mathbf{D}$: $R_{mj}<|x_j|<R_{Mj}$, x_j being the jth component of $\mathbf{x}$, for $j=1,2,\ldots,n$.

The following propositions are trivial to prove:

Proposition 3.1. *Let* $f(\mathbf{x})=g(\mathbf{x})+c\mathbf{x}^q$, *with*

$$\forall\mathbf{x}\in\mathbf{D}: \quad |g(\mathbf{x})|<A \quad \textit{and} \quad |c\mathbf{x}^q|>B=|c|\prod_{j=1}^{n} R_{mj}^{q_j}.$$

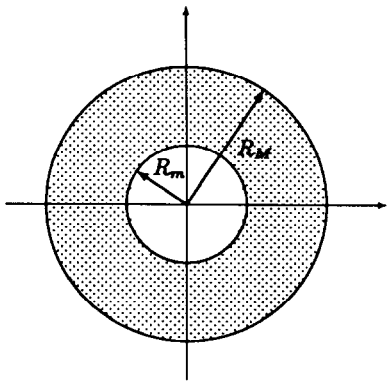

Fig. 1. $x \in D$: $R_m < |x| < R_M$.

Then

$$\forall \mathbf{x} \in \mathbf{D}: \quad |f(\mathbf{x})| \begin{cases} > B - A & \text{if } A < B, \\ \geqslant 0 & \text{otherwise.} \end{cases}$$

Proposition 3.2.

$$|f(\mathbf{x})| < \sum_{k=0}^{N} |c_k| \prod_{j=1}^{n} R_{Mj}^{q_{kj}}, \quad \forall \mathbf{x} \in \mathbf{D}.$$

Algorithm 1 applies Propositions 3.1 and 3.2, to estimate a lower bound for $|f(\mathbf{x})|$.

Algorithm 1. Computing a lower bound for $|f(\mathbf{x})|$.

1. Search for a term $c\mathbf{x}^{\mathbf{q}}$ in f for which $B = |c| \prod_{j=1}^{n} R_{mj}^{q_j}$ is maximal.
2. Let $f(\mathbf{x}) = g(\mathbf{x}) + c\mathbf{x}^{\mathbf{q}}$, as in Proposition 3.1.
   First apply Proposition 3.2 to compute A, an upper bound for g.
   Then Proposition 3.1 provides a lower bound for f.

The algorithm for searching for a dominant part $f_{\mathbf{D}}$ of a polynomial f over a domain $\mathbf{D}$ consists of considering all possible sums of k terms, starting at the term with the highest lower bound, for $k = 1, 2, \ldots, m$, where m equals the number of terms in f. When $f_{\mathbf{D}} = f$, f has no solutions in $\mathbf{D}$, as $|f_{\mathbf{D}}(\mathbf{x})| > 0$, $\forall \mathbf{x} \in \mathbf{D}$. This case can be referred to as a negative result, i.e. as an automatic proof that no solutions exist in $\mathbf{D}$.

Computing a dominant part $f_{\partial \mathbf{D}}$ on the border is presented in Algorithm 2.

Algorithm 2. Computing a dominant part $f_{\partial \mathbf{D}}$ on the border $\partial \mathbf{D}$.

for $k = 1, 2, \ldots, n$ do

1. Substitute x_k once by R_{mk} and once by R_{Mk}, values obtained when $x_k \in \partial D_k$.
   The resulting polynomials $g^{(k)}$ have $n-1$ unknowns and are to be considered over $(n-1)$-dimensional domains $\mathbf{D}^{(k)}$.

2. Compute $g_{\mathbf{D}^{(k)}}^{(k)}$ and collect the corresponding terms to construct $f_{\partial\mathbf{D}}^{(k)}$.
When all $2n$ dominant parts $f_{\partial\mathbf{D}}^{(k)}$ are the same, $f_{\partial\mathbf{D}} = f_{\partial\mathbf{D}}^{(k)}$,
otherwise no dominant part can be found in this way.

Example 3.1. Consider the following system:

$$F(\mathbf{x}) = \begin{cases} 4\,10^{-5}x_1^5x_2^2 + 2\,10^{-3}x_1x_2^4 + 2x_1^2x_2 - 2x_2 + 0.75 = 0, \\ 3\,10^{-4}x_1x_2^4 - 7\,10^{-6}x_1^3 + 2x_1x_2^2 - 2x_1 + 0.75 = 0. \end{cases}$$

According to Bézout's theorem, there are 35 isolated solution in two-dimensional complex space, while the total degree equals 35. The BKK bound equals 25, which means that for a general choice of the coefficients, this system would have 25 isolated solutions. Assume only the solutions for which $|x_k| < 1$, $k = 1, 2$ are wanted. Then the dominant part on the border of the domain is

$$F_{\partial\mathbf{D}}(\mathbf{x}) = \begin{cases} 2x_1^2x_2 - 2x_2 + 0.75 = 0, \\ 2x_1x_2^2 - 2x_1 + 0.75 = 0. \end{cases}$$

This system is sparser than F and has better scaled coefficients, which makes it easier to solve. It has exactly 5 real solutions, where only 2 of them lie inside the domain. Note that the 2-homogeneous Bézout number equals 5.

