

Fitting Curves and Surfaces With Constrained Implicit Polynomials

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Abstract—A problem which often arises while fitting implicit polynomials to 2D and 3D data sets is the following: Although the data set is simple, the fit exhibits undesired phenomena, such as loops, holes, extraneous components, etc. Previous work tackled these problems by optimizing heuristic cost functions, which penalize some of these topological problems in the fit. This paper suggests a different approach—to design parameterized families of polynomials whose zero-sets are *guaranteed* to satisfy certain topological properties. Namely, we construct families of polynomials with star-shaped zero-sets, as well as polynomials whose zero-sets are guaranteed not to intersect an ellipse circumscribing the data or to be entirely contained in such an ellipse. This is more rigorous than using heuristics which may fail and result in pathological zero-sets. The ability to parameterize these families depends heavily on the ability to parameterize positive polynomials. To achieve this, we use some powerful recent results from real algebraic geometry.

Index Terms—Implicit polynomials, fitting, free-form shapes, topological integrity, starshaped curves and surfaces, positive polynomials.

1 INTRODUCTION

FITTING analytic functions to sampled data is a common problem arising in many data modeling applications. In its most general form, the fitting problem is: Given a set of n data points

$$S = \{\bar{x}^i = (x_1^i, \dots, x_d^i) \in \mathcal{R}^d : i = 1, \dots, n\},$$

find an analytic surface that passes “close” to S . Common representations of such a surface are parametric surfaces defined on \mathcal{R}^{d-1} or zero-sets of a function $F: \mathcal{R}^d \rightarrow \mathcal{R}$. The latter is the locus of all points \bar{x} such that $F(\bar{x}) = 0$. Candidates for F are any interpolant over \mathcal{R}^d , e.g., radial basis functions, super-quadrics, thin-plate splines, or polynomials. In the latter, the number of degrees of freedom, i.e., polynomial coefficients, is

$$m = \binom{d+k}{k},$$

where k is the degree of the polynomial.

The advantages of using an implicit polynomial are its simplicity, the possibility to compute algebraic invariants [5], [4], [9], [7], [13], and the ease of containment computations (by computing the sign of the polynomial). The simplest way of fitting an implicit polynomial to the data set S is to solve the following least-squares problem for the coefficient vector \bar{a} of the polynomial $P_{\bar{a}}$:

$$\bar{a} = \arg \min_{\bar{a} \in \mathcal{R}^m} \sum_{i=1}^n P_{\bar{a}}(\bar{x}^i)^2. \quad (1)$$

This cost function minimized in (1) is simple; therefore, the problem may be solved easily by an eigenvector computation. However, the cost function does not necessarily express the Euclidean distances of the data points to the zero-surface; therefore, the fit might be somewhat unintuitive, especially in regions of high surface curvature, as has been shown in previous works [16], [8], [15]. A cost function that approximates the sum of the squares of the Euclidean distances is:

$$\bar{a} = \arg \min_{\bar{a} \in \mathcal{R}^m} \sum_i \left(\frac{P_{\bar{a}}(\bar{x}^i)}{\|\nabla P_{\bar{a}}(\bar{x}^i)\|} \right)^2, \quad (2)$$

where $\nabla P(\bar{x}) = (\partial P / \partial x_1, \dots, \partial P / \partial x_d)$ is the vector gradient function. Unfortunately, this cost function induces a nonlinear least-squares problem, whose numerical solution suffers from the usual non-linear optimization algorithmic pitfalls, namely, slow iterative solution, and local minima. If computation time is not a factor, as is the case in some applications, a solution to (2) is usually superior to that of (1). Because of its rational form, (2) may be solved iteratively as a sequence of *weighted* linear least squares problems [8], [15], [12], [2], which is a numerical procedure more efficient than general purpose optimization.

The disadvantages of using implicit polynomials as a modeling tool are the quality of the results commonly obtained when applying the above procedures, especially for high degrees. The zero-sets may consist of multiple components, be unbounded, or fit the data in very unnatural ways [8], [16], [15]. It is very difficult to predict the outcome of the fitting procedure, a problem compounded by the fact that the polynomial coefficients are geometrically meaningless. A typical data-fitting session consists of running the optimization procedure (2) again and again, obtaining local minima, and choosing that yielding the best solution. Many

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trials may be required until a pleasing fit is found. In some cases, the procedure seems to never end, in the sense that the pleasing local minima are so sparse, that it is virtually impossible to stumble on them at random. An open question is how to restrict the search space to a subset of “well-behaved” polynomials, thus reducing the number of trials until success.

The main question is how to compactly represent, i.e., parameterize, this family of well behaved polynomials by imposing some restrictions on the polynomial coefficients. In [8], [16], it is shown how to guarantee that the zero-set is bounded. These works also suggested heuristics to force the zero-set to be small and “tight” around the data set. The effort to achieve pleasing fits was carried further in [14], where it was suggested to use the geometric distance (as opposed to algebraic distance) in order to fit implicit polynomials. This resulted in better fits without holes. Also, a method to eliminate extraneous components was suggested. In [11], polynomials with a convex zero set are fitted to convex polygons so that their zero set contains the polygon; the degree of the polynomial is equal to the number of vertices in the polygon. In [1], polynomials whose zero set is guaranteed not to have folds within a certain region are constructed and many such “A-patches” are used to describe shapes. In work reported recently in [10], an attempt is made to force the zero-set to “stick” to the data, thus hopefully minimizing the number of branches, etc., in the zero-set.

However, the algorithms presented in [8], [16], [14] are heuristic in nature. They try to force the resulting fits to have certain “good” geometric properties (such as being “tight” around the data set) by minimizing a cost function that penalizes fits which are “not good.” In this work, we suggest a different approach—find a parameterization of a (large as possible) subfamily of polynomials whose zero-sets *always* have these “good” properties and restrict the search for a pleasing fit to this subfamily. This guarantees that the fit will be “good” and eliminates the necessity of using a penalizing function.

Some problems which arise quite often in the fitting process cannot be eliminated using previous methods, as demonstrated in Fig. 1, where an “area-minimizing” fit [8] was used. The cusps in the data result in loops in the zero-set—a rather common phenomena; note that this happens even though the data sets are not complicated. Previous methods, which penalized “holes” in the zero-set, as well as extraneous components, cannot eliminate these loops, as they pose a different type of problem. When the method for fitting star-shaped sets suggested in this paper was used, there were no such topological pathologies in the fits.

The purpose of this paper is to present novel algebraic techniques through which the coefficients of polynomials contained in well-behaved subsets may be parameterized. Specifically, we apply our techniques to generate star-shaped objects, and objects bounded within simpler objects, e.g., the unit sphere, or an ellipse.

We note that it is easy to modify the methods presented here to generate fits to convex objects, such that these fits will be guaranteed to be convex; however, we did not pursue this direction, since the assumption that the object is convex is a strong limitation.