The norm $\|F\| = |f_1| + |f_2|$ will be used in the demonstration that $F_{\partial\mathbf{D}}$ is dominant on the border of the domain. The 5 real solutions of $F_{\partial\mathbf{D}}$ are also zeros of the multivariate function $\|F_{\partial\mathbf{D}}(\mathbf{x})\|$. This function, returning a real value, is monotone increasing as the distance of its argument $\mathbf{x}$ to the zeros is growing. All zeros are real, so the larger the imaginary parts of the components of $\mathbf{x}$ become, the larger $\|F_{\partial\mathbf{D}}\|$ will be. As we search for a lower bound for $\|F_{\partial\mathbf{D}}(\mathbf{x})\|$, $\mathbf{x} \in \partial\mathbf{D}$, it is sufficient to consider the points on $\partial\mathbf{D}$ which lie closest to the real zeros. Then it turns out that only bounds for $x_1 = \pm 1$ or $x_2 = \pm 1$ need to be computed, which results in $\|F_{\partial\mathbf{D}}(\mathbf{x})\| > 0.75$. The rest of the system $F - F_{\partial\mathbf{D}}$ is bounded by $\|(F - F_{\partial\mathbf{D}})(\mathbf{x})\| < 3 \times 10^{-3}$, $\forall \mathbf{x} \in \mathbf{D}$.

Hence, $F_{\partial\mathbf{D}}$ is a reliable start system. It has exactly 5 solutions where only 2 solutions lie in the domain. These 2 solutions will be used as start solutions in the regional homotopy to compute the wanted solutions of F.

Note that a regional homotopy can be very appropriate to solve illconditioned polynomial systems. As in the example above, some terms can have coefficients that are very small compared to the other coefficients. Omitting these terms makes the system well conditioned and hence easier to solve and renders often the desired solutions, avoiding the computation of the spurious solutions.

3.2. Estimators based on radius and argument

The second domain consists of taking a slice of the band. In this way not only conditions on the radius can be imposed, but also on the argument of a solution. Fig. 2 pictures the domain for one component, using polar coordinates. In order to take advantage of the restrictions on the argument, $0 < \theta_M - \theta_m < \pi$.

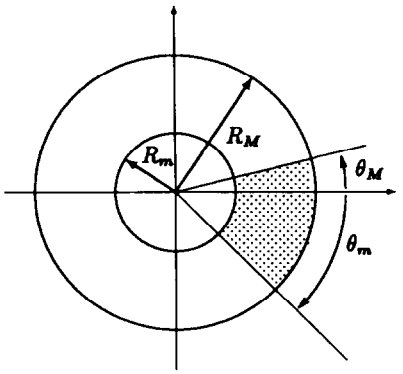

Fig. 2. $x = Re^{i\theta}$ with $R_m < R < R_M$, $\theta_m < \theta < \theta_M$.

More precise lower and upper bounds can now be given:

Proposition 3.3.

$$\forall a, b \in D: \; R_m |e^{i\theta_M} + e^{i\theta_m}| < |a+b| < 2R_M .$$

Proposition 3.4.

$$\forall a, b \in D: \; 0 \leqslant |a-b| < |R_M e^{i\theta_M} + R_m e^{i\theta_m}| .$$

These propositions introduce the line of thought for estimating bounds in the domain. Again, the proofs are visible.

First lower and upper bounds will be given for pairs of multivariate terms. The idea is to consider the terms as ordinary numbers in the complex plane as follows. Consider a term $c\mathbf{x}^{\mathbf{q}}$, with bounds on the kth unknown $x_k = R_k e^{i\theta_k}$: $R_{mk} < |x_k| < R_{Mk}$ and $\theta_{mk} < \theta_k < \theta_{Mk}$, for $k = 1, 2, \ldots, n$. When $c = |c| e^{i\gamma}$, then for radius R and argument θ of the term $c\mathbf{x}^{\mathbf{q}}$, one has the following bounds:

$$|c| \prod_{j=1}^{n} R_{mj}^{q_j} < R < |c| \prod_{j=1}^{n} R_{Mj}^{q_j} \quad \text{and} \quad \gamma + \sum_{j=1}^{n} q_j \theta_{mj} < \theta < \gamma + \sum_{j=1}^{n} q_j \theta_{Mj} . \tag{1}$$

The bounds (1) define a domain in the complex plane for a complex number $a = Re^{i\theta}$, which can replace the term $c\mathbf{x}^{\mathbf{q}}$. Computing lower and upper bounds for a multivariate polynomial is then transformed into estimating bounds for a sum of complex numbers.

Fig. 3 pictures two different domains $D_k = \{Re^{i\theta} \mid R_{mk} < R < R_{Mk}, \; \theta_{mk} < \theta < \theta_{Mk}\}$, $k = 1, 2$. Lower and upper bounds are provided by

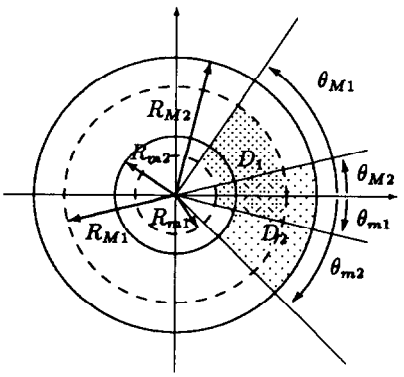

Fig. 3 Two different domains.

Proposition 3.5. $\forall a \in D_1, \forall b \in D_2$:

$$|a+b| \begin{cases} > \left| \sum_{k=1}^{2} R_{mk} e^{i\theta_k} \right| & \text{if } |\theta_{mk} - \theta_{M3-k}| < \pi, \text{ with } \theta_{mk} < \theta_k < \theta_{Mk}, \text{ for } k = 1,2, \text{ so that } |\theta_2 - \theta_1| \text{ is maximal,} \\ > R_{mk} - R_{M3-k} & \text{if } |\theta_{mk} - \theta_{M3-k}| \geqslant \pi, \text{ and } R_{mk} > R_{M3-k}, \text{ for } k = 1 \text{ or } 2, \\ \geqslant 0 & \text{otherwise} \end{cases}$$

Proposition 3.6.

$$\forall a \in D_1, \forall b \in D_2: \quad |a+b| < \left| \sum_{k=1}^{2} R_{Mk} e^{i\theta_k} \right|$$

with $\theta_{mk} < \theta_k < \theta_{Mk}$, $k = 1,2$, *so that* $|\theta_2 - \theta_1|$ *is minimal.*

The price for more precise bounds is the solution of an optimization problem. Propositions 3.5 and 3.6 can be generalized as follows:

Proposition 3.7. $\forall a_k \in D_k$:

$$\left| \sum_{k=1}^{N} a_k \right| \begin{cases} > \sqrt{\sum_{k=1}^{N} R_{mk}^2 + \sum_{k=1}^{N} \sum_{k \neq l} 2R_{mk} R_{ml} \cos(\theta_k - \theta_l)} \\ \qquad \text{if } |\theta_{mk} - \theta_{Ml}| < \pi, \ \forall k,l = 1,2,\ldots,N, \text{ with } \theta_{mk} < \theta_k < \theta_{Mk}, \\ \qquad \forall k = 1,2,\ldots,N, \text{ so that the right-hand side becomes minimal;} \\ > R - R_{Mk} \quad \text{if } |\theta_{mk} - \theta_{Ml}| \geqslant \pi \text{ for } k,l \in \{1,2,\ldots,N\}, \text{ with } \left| \sum_{j \neq k} a_j \right| > R > R_{Mk}; \\ \geqslant 0 \quad \text{otherwise.} \end{cases}$$

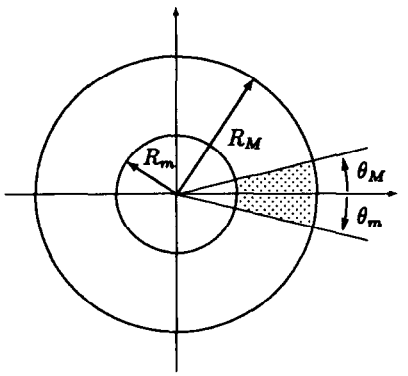

Fig. 4. A positive real domain.