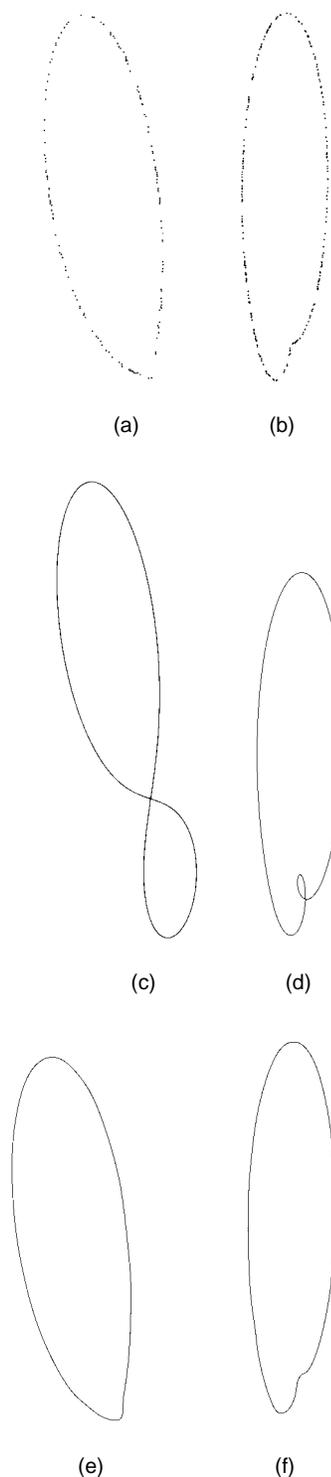


Fig. 1. (a), (b) Data sets and (c), (d) “area minimizing” fits to them; note spurious loops which the fitting process cannot eliminate. (e) and (f) are fits obtained using the “focus of expansion” method suggested in this paper (see Section 3.3).

2 THE GENERAL METHOD

We are interested in restricting our search to a subset of the polynomials with given characteristics. The question becomes how to easily parameterize that subset. In general, we will not be able to parameterize precisely the subset we are interested in, but a smaller subset of it, since we are able

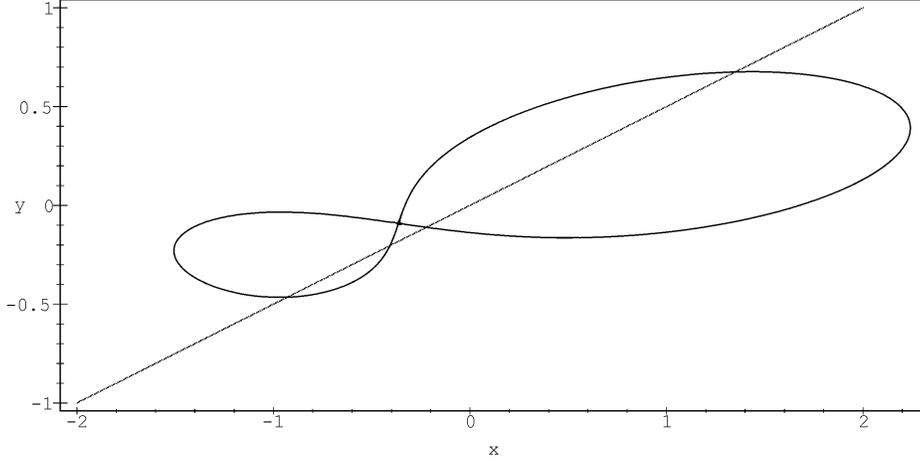


Fig. 2. An illustration of how the line convexity condition eliminates extraneous loops in the zero-set.

to formulate only sufficient (but not necessary) conditions for a polynomial to have the given characteristics. These conditions lead to an unconstrained search on a parameter space, whose dimension might be larger than the dimension of the original polynomial space. This is because our techniques lead to an *over-representation* of the subset. This imposes some extra numerical overhead.

3 STAR-SHAPED OBJECTS

In this section, methods to enforce the zero-set to be star-shaped will be described. Recall that a closed curve is star-shaped if there is an interior point S from which the whole curve is visible; that is, every ray emanating from S intersects the curve exactly once. Such a point is called a *kernel point*. For simplicity, we shall assume that this point is the origin; however, it is trivial to incorporate into the algorithm a step which will attempt to look for a different kernel point, by simply allowing the fitted polynomial to translate.

As demonstrated in Figs. 1c and 1d and in [8], some fits to star-shaped data sets may have pathologies in them—holes, loops, “folds,” extraneous components. Such pathologies are avoided by forcing the “line convexity” and “focus of expansion” conditions we now introduce; these conditions, together with the fact that the data set is star-shaped, ensure that the fit will also be star-shaped and, therefore, devoid of such pathologies.

3.1 First Method: Line Convexity

This method forces the zero-set to be star-shaped by allowing every line through a given point to intersect it only twice. For instance, let us see how the extraneous loop in Fig. 1c would be eliminated; note, in Fig. 2, how the line through the origin intersects the zero-set four times. Similarly, extraneous components will also be eliminated.

We can force this condition in the following way, demonstrated for a quartic polynomial in two variables x and y :

$$P(x, y) = a_{40}x^4 + a_{31}x^3y + a_{22}x^2y^2 + a_{13}xy^3 + a_{04}y^4 + a_{30}x^3 + a_{21}x^2y + a_{12}xy^2 + a_{03}y^3 + a_{20}x^2 + a_{11}xy + a_{02}y^2 + a_{10}x + a_{01}y + a_{00}.$$

The value of $P(x, y)$ on a line $y = \alpha x$ through the origin is

$$P_\alpha(x) = (a_{40} + a_{31}\alpha + a_{22}\alpha^2 + a_{13}\alpha^3 + a_{04}\alpha^4)x^4 + (a_{30} + a_{21}\alpha + a_{12}\alpha^2 + a_{03}\alpha^3)x^3 + (a_{20} + a_{11}\alpha + a_{02}\alpha^2)x^2 + (a_{10} + a_{01}\alpha)x + a_{00}.$$

If a line through the origin intersects the zero-set in more than two points, then $P_\alpha(x)$ will have more than two roots. By applying Roll’s theorem twice, it follows that $\frac{d^2}{dx^2}P_\alpha(x)$ should have at least one root. To prevent this, we require that $\frac{d^2}{dx^2}P_\alpha(x)$ be positive for every x and α . This actually forces the restriction of $P(x, y)$ to every straight line through the origin to be convex (as a function of one variable), hence the term “line convexity”.

$$\frac{d^2}{dx^2}P_\alpha(x) = 12(a_{40} + a_{31}\alpha + a_{22}\alpha^2 + a_{13}\alpha^3 + a_{04}\alpha^4)x^2 + 6(a_{30} + a_{21}\alpha + a_{12}\alpha^2 + a_{03}\alpha^3)x + 2(a_{20} + a_{11}\alpha + a_{02}\alpha^2),$$

which, for brevity, we will denote by

$$P_4(\alpha)x^2 + P_3(\alpha)x + P_2(\alpha).$$

Now, suppose that there exist polynomial functions $K(\alpha)$, $L(\alpha)$, and $M(\alpha)$ such that

$$P_4(\alpha) = K^2(\alpha) + L^2(\alpha)$$

$$P_3(\alpha) = 2L(\alpha)(K(\alpha) + M(\alpha)) \quad (3)$$

$$P_2(\alpha) = L^2(\alpha) + M^2(\alpha).$$

Then, for every α , $\frac{d^2}{dx^2}P_\alpha(x)$ is a polynomial in x with a discriminant equal to

$$P_3(\alpha)^2 - 4P_4(\alpha)P_2(\alpha) = -4(L^2(\alpha) - K(\alpha)M(\alpha))^2,$$

which is negative for every α . This means that, when viewed as a polynomial in x , the second derivative is everywhere positive, from which it follows that $P_\alpha(x)$ is indeed convex along every line that passes through the origin.