Proposition 3.8.

$$\forall a_k \in D_k: \left| \sum_{k=1}^{N} a_k \right| < \sqrt{\sum_{k=1}^{N} R_{Mk}^2 + \sum_{k=1}^{N} \sum_{k \neq l} 2R_{Mk}R_{Ml}\cos(\theta_k - \theta_l)}$$

with $\theta_{mk} < \theta_k < \theta_{Mk}$, $k = 1, 2, \ldots, N$, *so that the right-hand side becomes maximal.*

The formulas in Propositions 3.7 and 3.8 do not look very encouraging for implementation. Therefore, a particular case will now be investigated. When all coefficients are real numbers and when only real solutions in a certain domain are desired, then it is sufficient to consider real domains, where the slices are centered around the real axis. Fig. 4 shows *a positive real domain* in one dimension, i.e. $\theta_m = -\theta_M$ and $|R_m \cos\theta_M| \approx R_m$. By reflection around the complex axis *a negative real domain* is obtained.

Proposition 3.9. *Let* D *be a real domain and* $\varepsilon = R_m - |R_m \cos\theta_M|$, *then* $\forall a, b \in D$: $2(R_m - \varepsilon) < |a+b| < 2R_M$.

Proposition 3.10. *Let* D_1 *and* D_2 *be two different real domains, both negative or positive. Let* $\varepsilon = \max(R_{m1} - |R_{m1}\cos\theta_{M1}|, \; R_{m2} - |R_{m2}\cos\theta_{M2}|)$, *then* $\forall a \in D_1$, $\forall b \in D_2$: $R_{m1} + R_{m2} - 2\varepsilon < |a+b| < R_{M1} + R_{M2}$.

The generalization to sums of N terms is straightforward.

Bounds for a polynomial f with real coefficients and unknowns belonging to the multidimensional real domain **D** can be estimated as proposed in Algorithm 3.

Algorithm 3. Computing bounds for $|f(\mathbf{x})|$ over **D**.

1. Apply transformations (1) to obtain new bounds which define one-dimensional real domains for the individual terms in the sum S.
2. Write S as $S = S_P + S_N$, where S_P groups the terms belonging to positive domains and S_N contains those in negative domains.

3. By application of the generalized version of Proposition 3.10, lower and upper bounds can be computed, which results in $A_N < |S_N| < B_N$ and $A_P < |S_P| < B_P$.
4. Then $\forall \mathbf{x} \in \mathbf{D}$:

$$|f(\mathbf{x})| < \max(|B_P - A_N|, |B_N - A_P|) \quad \text{and} \quad |f(\mathbf{x})| \begin{cases} > |A_P - B_N| & \text{if } A_P > B_N, \\ > |A_N - B_P| & \text{if } A_N > B_P, \\ \geqslant 0 & \text{otherwise.} \end{cases}$$

Algorithm 4 proposes a way for computing a dominant part of f over a real domain $\mathbf{D}$.

Algorithm 4. Computing a dominant part $f_{\mathbf{D}}$ over a real domain $\mathbf{D}$.

1. Apply transformations (1) and group the terms in the sum S as $S = S_P + S_N$, as in Algorithm 3, to obtain lower bounds A_P and A_N and upper bounds B_P and B_N for S_P and S_N respectively.
2. If $A_P > B_N$ or $A_N > B_P$,
   then a dominant part $f_{\mathbf{D}}$ consist of the terms which lie
   after transformation in the positive or the negative domains,
   otherwise terms should be moved from the one part into the other one.
3. In case $f_{\mathbf{D}}$ has been found, one can try to enumerate all possible subsets of its terms in order to find a dominant part with the smallest number of terms.

Algorithm 2, proposed at the end of Section 3.1, can be applied for computing a dominant part $f_{\partial \mathbf{D}}$. But then only where the geometry of the border coincides with that of the first type of domain, as pictured in Fig. 1. Here the second type of domain, drawn in Fig. 2 for one dimension, is considered. A point on the border of the domain of the second type, denoted by $x = Re^{i\theta}$, belongs either to a circular part, when its modulus R remains constant ($R \in \{R_m, R_M\}$), or lies on a diagonal part of $\partial \mathbf{D}$, when its argument θ is fixed ($\theta \in \{\theta_m, \theta_M\}$). In order to deal with these diagonal parts of the border, one has to work with real homotopies, as is explained next.

3.3. Real homotopies over real domains

The great advantage of real domains is the possibility of obtaining more precise estimates for the polynomials over a certain domain. The problem with real domains is the fact that estimating over the border $\partial \mathbf{D}$ can be real burden, when it comes to considering the diagonal parts close to the real axis. Applying real homotopies provides an effective solution.

The behavior of the solution paths of real homotopies for solving real polynomial systems has been studied by Li and Wang, see [23], and applied in [18, 24]. The main result of their paper shows that, generically, the solution set of a real homotopy contains no singular point other than a finite number of quadratic turning points. We refer to [23] for technical and theoretical details. Here only the practical importance of the result of Li and Wang will be discussed.

In a real homotopy, each complex solution path has a conjugate solution path. At a quadratic turning point, the two conjugate complex solution paths meet. When passing through such a point, the two complex paths turn into two real paths. The reverse process is sketched in Fig. 5, in the complex plane, for one unknown.

As $t: t_0 \to t_1$, the two real solutions $\triangleright$ and $\triangleleft$ approach each other along the real axis. They meet at the quadratic turning point, when $t = t_1$, and turn into the complex plane, where they move further as a conjugate pair, as $t: t_1 \to t_2$.

In many practical applications, the components of real solutions are scattered in different real domains. Fig. 6 shows the behaviour of the paths for a real homotopy when the two real solutions lie initially in two different (one positive and one negative) real domains.

There is only one way for the solutions to meet and to turn into the complex plane. Namely, by violating the circular inner borders of the domain. Which is impossible, as the start system is dominant on the border.

In general, if the dominant part of the system has for each component at most one solution in a real domain, then all solutions will remain in their domain during continuation, provided of course that a real homotopy is used. Hence, when dealing with real domains, real homotopies are required.

When two real solutions lie initially in the same domain, the two solutions can meet each other inside the real domain and turn over to the complex plane after crossing the diagonal lines close to the real axis. This case can be avoided, by applying a linear

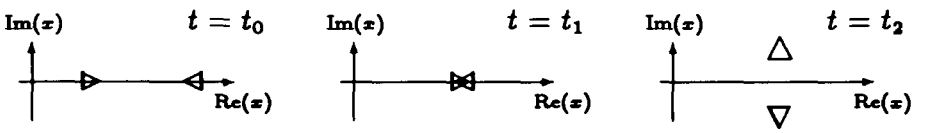

Fig. 5. Behavior at a quadratic turning point.

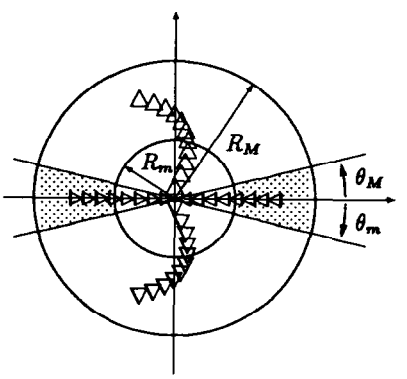

Fig. 6. A real homotopy.

transformation on the system, which places the origin between the solutions, as in Fig. 6.

3.4. *Customizing the norm* $\|\cdot\|$

Recall that the third condition of the multivariate Rouché's theorem has to be valid for *some* norm $\|\cdot\|$. This subsection is concerned about customizing the norm to the given problem by the solution of a linear program.

Consider the following class of norms:

$$\|F\| = \sum_{l=1}^{n} a_l |f_l|, \quad \text{with } a_l \geqslant 0 \text{ and } \prod_{l=1}^{n} a_l \neq 0. \tag{2}$$

Let the following bounds be given: $R_{mk} < |x_k| < R_{Mk}$, for $k = 1, 2, \ldots, n$, which define a domain $\mathbf{D}$. Given a part $F_{\partial \mathbf{D}}$ of the system F, one can formulate conditions on the constants a_l in (2) so that $F_{\partial \mathbf{D}}$ is dominant on the border of the domain $\mathbf{D}$, w.r.t. the norm defined by those constants.

In order that $F_{\partial \mathbf{D}}$ is dominant on the border, the following conditions should be satisfied:

$$\forall \mathbf{x} \in \partial \mathbf{D}: \quad \|F_{\partial \mathbf{D}}(\mathbf{x})\| > \|F(\mathbf{x})\|. \tag{3}$$

With the results of the previous subsection in mind, one has only to consider the circular parts of the domain. The conditions (3) are then equivalent to the following set of inequalities.:

$$\begin{aligned} \forall \mathbf{x} \in \partial \mathbf{D}: \quad & \sum_{l=1}^{n} a_l |f_{\partial \mathbf{D}1}(x_1, \ldots, x_k = R, \ldots, x_n)| \\ & > \sum_{l=1}^{n} a_l |(f_l - f_{\partial \mathbf{D}1})(x_1, \ldots, x_k = R, \ldots, x_n)|, \end{aligned} \tag{4}$$

with $R \in \{R_{mk}, R_{Mk}\}$, $k = 1, 2, \ldots, n$, $l = 1, 2, \ldots, n$.