Since $P_2(\alpha)$ is a quadratic in α , it follows that $K(\alpha)$ and $M(\alpha)$ cannot be more than linear in α . Similarly, since $P_4(\alpha)$

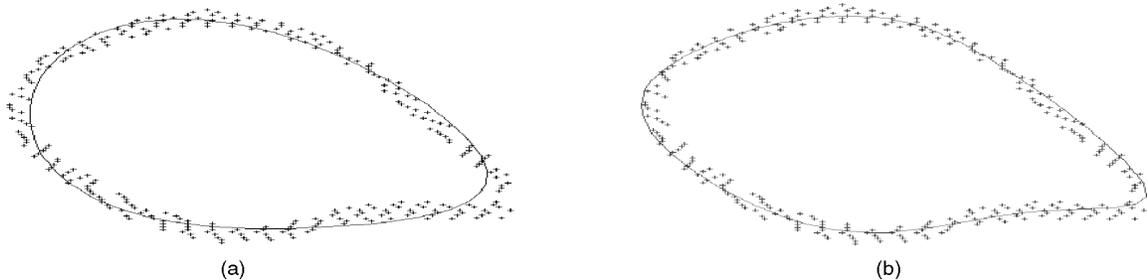


Fig. 3. Fitting an eye with (a) a quartic having 10 degrees of freedom and (b) with a quartic which also satisfies the "line convexity" condition, but has the full 15 degrees of freedom, described by (4).

is a quartic in α , $K(\alpha)$ cannot be more than quadratic in α .

Denoting $L(\alpha) = l_1\alpha + l_0$, $M(\alpha) = m_1\alpha + l_0$, and $K(\alpha) = k_2\alpha^2 + k_1\alpha + k_0$, results in the following parameterization for $P(x, y)$:

$$\begin{aligned} a_{04} &= \frac{k_2^2}{12}, a_{13} = \frac{k_2k_1}{6}, a_{22} = \frac{k_1^2}{12} + \frac{l_1^2}{12} + \frac{k_2k_0}{6} \\ a_{31} &= \frac{k_1k_0}{6} + \frac{l_1l_0}{6}, a_{40} = \frac{k_0^2}{12} + \frac{l_0^2}{12}, a_{03} = \frac{l_1k_2}{3} \\ a_{12} &= \frac{l_1k_1}{3} + \frac{l_1m_1}{3} + \frac{l_0k_2}{3}, a_{21} = \frac{l_1k_0}{3} + \frac{l_1m_0}{3} + \frac{l_0k_1}{3} + \frac{l_0m_1}{3}, \\ a_{30} &= \frac{l_0k_0}{3} + \frac{l_0m_0}{3}, a_{02} = \frac{l_1^2}{2} + \frac{m_1^2}{2}, a_{11} = l_1l_0 + m_1m_0, \\ a_{20} &= \frac{l_0^2}{2} + \frac{m_0^2}{2} \end{aligned}$$

and a_{10} , a_{01} , a_{00} are free.

This is a parameterization for a subset of the family of quartics in two variables which have star-shaped zero-sets.

However, the dimension of the space of quartics in two variables is 15, while the above parameterization has only 10 degrees of freedom. So, while we have obtained a very simple and compact parameterization of a subset of "good" polynomials, we have lost 5 degrees of freedom. This is, of course, highly undesirable. Such a degenerate parameterization may succeed in describing simple objects; however, Fig. 3a shows a fit to data corresponding to the contour of a human eye, obtained using this parameterization; it's clearly inferior to the quartic fit obtained using the more sophisticated methods described in the sequel (see Fig. 3b).

The challenge is, therefore, to find a parameterization which will cover as many polynomials as possible; in particular, we want it to have 15 degrees of freedom.

When written in general form (without the scalars resulting from taking derivatives by x), all possible $\frac{d^2}{dx^2} P_\alpha(x)$ are a subset of the set of sextic polynomials in x and α of the following type:

$$(a_{40} + a_{31}\alpha + a_{22}\alpha^2 + a_{13}\alpha^3 + a_{04}\alpha^4)x^2 + (a_{30} + a_{21}\alpha + a_{12}\alpha^2 + a_{03}\alpha^3)x + (a_{20} + a_{11}\alpha + a_{02}\alpha^2).$$

We seek a parameterization of polynomials of this type which are everywhere positive. Denote this class of polynomials by POS_2^4 .

The question, therefore, is: how to parameterize some

subset of POS_2^4 ? Obviously, we want this subset to be as large as possible to allow us as much flexibility as possible in the fitting process. The larger the subset, the larger number of shapes which can be described by zero-sets of polynomials in it.

We can generate polynomials that are everywhere positive by summing the squares of other polynomials. Thus, a sum of squares of polynomials of the type

$$L_{21}\alpha^2x + L_{11}\alpha x + L_{10}\alpha + L_{01}x + L_{00}$$

is certainly an element of POS_2^4 .

The sum

$$\sum_i \left[L_{21}^{(i)}\alpha^2x + L_{11}^{(i)}\alpha x + L_{10}^{(i)}\alpha + L_{01}^{(i)}x + L_{00}^{(i)} \right]^2$$

results in the following parameterization for a subset of POS_2^4 :

$$\begin{aligned} a_{04} &= \sum_i L_{21}^{(i)2}, a_{13} = 2 \sum_i L_{21}^{(i)}L_{11}^{(i)}, a_{22} = \sum_i \left(L_{11}^{(i)2} + 2L_{21}^{(i)}L_{01}^{(i)} \right) \\ a_{31} &= 2 \sum_i L_{11}^{(i)}L_{01}^{(i)}, a_{40} = \sum_i L_{01}^{(i)2}, \\ a_{03} &= 2 \sum_i L_{21}^{(i)}L_{10}^{(i)} \\ a_{12} &= 2 \sum_i \left(L_{11}^{(i)}L_{10}^{(i)} + L_{21}^{(i)}L_{00}^{(i)} \right) \\ a_{21} &= 2 \sum_i \left(L_{10}^{(i)}L_{01}^{(i)} + L_{11}^{(i)}L_{00}^{(i)} \right), a_{30} = 2 \sum_i L_{01}^{(i)}L_{00}^{(i)} \\ a_{02} &= 2 \sum_i L_{10}^{(i)2}, a_{11} = 2 \sum_i L_{10}^{(i)}L_{00}^{(i)}, a_{20} = \sum_i L_{00}^{(i)2} \end{aligned} \quad (4)$$

and, as before, a_{10} , a_{01} , a_{00} are free.

Denote the polynomials of the type $L_{21}\alpha^2x + L_{11}\alpha x + L_{10}\alpha + L_{01}x + L_{00}$ as $ROOT_2^4$. Some elements of POS_2^4 are sums of squares of elements of $ROOT_2^4$. Note that POS_2^4 is a subset of the quintic polynomials in α and x , and $ROOT_2^4$ is a subset of the cubic polynomials in α and x .

Finally, let us denote by $SUMSQ_2^4$ the subset of the polynomials in POS_2^4 which are sums of squares of polynomials in $ROOT_2^4$.

Some questions immediately arise:

- Is every element of POS_2^4 a sum of squares of elements of $ROOT_2^4$? Namely, are the sets $SUMSQ_2^4$ and POS_2^4 identical?
- If not, does $SUMSQ_2^4$ have a “full dimension”? That is, what is its dimension (or, equivalently, how many degrees of freedom does it have)? Naturally, we hope that its dimension is 15, as this will guarantee that we are not losing any degrees of freedom, as with the simple parameterization with 10 degrees of freedom.
- What is the minimal number (if it exists at all) of elements of $ROOT_2^4$ which must be squared and summed in order to obtain all elements of $SUMSQ_2^4$? This is important when implementing the fitting procedure, for we have to know how $SUMSQ_2^4$ is to be parameterized. The optimal choice would be to sum as many squares of elements of $ROOT_2^4$ which will guarantee that we have covered all elements of $SUMSQ_2^4$. If we sum too many, we are complicating the fitting procedure without gaining anything. If we sum too few, we are losing part of $SUMSQ_2^4$, and the results of the fitting process will not be optimal.