Apply Algorithm 3 to compute estimates A_{lkj} and B_{lkj} for lower bounds for $|f_{\partial \mathbf{D}1}|$ and for upper bounds for $|f_l - f_{\partial \mathbf{D}1}|$ respectively. Let $j = 1$ when $x_k = R_m$ and $j = 2$ when $x_k = R_M$. The inequalities (4) can then be rewritten as

$$\sum_{l=1}^{n} a_l A_{lkj} > \sum_{l=1}^{n} a_l B_{lkj}, \quad \text{with } k = 1, 2, \ldots, n \text{ and } j = 1, 2. \tag{5}$$

Equivalently,

$$\sum_{l=1}^{n} a_l (B_{lkj} - A_{lkj}) < 0, \quad \text{with } k = 1, 2, \ldots, n \text{ and } j = 1, 2. \tag{6}$$

In order to keep the coefficients a_l bounded, add $\sum_{l=1}^{n} a_l \leqslant C$, $C > 0$ to the constraints (6). Choose a small positive constant ε. Then the following standard linear

program is left to solve:

$$\max \sum_{l=1}^{n} a_l \text{ subject to } \begin{cases} \sum_{l=1}^{n} a_l(B_{lkj} - A_{lkj}) \leqslant \varepsilon, \quad k = 1,2,\ldots,n, \ j = 1,2 \\ \sum_{l=1}^{n} a_l \leqslant C \quad \text{and} \quad a_l \geqslant 0, \ l = 1,2,\ldots,n \end{cases} \tag{7}$$

If a feasible solution is found, $F_{\partial \mathbf{D}}$ dominates the rest of F on the circular parts of the border.

4. Applications

Two classes of applications can efficiently be attacked by regional homotopy methods: illconditioned systems and systems with a special structure. The first class seems to be typical for chemical equilibrium problems, where the existence of some terms with extreme coefficients introduce spurious solutions making the system hard to solve. The second class consists of special structured systems, such as eigenvalue problems and matrix polynomials. The start system can here be either a linear system or a decoupled system of univariate polynomials. For both classes, the choice of the dominant part is obvious, but of course applications exist where the combinatorial dominant part computing algorithms presented in the previous section can lead to discoveries.

The problems considered here have been taken out of the literature. So, no original problems will be solved. The importance of this section lies in the unifying approach of the methods presented. Regional homotopy methods seem to be applicable to different problem areas where polynomial systems occur.

Before proceeding, let us take a look at the armament used in attacking the problems. First of all, a software package [38] providing a homotopy continuation environment and equipped with homotopy methods exploiting Newton polytopes, developed in [41], are at our disposal. The implementations of the algorithms for estimating bounds have been added to the software environment, as also some elementary LP routines.

(1) Consider the following system:

$$F_1(\mathbf{x}) = \begin{cases} 1.069\,10^{-4}x_1^4 + 2\,10^4 x_1^3 x_2 + x_1^3 - 1.8\,10^{-10}x_1 - 1.283\,10^{-24} = 0, \\ 2\,10^{16}x_1 x_2^2 + 10^{14}x_2^2 - 1 = 0. \end{cases}$$

This is a chemical equilibrium problem, known as Butler's problem. See [27, Ch. 9] for a general introduction to the derivation of polynomial systems out of chemical problems. In [25, 26], a description of the solution list can be found. There are 7 real solutions and 2 complex solutions. 4 real solutions have a physical meaning and appear in a symmetrical pattern. They are bounded by $10^{-6} < |x_1| < 10^{-4}$ and $10^{-9} < |x_2| < 10^{-6}$. The other 3 real solutions lie our of range: 2 too small, 1 too large.

The total degree equals 12, the BKK bound is 9. As this number is small, the system could be solved easily. However, the extreme coefficients cause great numerical difficulties to most path trackers. Therefore scaling the homotopy is a necessity. As the location of the roots is important, only equation scaling will be used, not variable scaling, see [27, Ch. 5]. The first equation will be divided by 10^4, the second one by 10^{16}.

On the negative real domain, with bounds on radii $10^{-7}<|x_k|<1$, $k=1,2$, the following system is dominant on the border:

$$F'_{1\partial\mathbf{D}}(\mathbf{x})=\begin{cases} 2x_1^3x_2+10^{-4}x_1^3=0 \\ 2x_1x_2^2+10^{-2}x_2^2=0 \end{cases} \quad \text{or equivalently} \quad \begin{cases} x_1^3(2x_2+10^{-4})=0 \\ x_2^2(2x_1+10^{-2})=0. \end{cases}$$

This system has 7 real solutions: $(0,0)$ with multiplicity 6 and $(-0.5\,10^{-3}, -0.5\,10^{-5})$. The last solution is the spurious solution that is too large. Note that the pair of complex solutions is already left out. But $F'_{1\partial\mathbf{D}}$ contains too few terms, as it is now impossible to distinguish the physical solutions from the two other solutions and moreover, the singular solution $(0,0)$ cannot be used as a start solution.

The dominant part of F_1 should contain more terms. We can add more terms to $F'_{1\partial\mathbf{D}}$, preserving the product structure, so that it remains trivial to solve it. On the positive real domain bounded by $10^{-6}<|x_1|<10^{-4}$ and $10^{-9}<|x_2|<10^{-6}$, consider the following:

$$F_{1\partial\mathbf{D}}(\mathbf{x})=\begin{cases} x_1(x_1-10^{-5})(x_1+10^{-5})(2x_2+10^{-4})=0, \\ (x_2-10^{-7})(x_2+10^{-7})(2x_1+10^{-2})=0. \end{cases}$$

Then

$$(F_1-F_{1\partial\mathbf{D}})(\mathbf{x})=\begin{cases} 2\,10^{-10}x_1x_2-0.80\,10^{-14}x_1-1.283\,10^{-28}=0, \\ 2\,10^{-14}x_1=0. \end{cases}$$

$F_{1\partial\mathbf{D}}$ has again 7 real solutions, but now the 4 physical solutions are clearly separated from the other ones. To prove that $F_{1\partial\mathbf{D}}$ dominates $F_1-F_{1\partial\mathbf{D}}$ on the border of the domain, it is important to preserve the product structure of $F_{1\partial\mathbf{D}}$ while estimating. The implemented algorithms gave too low lower bounds, especially for the first equation, on the borders for x_1. The start solutions are that good, that no continuation is needed, a couple of simple Newton–Raphson iterations are sufficient to calculate the desired solutions.

(2) Another chemical equilibrium problem has been stated in [26]:

$$F_2(\mathbf{x})=\begin{cases} x_1x_2+x_1-3x_5=0, \\ 2x_1x_2+x_1+2R_{10}x_2^2+x_2x_3^2+R_7x_2x_3+R_9x_2x_4+R_8x_2-Rx_5=0, \\ 2x_2x_3^2+R_7x_2x_3+2R_5x_3^2+R_6x_3-8x_5=0, \\ R_9x_2x_4+2x_4^2+4Rx_5=0, \\ x_1x_2+x_1+R_{10}x_2^2+x_2x_3^2+R_7x_2x_3+R_9x_2x_4 \\ \qquad +R_8x_2+R_5x_3^2+R_6x_3+x_4^2-1=0. \end{cases}$$

The total degree equals 108, but there are only 4 real and 12 complex solutions.

Table 1
The coefficients for F_2

R	10
R_5	$1.9300\,10^{-1}$
R_6	$4.1062\,10^{-4}$
R_7	$5.4518\,10^{-4}$
R_8	$4.4975\,10^{-7}$
R_9	$3.4074\,10^{-5}$
R_{10}	$9.6150\,10^{-7}$

The BKK bound equals 16. The constants R and R_j, $j=5,6,\ldots,10$ are listed in Table 1.

Only the 4 real solutions have a physical meaning. Define a real domain **D** with the following bounds on the radii: $10^{-3}<|x_k|<10^2$, $\forall k=1,2,\ldots,5$.

Considering the system, given the coefficients in Table 1, one notes that the constants R_j, $j=6,\ldots,10$, introduce coefficients in the system which are of a lower magnitude than the other ones. It is natural to eliminate those terms whose coefficients are in modulus smaller than 10^{-3}. The result is the system $F_{2\partial\mathbf{D}}$ which is dominant on the border of the domain.

$$F_{2\partial\mathbf{D}}(\mathbf{x})=\begin{cases} x_1x_2+x_1-3x_5=0,\\ 2x_1x_2+x_1+x_2x_3^2-Rx_5=0,\\ 2x_2x_3^2+2R_5x_3^2-8x_5=0,\\ 2x_4^2+4Rx_5=0,\\ x_1x_2+x_1+x_2x_3^2+R_5x_3^2+x_4^2-1=0. \end{cases}$$

The system $F_{2\partial\mathbf{D}}$ has fewer terms and a BKK bound equal to 8. There are 4 real solutions, which serve as start solutions for computing the desired solutions to F.