Next, the answers to these questions—for $SUMSQ_2^4$ as well as for more general families of polynomials—will be presented, together with some recent results about positive polynomials.

3.2 Polynomials Represented as Sums of Squares

Most of the material in this subsection is a short summary of some notions and a few recent powerful results in real algebraic geometry, summarized from [3]. We restrict ourselves to definitions and results which are necessary for the sequel.

First, some terminology:

- Given a ring R , its *Pythagoras number*, $P(R)$, is defined to be the lower bound on the number of squares which must be summed in order to obtain every element of R which is a sum of squares. That is, if any element of R is a sum of squares of elements of R , it can be expressed as a sum of no more than $P(R)$ squares, and $P(R)$ is the minimal number with this property. There is no general bound on $P(R)$ and, for some rings, it equals infinity; fortunately, that is not the case for the rings of polynomials which are relevant to the fitting paradigm described here.

The Pythagoras number $P(R)$ is very important for parameterizing the elements of $SUMSQ_2^4$ (as well as polynomials which are sums of squares of higher degree polynomials). This is because the parameterization given in the previous section requires summing exactly $P(R)$ squares and no more. Naturally, the smaller $P(R)$ is, the better; and, fortunately, some powerful lower bounds for $P(R)$ have been recently obtained for some polynomials rings.

- A *form* is a homogeneous polynomial. The ring of

forms of degree m in n variables is denoted $F_{n,m}$, and its Pythagoras number is denoted $P(n, m)$.

- Suppose we are given a subset A of $F_{n,m}$. The *cage* associated with it is the set of n -tuples of coefficients which are non-zero for some element of A . For example, look at the polynomials we have discussed before

$$(a_{40} + a_{31}\alpha + a_{22}\alpha^2 + a_{13}\alpha^3 + a_{04}\alpha^4)x^2 + (a_{30} + a_{21}\alpha + a_{12}\alpha^2 + a_{03}\alpha^3)x + (a_{20} + a_{11}\alpha + a_{02}\alpha^2).$$

When homogenized, these polynomials assume the shape

$$a_{40}x^2w^4 + a_{31}\alpha x^2w + a_{22}\alpha^2x^2w^2 + a_{13}\alpha^3x^2w + a_{04}\alpha^4x^2 + a_{30}\alpha w^5 + a_{21}\alpha xw^4 + a_{12}\alpha^2xw^3 + a_{03}\alpha^3xw^2 + a_{20}w^6 + a_{11}\alpha w^5 + a_{02}\alpha^2w^4,$$

and their cage, when viewed as a subset of $F_{3,6}$, is equal to $\{(4, 2, 0), (3, 2, 1), (2, 2, 2), (1, 2, 3), (0, 2, 4), (3, 1, 2), (2, 1, 3), (1, 1, 4), (0, 1, 5), (2, 0, 4), (1, 0, 5), (0, 0, 6)\}$.

- For a cage C , let us denote by $l = l(C)$ the number of monomials in C , by $e = e(C)$ the number of even monomials in C (that is, the n -tuples all of whose elements are even), and by $a = a(C)$ the number of distinct means of even monomials.

For example, for the cage described above, $l = 12$, $e = 5$, and $a = 12$. This is because every monomial in the cage can be expressed as an average of two even monomials; for instance, $(1, 2, 3)$ is the average of $(4, 2, 0)$ and $(0, 0, 6)$, both of which are even monomials in the cage.

Let us also denote by $F^+(C)$ the set of everywhere positive polynomials with coefficients in C , and by $F(C)$ those polynomials in $F^+(C)$ which are sums of squares.

Last, let us define the Pythagoras number of a cage C , $P(C)$, in exactly the same fashion as the Pythagoras number of a ring R , that is, as the maximal number of squares that we need to sum in order to obtain all the elements of $F(C)$.

Now, we are ready to present some results from [3]:

LEMMA 1. *The dimension of $F^+(C)$ is l , and the dimension of $F(C)$ is a .*

THEOREM 1. *For any cage C , the following inequality holds:*

$$\frac{a}{e} \leq \lambda \leq P(C) \leq \Lambda \leq e,$$

$$\text{where } \Lambda = \frac{\sqrt{1+8a}-1}{2} \text{ and } \lambda = \frac{2e+1-\sqrt{(2e+1)^2-8a}}{2}.$$

LEMMA 2. *For any m , $P(3, m) \leq \frac{m}{2} + 2$ (this result was obtained by David Leep).*

LEMMA 3. $P(3, 4) = 3$ (this is a famous theorem of David Hilbert [6]).

LEMMA 4. *For every n , $P(2, n) = 2$.*

LEMMA 5. *In general, $F^+(C) \neq F(C)$, that is, there are polynomials which are everywhere positive but are not sums of squares.*

Let us see how these results apply to the simplest case we have studied, quartics in two variables:

- The dimension of $SUMSQ_2^4$ is 12. To this, we should add 3 degrees of freedom (because the linear coefficients a_{10} , a_{01} , and the constant coefficient a_{00} are not constrained). Since this gives, altogether, 15 degrees of freedom, we lose no degrees of freedom by using the parameterization of (4) for quartics in two variables, because they also have 15 degrees of freedom.
- $POS_2^4 \neq SUMSQ_2^4$. Hence, although we lose no degrees of freedom, there are everywhere positive polynomials which cannot be represented as sums of squares.
- Since $P(3, m) \leq \frac{m}{2} + 2$ and, in our case, $m = 6$, we need a sum of five squares of elements of $ROOT_2^4$ to guarantee that we have indeed covered all of $SUMSQ_2^4$.

The first and second observations carry over to higher-degree polynomials and polynomials in three variables, the only change being the upper bound on the Pythagoras number. Note that, because we have to homogenize the polynomials, polynomials in two variables transform into forms in three variables, and polynomials in three variables transform into forms in four variables. For the first, the bound $P(3, m) \leq \frac{m}{2} + 2$ is sharper than the one given by Theorem 1. For the latter, we use Theorem 1 to obtain a lower bound; for instance, the lower bound for quartics in three variables turns out to be 11. This means that we have to sum 11 squares of polynomials of the appropriate type to guarantee that we obtain all the polynomials which are sums of squares.

3.3 Second Method: Focus of Expansion

Another method of forcing the zero-set to be star-shaped is to force the fitted polynomial to have a *focus of expansion*. By that, we mean a point O which has the following property: the fitted polynomial has to increase on every ray emanating from O . In a typical scenario, O will belong to the interior of the set of points to be fitted and the value of the polynomial in O will be negative. Obviously, the zero-set has to be star-shaped in that case; if not, some ray emanating from O will intersect it twice, but this is impossible, as the polynomial is increasing on every such ray. In [14], a method of using rays to prevent extraneous components proceeds as follows: A finite number of rays are created during the iterative process, emanating outside from a sphere bounding the data set. The rays are tested for intersection with the zero-set; if such an intersection takes place, the current polynomial is penalized. This method, however, may fail to detect and penalize loops, holes, or components *inside* the data. For instance, the *internal* loop in Fig. 1d cannot be detected and removed by using rays which emanate from a sphere bounding the data. Also, it is impossible to cover the entire space with a finite number of rays and extraneous components may exist between them. What would be desirable is to ensure that such conditions on the intersection of rays with the

zero-set will be guaranteed to hold for every ray and that no checking will be required.