(3) Systems occurring in the analysis of nonlinear circuits and neural networks [36] have a typical structure like

$$F(\mathbf{x})=\mathbf{A}G(\mathbf{x})+\mathbf{B}\mathbf{x}+\mathbf{c}=\mathbf{0}, \quad \text{with } \mathbf{A},\mathbf{B}\in\mathbb{R}^{n\times n}, \quad \mathbf{c}\in\mathbb{R}^n,$$

and $g_k(\mathbf{x})=g_k(x_k)$, where the polynomials g_k are univariate, for $k=1,2,\ldots,n$.

One of the most simple examples [36, p. 74] is the following

$$F_3(\mathbf{x})=\begin{cases} 0.081x_1^3-2.04x_1^2+13.6x_1+x_1+x_2-69=0,\\ 0.081x_2^3-2.04x_2^2+13.6x_2+x_1+x_2-75=0. \end{cases}$$

It has 1 real solution and 8 complex ones. A regional homotopy continuation method can provide a start solution, already very close to the real solution. It is natural to take the decoupled system of univariate polynomials as dominant part, leaving all terms x_l, $l\neq k$ to the kth equation of the rest of the system. Solving 2 third degree equations yields a start solution. For F_3, the considered real domain imposed

the following restrictions on the radius of the unknowns: $|x_k| < 50$, $k = 1, 2$. Over this domain, the linear program turned out to have feasible solution, hereby proving that the decoupled system is dominant on the border. By the choice of appropriate bounds, the first significant number of each solution component was already correct, which makes the continuation process fast and reliable. It has one real solution and 8 complex ones.

When the classical homotopy is used, based on the total degree, no diverging paths will occur, but for general n, the complexity of computing 3^n paths is a cost too large for obtaining one real solution. As the univariate equations are symmetrical, one has only to solve one instead of n third degree equations.

(4) Homotopy continuation methods for solving (generalized) eigenvalue problems were first presented in [5], the polynomial system can be described as

$$F(\mathbf{x}, \lambda) = \begin{cases} \left(\sum_{l=0}^{k} A_l \lambda^l \right) \mathbf{x} = \mathbf{0}, \\ \sum_{l=1}^{n} x_l^2 - 1 = 0. \end{cases}$$

For general matrices A_l, there are kn eigenpairs. They can be computed by using the homotopy developed in [5]. For the classical eigenvalue problem $\mathbf{Ax} = \lambda \mathbf{x}$, it only seldomly occurs that all eigenpairs are wanted. In [18] the concept of Order Preserving Property was introduced, stating that the real homotopies presented there preserve the order between different eigenvalues, as solution paths each other never cross during continuation. This line of thought has in [24] been generalized and applied to nonsymmetric matrices. In [23], the approach of real homotopies has been worked out in general for real polynomial systems.

Consider the following simple eigenvalue problem:

$$\lambda \mathbf{x} = \mathbf{A}\mathbf{x} \quad \text{with } \mathbf{A} = \begin{bmatrix} 10 & -1 & 0.5 \\ -1 & 20 & -4 \\ 2 & -1.5 & 38 \end{bmatrix}$$

Suppose only the largest eigenvalue is desired. As the elements on the diagonal of $\mathbf{A}$ are larger then the other entries, it is natural to take $\mathbf{D} = \text{diag}(10, 20, 38)$ as matrix for the initial eigenvalue problem.

The largest eigenvalue of $\mathbf{D}$ equals 38 and can be associated with the third unit vector $(0, 0, 1)$. Take as norm $\|F\| = |f_3|$. Then on the border of the real domain, defined by

$$0 < |\lambda| < 30, \qquad 0 < |x_k| < 1.001, \qquad k = 1, 2 \quad \text{and} \quad 0.999 < |x_3| < 1.001,$$

the system $\lambda \mathbf{x} - \mathbf{D}\mathbf{x} = \mathbf{0}$ is dominant over the rest of the original eigenvalue problem.

Assume the first or second eigenvalue becomes the largest during continuation. Then for some $t = t_0$, $|t_0| \leqslant 1$, there is a solution path with $\lambda = 30$, because a real homotopy will be used. But on $\partial \mathbf{D}$, $H(\mathbf{x}, t) \neq 0$. Hence, it is sufficient to compute only the path starting at the largest eigenvalue of $\lambda \mathbf{x} - \mathbf{D}\mathbf{x} = \mathbf{0}$.

5. Conclusion

It is possible to construct homotopies for computing only the solutions in a bounded domain. This paper gives conditions on the homotopy and proposes homotopy construction methods. When it comes to computing the real solutions of real polynomial systems, the regional homotopy has to be a real homotopy. In this case, regional homotopies can on the one hand be considered as a general application of real homotopies. On the other hand, the conditions of Rouché's theorem provide a useful tool for the construction of a reliable real homotopy.

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