Next, we show how to enforce such a condition. Assume for the moment that the focus of expansion O is the origin $(0, 0)$. Denote once again the restriction of the polynomial $P(x, y)$ to the line $y = \alpha x$ by $P_\alpha(x)$. Now, assume that $\frac{dP_\alpha(x)}{dx} = xQ_\alpha(x)$ for every α and x , where $Q_\alpha(x)$ is positive for every α and x . Then, for every fixed α , it is easy to see that, as we move away from the origin on the rays $y = \alpha x$, $x > 0$, and $y = \alpha x$, $x < 0$, $P_\alpha(x)$ is increasing (because, as a function of x , its derivative is positive). Therefore, the origin is a focus of expansion for $P(x, y)$, and its zero-set will be star-shaped.

Let us demonstrate these notions for the simplest case, a quartic in x and y :

$$\begin{aligned} P(x, y) &= a_{40}x^4 + a_{31}x^4\alpha + a_{22}x^4\alpha^2 + a_{13}x^4\alpha^3 + a_{04}\alpha^4x^4 \\ &\quad + a_{30}x^3 + a_{21}x^3\alpha + a_{12}x^3\alpha^2 + a_{03}\alpha^3x^3 + a_{20}x^2 \\ &\quad + a_{11}x^2\alpha + a_{02}\alpha^2x^2 + a_{10}x + a_{00} \\ \frac{dP_\alpha(x)}{dx} &= 4a_{40}x^3 + 4a_{31}x^3\alpha + 4a_{22}x^3\alpha^2 + 4a_{13}x^3\alpha^3 + 4a_{04}\alpha^4x^3 \\ &\quad + 3a_{30}x^2 + 3a_{21}x^2\alpha + 3a_{12}x^2\alpha^2 + 3a_{03}\alpha^3x^2 + 2a_{20}x \\ &\quad + 2a_{11}x\alpha + 2a_{02}\alpha^2x + a_{10} + a_{01}\alpha. \end{aligned}$$

For the equality $\frac{dP_\alpha(x)}{dx} = xQ_\alpha(x)$ to hold, assume for the moment that $a_{10} = a_{01} = 0$ and, then,

$$\begin{aligned} \frac{dP_\alpha(x)}{dx} &= 4a_{40}x^3 + 4a_{31}x^3\alpha + 4a_{22}x^3\alpha^2 + 4a_{13}x^3\alpha^3 \\ &\quad + 4a_{04}\alpha^4x^3 + 3a_{30}x^2 + 3a_{21}x^2\alpha + 3a_{12}x^2\alpha^2 \\ &\quad + 3a_{03}\alpha^3x^2 + 2a_{20}x + 2a_{11}x\alpha + 2a_{02}\alpha^2x \end{aligned}$$

from which it follows that

$$\begin{aligned} Q_\alpha(x) &= 4a_{40}x^2 + 4a_{31}x^2\alpha + 4a_{22}x^2\alpha^2 + 4a_{13}x^2\alpha^3 \\ &\quad + 4a_{04}\alpha^4x^2 + 3a_{30}x + 3a_{21}x\alpha + 3a_{12}x\alpha^2 \\ &\quad + 3a_{03}\alpha^3x + 2a_{20} + 2a_{11}\alpha + 2a_{02}\alpha^2. \end{aligned}$$

To force $Q_\alpha(x)$ to be positive, we parameterize the a_{ij} s as before, as coefficients of elements of $SUMSQ_2^4$. In order not to lose the two degrees of freedom because of the constraint $a_{10} = a_{01} = 0$, we add to the optimization program a step which allows to translate the polynomial; this is equivalent to allowing any point, not just the origin, to be the focus of expansion.

In Fig. 4, an example of fitting a polynomial of degree 8 with the focus of expansion method is presented. The curve is an outline of a violin (the data points are white, and the zero-set of the fit is gray). Although the data contains cusps, the fit is reasonable and does not suffer from loops and other pathologies.

For this shape, the focus of expansion method resulted in a much better fit than the line convexity method (Fig. 5).

We do not include the parameterizations for higher degree polynomials here, as the expressions are somewhat long. They are, however, obtained simply by summing

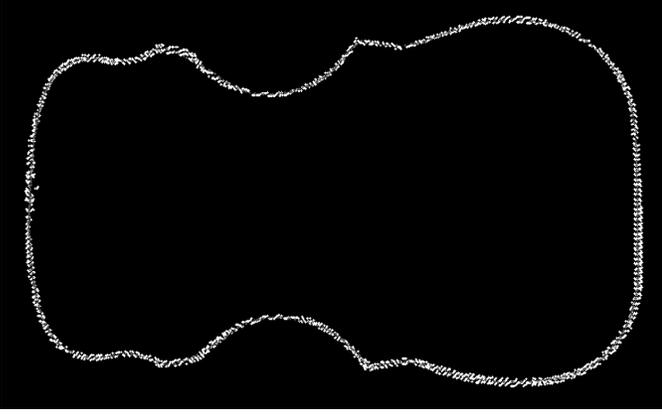


Fig. 4. Fitting a violin with the zero-set of an eight-degree polynomial, using the focus of expansion method.

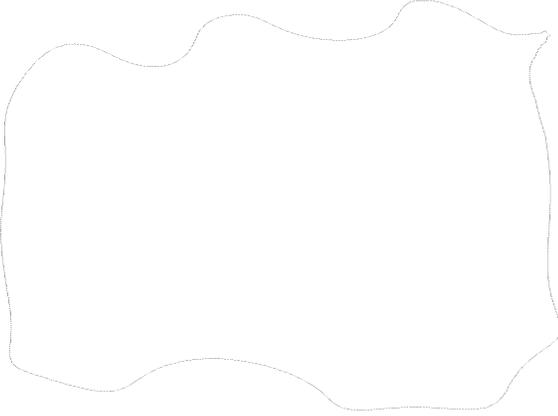


Fig. 5. Fitting a violin with the zero-set of an eight-degree polynomial, using the line convexity method.

squares of appropriate polynomials, the number of which is given by the appropriate Pythagoras number.

4 BOUNDED OBJECTS

Forcing zero-sets of polynomials to be star-shaped has been shown to be possible, but is not appropriate for all real-world objects. Assume the data set $S = \{\bar{x}^i\}$ is contained in a bounded region of \mathcal{R}^d , e.g., the unit sphere. It would be natural to require that the polynomial zero-set also be confined to the unit sphere. For many practical purposes, though, it suffices to require that the surface of the unit sphere *separates* the different components of the zero-set. Hopefully there will be only one component inside the sphere, and any other superfluous components outside the sphere may be “clipped” away cleanly. In terms of the polynomial P , this translates to the constraint $P(\bar{x}) > 0$ for $\bar{x} \in C$, where C is the surface of the unit sphere.

At first glance, it seems that this “continuous” constraint may be approximated by a large set of discrete constraints by densely sampling the unit sphere surface at the points $\left\{ \bar{y}_j = (y_1^j, \dots, y_d^j) : \sum_{i=1}^d (y_i^j)^2 = 1, j = 1, \dots, s \right\}$. These con-

straints imply the following *linearly constrained* version of the least squares problem (2)

$$\bar{a} = \arg \min_{\bar{a} \in \mathcal{R}^m} \sum_i \left(\frac{P_{\bar{a}}(\bar{x}^i)}{\|\nabla P_{\bar{a}}(\bar{x}^i)\|} \right)^2$$

$$\text{subject to } P_{\bar{a}}(\bar{y}^i) > 0 \quad i = 1, \dots, s. \quad (5)$$

This problem may be solved numerically by standard optimization techniques, with the hope that the resulting zero-set will indeed be contained in the unit sphere. However, the complexity of the numerical procedure increases with the number of constraints s , which must be very large in order to ensure, with high probability, that the zero-set not “escape” between the discrete samples of the sphere. Fortunately, this naive method may be significantly improved by analytic methods.

4.1 The 2D Case

The 2D case permits the following solution: Parameterize the unit circle by: $C = \left\{ (x(t), y(t)) = \left(\frac{t^2-1}{t^2+1}, \frac{2t}{t^2+1} \right) : t \in \mathcal{R} \right\}$. We are interested only in the polynomials $P(x, y)$ such that $P(x(t), y(t)) > 0$ for all $t \in \mathcal{R}$. Assume P is quartic.

$$P(x, y) = \sum_{d_1+d_2 \leq 4} a_{d_1, d_2} x^{d_1} y^{d_2}$$

P reduced to C , parameterized by t , is

$$Q(t) = P\left(\frac{t^2-1}{t^2+1}, \frac{2t}{t^2+1}\right) = \sum_{d_1+d_2 \leq 4} a_{d_1, d_2} \frac{(t^2-1)^{d_1} (2t)^{d_2}}{(t^2+1)^{d_1+d_2}}.$$

Requiring that $Q(t) > 0$ for all $t \in \mathcal{R}$ is equivalent to requiring that

$$\sum_{d_1+d_2 \leq 4} a_{d_1, d_2} (t^2-1)^{d_1} (2t)^{d_2} (t^2+1)^{4-d_1-d_2} > 0 \quad t \in \mathcal{R}. \quad (6)$$

Since $P(2, 8) = 2$ (Lemma 4, Section 3.2), a sufficient condition for (6) to hold is the identity

$$\sum_{d_1+d_2 \leq 4} a_{d_1, d_2} (t^2-1)^{d_1} (2t)^{d_2} \equiv R_1(t)^2 + R_2(t)^2. \quad (7)$$

where R_1 and R_2 are one-dimensional quartic polynomials, determined by 10 free parameters, which we denote by L_1, \dots, L_{10} . Expanding the left side of (7) and equating the coefficients of the nine monomials on both sides yields nine linear equations for the 14 a_{d_1, d_2} in terms of the ten L_i , which may be solved easily (see Appendix). Since the system is degenerate, five of the a_{d_1, d_2} are left free, or equivalently, equal to L_{11}, \dots, L_{15} , five extra degrees of freedom. Note that the solutions are not linear in L_i . Substituting any real values for the L_i yield coefficients a_{d_1, d_2} of a two-dimensional quartic polynomial which is positive on the unit circle. This means that the optimization procedure searches \mathcal{R}^{15} , the \bar{L} space, unconstrained, instead of the equivalent (but unknown) \bar{a} subset of \mathcal{R}^{15} .

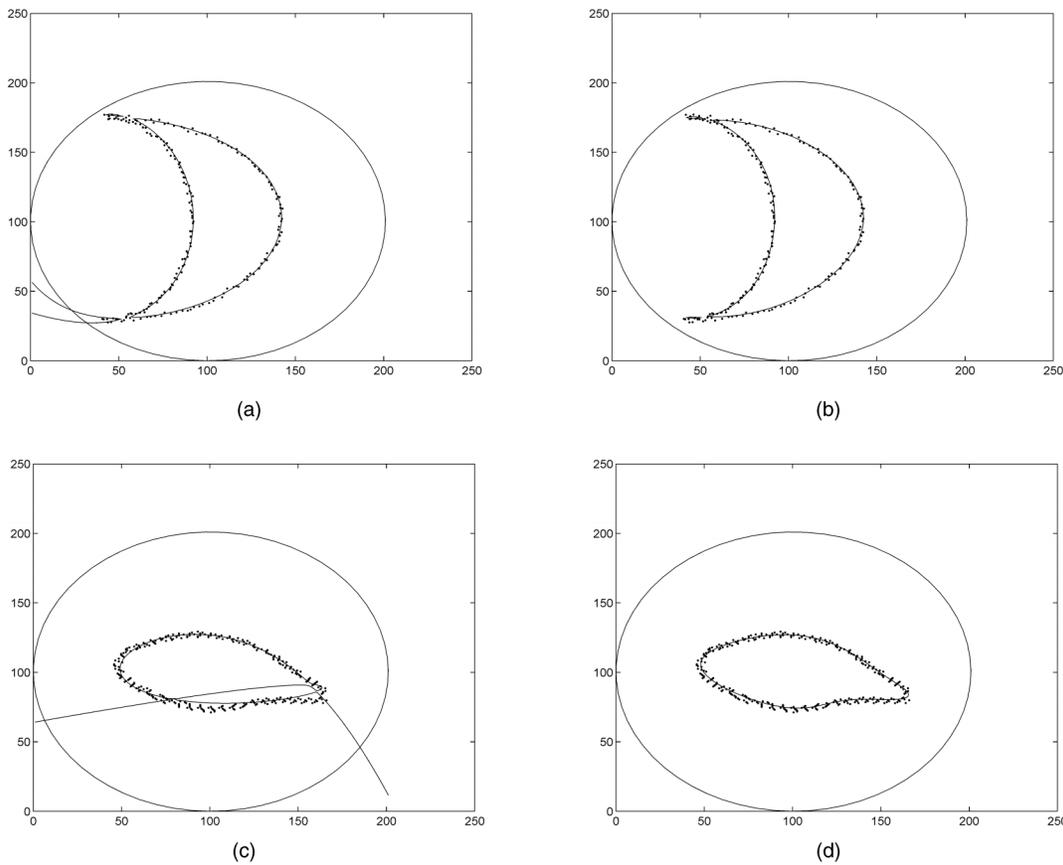


Fig. 6. (a), (c) Unconstrained and (b), (d) constrained fits to the “moon” and “eye” data sets, where the constraint is positivity on the marked unit circle.

Fig. 6 shows some results of our method applied to fitting quartic polynomials to some 2D data sets, compared to the results obtained by an unconstrained fitting procedure. The results of our procedure are obviously superior.

4.2 The 3D Case

The obvious extension of the 2D solution to the 3D case is to parameterize the unit sphere using two parameters (u, v), and follow a procedure similar to the above to parameterize the 35 coefficients of a quartic 3D polynomial by a (possibly larger) number of L s. However, this turns out to be impossible, as the procedure generates 66 linear equations for the 34 coefficients in terms of the L s. Theoretically, this difficulty may be alleviated by increasing the degree of the polynomial, so a solution exists for $d \geq 10$. These degrees are, however, impractical.

A slightly different approach enables a solution, even for lower degree polynomials. Assume that P can be written as

$$P(x, y, z) = Q_1(x^2 + y^2 + z^2 - 1, y, z) + Q_2(x, x^2 + y^2 + z^2 - 1, z) + Q_3(x, y, x^2 + y^2 + z^2 - 1).$$

A sufficient condition for the positivity on the unit sphere constraint to hold is

$$\begin{aligned} Q_1(0, v, w) > 0 \quad Q_2(u, 0, w) > 0 \quad Q_3(u, v, 0) > 0 \\ \text{for all } (u, v, w) \in \mathcal{R}^3 \end{aligned} \quad (8)$$

Naively, in order that P be quartic, Q_i cannot be more than

quadratic. However, this means that the resulting P will have at most $3 \times 6 = 18$ degrees of freedom, which is much less than the 35 it should have. A more promising way of generating P is allowing Q_i to be quartic, but with vanishing coefficients for the monomials, which would cause P to have a degree higher than four, i.e., retain only the following 22 coefficients:

$$\begin{aligned} Q_1(u, v, w) = & a_{040}v^4 + a_{031}v^3w + a_{022}v^2w^2 + a_{013}vw^3 \\ & + a_{004}w^4 + a_{120}uv^2 + a_{111}uvw + a_{102}uw^2 \\ & + a_{003}v^3 + a_{021}v^2w + a_{012}vw^2 + a_{003}w^3 \\ & + a_{200}u^2 + a_{020}v^2 + a_{002}w^2 + a_{110}uw \\ & + a_{101}uw + a_{011}vw + a_{100}u + a_{010}v + a_{001}w + a_{000}. \end{aligned}$$

For instance, $a_{400}u^4$ has been removed, as the term $a_{400}(x^2 + y^2 + z^2 - 1)^4$ would cause the degree of P to be 8. Q_2 and Q_3 have analogous type. The resulting P is quartic with the full 35 degrees of freedom. The constraints of (8) may be translated into the identities

$$\begin{aligned} Q_1(0, v, w) &= R_1(v, w)^2 + R_2(v, w)^2 + R_3(v, w)^2 \\ Q_2(u, 0, w) &= R_4(u, w)^2 + R_5(u, w)^2 + R_6(u, w)^2 \\ Q_3(u, v, 0) &= R_7(u, v)^2 + R_8(u, v)^2 + R_9(u, v)^2, \end{aligned}$$

where the R_i are quadratic 2D polynomials, having $9 \times 6 = 54$ coefficients L_i in total. (It suffices to sum three squares

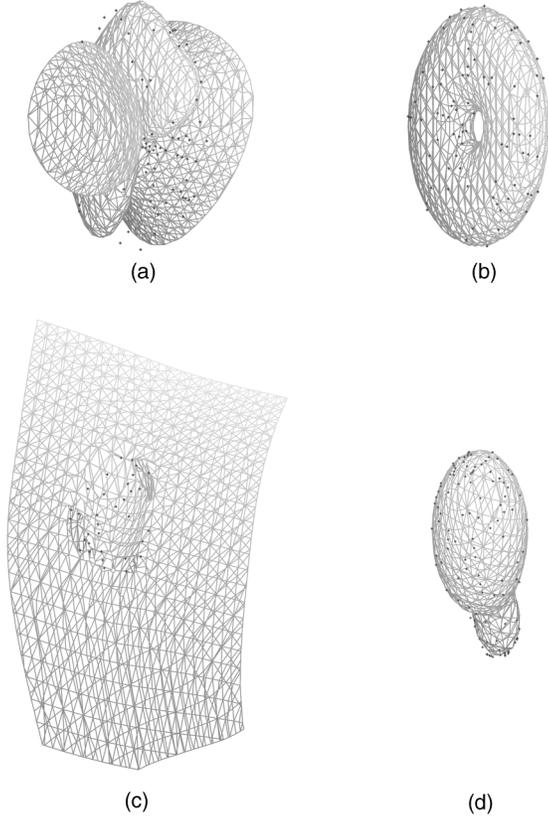


Fig. 7. (a), (c) Unconstrained and (b), (d) constrained quartic fits to the “torus” and “bulb” data sets.

since $P(3, 4) = 3$ —Lemma 3, Section 3.2).

As opposed to the solution in the 2D case, there is no need to solve equations in order to express the a_{d_1, d_2, d_3} in terms of the L_r . This reduces the optimization procedure to an unconstrained search over \mathcal{R}^{54} .

Fig. 7 shows some results of our method applied to fitting quartic polynomials to some 3D data sets, compared to the results obtained by an unconstrained fitting procedure. The results of our procedure are obviously superior.

Another example follows in Fig. 8. The 3D data was sampled from the handle of a screwdriver.

4.3 Forcing the Zero-Set to Lie Entirely Within a Circle

Methods similar to those described in Sections 4.1 and 4.2 can be used to force a stronger condition on a polynomial’s zero-set—namely, that it is positive everywhere on and outside a given ellipse, not just on the ellipse. As before, it will be demonstrated how to force the zero-set to be positive everywhere on and outside the unit circle; the generalization to any ellipse, and to polynomials in three variables, is straightforward. The method can also be extended to other algebraic curves, in exactly the same way; however, the resulting parametrization will be more complicated.

Let us look at the case of a quartic in two variables. We start with the following degenerate quartic $P(x, u)$:

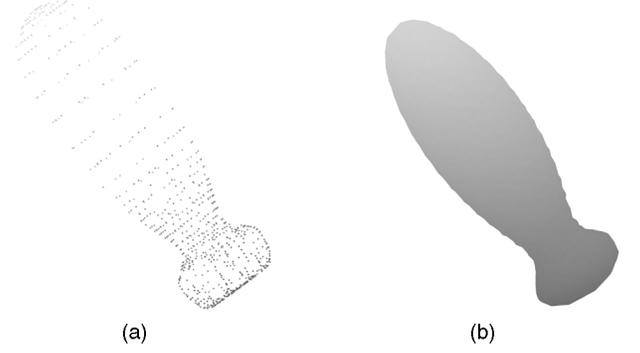


Fig. 8. Quartic 3D: (a) screwdriver data, (b) fit to data.

$$P(x, u) = a40x^4 + a30x^3 + a21x^2u + a20x^2 + a11xu + a02u^2 + a10x + a01u + a00.$$

As in Section 4.2, u will eventually be replaced by $x^2 + y^2 - 1$; this is why monomials which would increase the degree beyond 4 were removed. If $P(x, u)$ is to be positive outside of the unit circle, it is necessary that $P(x, u)$ be positive for $u > 0$.

The corresponding cage has nine elements. It is easy to verify, using the notation of Theorem 1, that $a = 9$ and, therefore, the corresponding Pythagoras number is bounded by $\frac{\sqrt{1+72}-1}{2} = 3.77$; since it has to be an integer, 3 is an upper bound on the Pythagoras number. We can, therefore, parameterize an everywhere positive $P(x, u)$ by

$$(L_1x^2 + L_2u + L_3x + L_4)^2 + (L_5x^2 + L_6u + L_7x + L_8)^2 + (L_9x^2 + L_{10}u + L_{11}x + L_{12})^2$$

In order to allow the polynomial to be negative for negative values of u (that is, inside the unit circle), we simply add to $P(x, u)$ the term L_{13}^2u . Note that $P(x, u)$ will still be positive on and outside the unit circle, as desired. All in all, we obtain

$$\begin{aligned} & (L_1^2 + L_5^2 + L_9^2)x^4 + (2L_1L_3 + 2L_5L_7 + 2L_9L_{11})x^3 \\ & + (2L_1L_2 + 2L_5L_6 + 2L_9L_{10})x^2u \\ & + (L_3^2 + 2L_9L_{12} + L_7^2 + L_{11}^2 + 2L_1L_4 + 2L_5L_8)x^2 \\ & + (2L_2L_3 + 2L_6L_7 + 2L_{10}L_{11})xu + (L_2^2 + L_6^2 + L_{10}^2)u^2 \\ & + (2L_{11}L_{12} + 2L_3L_4 + 2L_7L_8)x \\ & + (L_{13}^2 + 2L_2L_4 + 2L_6L_8 + 2L_{10}L_{12})u + L_4^2 + L_{12}^2 + L_8^2 + L_{13}^2u. \end{aligned}$$

Finally, after substituting $u = x^2 + y^2 - 1$, we obtain the following parameterization for quartics which are positive everywhere on and outside of the unit circle:

$$\begin{aligned}
& 2x^4L_9L_{10} + 2x^4L_5L_6 - 2xL_{10}L_{11} - 2xL_6L_7 - 2xL_2L_3 \\
& + 2L_{10}L_{11}x^3 + 2L_6L_7x^3 + L_1^2x^4 + L_3^2x^2 + 2L_2L_3x^3 \\
& + 2L_1x^3L_3 + 2L_6L_8x^2 + L_4^2 + 2L_2L_4y^2 + 2L_2L_4x^2 \\
& + 2L_{10}^2x^2y^2 + 2L_6^2x^2y^2 + 2L_2^2x^2y^2 + 2L_{11}xL_{12} + 2L_{10}L_{12}y^2 \\
& + L_6^2y^4 + 2L_{10}L_{12}x^2 + 2L_6L_8y^2 + 2L_3xL_4 + 2x^4L_1L_2 \\
& + 2L_9x^2L_{12} + L_6^2 + L_5^2x^4 + L_7^2x^2 + L_3^2x^4 + L_{11}^2x^2 \\
& + L_{12}^2 - 2L_6L_8 - 2L_2L_4 - 2L_{10}L_{12} + L_8^2 + L_2^2 + 2L_1x^2L_4 \\
& + 2L_5x^3L_7 + 2L_5x^2L_8 + 2L_7xL_8 + 2L_9x^3L_{11} + L_{10}^2 \\
& - 2L_1L_2x^2 - 2L_{13}^2 - 2L_5L_6x^2 - 2L_9L_{10}x^2 - 2L_6^2y^2 + 2L_{13}^2x^2 \\
& + 2L_{13}^2y^2 + L_{10}^2x^4 - 2L_{10}^2x^2 + L_{10}^2y^4 - 2L_{10}^2y^2 + L_2^2y^4 - 2L_2^2y^2 \\
& - 2L_6^2x^2 + L_6^2x^4 + L_2^2x^4 - 2L_2^2x^2 + 2xL_2L_3y^2 + 2xL_6L_7y^2 \\
& + 2xL_{10}L_{11}y^2 + 2x^2L_1L_2y^2 + 2x^2L_5L_6y^2 + 2x^2L_9L_{10}y^2.
\end{aligned}$$

Note that this family is degenerate (for instance, the coefficient of y is always 0). By adding another quartic of this type—with x replaced by y during the construction—we obtained a family of quartics which have the full 15 degrees of freedom and satisfy the condition of being positive everywhere outside the unit circle. However, more parameters are required to describe this family than to describe the quartics which are only guaranteed to be positive on the unit circle (Section 4.1).

In Fig. 9, a fit to the “vase” data set using this parameterization is shown. Unconstrained fits to this data set, even those with a globally bounded zero set, had extraneous components [8]. These had to be removed using heuristic methods. The method presented here guarantees that no such extraneous components can possibly occur outside of a bounding ellipse.

5 CONCLUSIONS AND FUTURE WORK

We have presented novel parameterizations for families of polynomials, which have certain desirable topological properties. This eliminates the need to use failure-prone heuristics to achieve these properties when fitting implicit polynomials to discrete data. In this regard, this work can be viewed as a continuation of [8], [16], [14]. The fitting algorithms presented here were implemented and tested on real data sets, with satisfactory results.

In the future, we hope to discover additional parameterized families of polynomials, which will satisfy other topological properties (such as connectedness).

APPENDIX

The parameterization obtained by solving the equations resulting from (7) is:

$$\begin{aligned}
a_{04} = & \frac{1}{16} \left(-L_2^2 + L_5^2 + L_{10}^2 - 2L_1L_3 + 2L_1L_5 + 2L_2L_4 \right. \\
& + 2L_7L_9 + 2L_6L_{10} - 2L_3L_5 - 2L_8L_{10} + L_6^2 \\
& \left. + L_1^2 - L_7^2 - L_4^2 + L_8^2 + L_3^2 - L_9^2 - L_{11} + L_{13} - 2L_6L_8 \right)
\end{aligned}$$



Fig. 9. Bounded fit to “vase” data.

$$\begin{aligned}
a_{31} = & \frac{1}{16} \left(-2L_7L_8 + 2L_6L_7 + 2L_1L_2 + 2L_3L_4 + 2L_2L_5 \right. \\
& + 2L_8L_9 + 2L_7L_{10} + L_{14} - 2L_9L_{10} - 2L_4L_5 \\
& \left. - 2L_1L_4 - 2L_2L_3 - 2L_6L_9 \right)
\end{aligned}$$

$$\begin{aligned}
a_{12} = & \frac{1}{16} \left(-2L_7L_8 + 6L_6L_7 + 6L_1L_2 - 2L_3L_4 - 2L_2L_5 \right. \\
& - 2L_8L_9 - 2L_7L_{10} + 6L_9L_{10} + 6L_4L_5 - 2L_1L_4 \\
& \left. - 2L_2L_3 - 2L_6L_9 + L_{12} \right)
\end{aligned}$$

$$\begin{aligned}
a_{20} = & \frac{1}{16} \left(1 + L_5^2 + L_{10}^2 + 2L_1L_3 + 2L_1L_5 + 2L_2L_4 + 2L_7L_9 \right. \\
& + 2L_6L_{10} + 2L_3L_5 + 2L_8L_{10} + L_6^2 + L_1^2 + L_7^2 + L_2^2 \\
& \left. + L_8^2 + L_3^2 + L_9^2 + L_4^2 - L_{11} + 2L_6L_8 \right)
\end{aligned}$$

$$\begin{aligned}
a_{03} = & \frac{1}{16} \left(4L_5^2 + 4L_{10}^2 + 4L_1L_3 - 4L_3L_5 - 4L_8L_{14}L_6^2 \right. \\
& \left. - 4L_1^2 + 2L_7^2 + 2L_2^2 - 2L_9^2 - 2L_4^2 + L_{15} + 4L_6L_8 \right)
\end{aligned}$$

$$a_{11} = \frac{1}{16} \left(-8L_6L_7 - L_{14} - 8L_1L_2 + 8L_9L_{10} + 8L_4L_8 \right)$$

$$\begin{aligned}
a_{02} = & \frac{1}{16} \left(1 + 7L_5^2 + 7L_{10}^2 + 2L_1L_3 - 2L_1L_5 - 2L_2L_4 - L_7L_9 \right. \\
& - 2L_6L_{10} + 2L_3L_5 + 2L_8L_{10} + 7L_6^2 + 7L_1^2 + L_7^2 - L_8^2 \\
& \left. - L_3^2 + L_9^2 + L_4^2 + L_{11} - L_{13} + 2L_6L_8 \right)
\end{aligned}$$

$$\begin{aligned}
a_{10} = & \frac{1}{16} \left(2L_6L_7 + 2L_7L_8 + 2L_1L_2 + 2L_3L_4 + 2L_2L_5 + 2L_8L_9 \right. \\
& \left. + 2L_7L_{10} + 2L_9L_{10} + 2L_4L_5 + 2L_1L_4 + 2L_2L_3 + 2L_6L_9 - L_{12} \right)
\end{aligned}$$

$$a_{01} = \frac{1}{16} \left(4L_5^2 + 4L_{10}^2 - 4L_1L_3 + 4L_3L_5 + 4L_8L_{10} - 4L_6^2 \right. \\ \left. - 4L_1^2 - 2L_7^2 - 2L_2^2 + 2L_9^2 + 2L_4^2 - L_{15} - 4L_6L_8 \right)$$

$$a_{40} = L_{11}, a_{30} = L_{12}, a_{22} = L_{13}, a_{13} = L_{14}, a_{21} = L_{15}.$$

The solution was obtained using the Maple symbolic computation package.

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