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Rational approximation of vertical segments

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Abstract In many applications, observations are prone to imprecise measurements. When constructing a model based on such data, an approximation rather than an interpolation approach is needed. Very often a least squares approximation is used. Here we follow a different approach. A natural way for dealing with uncertainty in the data is by means of an uncertainty interval. We assume that the uncertainty in the independent variables is negligible and that for each observation an uncertainty interval can be given which contains the (unknown) exact value. To approximate such data we look for functions which intersect all uncertainty intervals. In the past this problem has been studied for polynomials, or more generally for functions which are linear in the unknown coefficients. Here we study the problem for a particular class of functions which are nonlinear in the unknown coefficients, namely rational functions. We show how to reduce the problem to a quadratic programming problem with a strictly convex objective function, yielding a unique rational function which intersects all uncertainty intervals and satisfies some additional properties. Compared to rational least squares approximation which reduces to a nonlinear optimization

Dedicated to Walter Gautschi for his 50 years of valuable work in rational approximation theory.

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problem where the objective function may have many local minima, this makes the new approach attractive.

Keywords Rational approximation · Rational interpolation · Noise interval · Modeling · Polyhedral cone · Optimization · Quadratic programming

1 Problem statement

To approximate noisy or imprecise data, very often a least squares approach is used. The idea here is to deal with uncertainty in another, very natural way: by means of an uncertainty interval. We assume that the uncertainty in the independent variables is negligible and that for each observation, an uncertainty interval can be given which contains the (unknown) exact value. We study the problem of approximating these data with a rational function which intersects the given uncertainty intervals.

Both the problem statement and the algorithm that we develop to solve it can be written down for any number of independent variables. For ease of notation, we consider the bivariate instead of the general high dimensional case. Consider the set of $n+1$ vertical segments

$$S_n = \{(x_0, y_0, F_0), (x_1, y_1, F_1), \ldots, (x_n, y_n, F_n)\}, \tag{1}$$

where $F_i = [\underline{f}_i, \overline{f}_i]$ are real finite intervals with $\underline{f}_i < \overline{f}_i$ $(i = 0, \ldots, n)$ and none of the points $(x_i, y_i) \in \mathbb{R}^2$ coincide. Let N_ℓ and D_m be two finite subsets of $\mathbb{N}^2$ of the form

$$N_\ell = \{(i_0, j_0), \ldots, (i_\ell, j_\ell)\}, \tag{2}$$

$$D_m = \{(d_0, e_0), \ldots, (d_m, e_m)\}, \tag{3}$$

with which we associate the bivariate polynomials

$$p(x, y) = \sum_{k=0}^{\ell} a_k x^{i_k} y^{j_k},$$

$$q(x, y) = \sum_{k=0}^{m} b_k x^{d_k} y^{e_k}. \tag{4}$$

Further, denote the irreducible form of $p(x, y)/q(x, y)$ by $r_{\ell,m}(x, y)$ and let

$$\mathcal{R}_{\ell,m}(S_n) = \{r_{\ell,m}(x, y) \mid r_{\ell,m}(x_i, y_i) \in F_i,\ q(x_i, y_i) > 0, i = 0, \ldots, n\}. \tag{5}$$

As we see in the next section, changing the conditions on the sign of $q(x_i, y_i)$ does not change the nature of the problem. Therefore there is no loss of generality in describing the problem with the conditions $q(x_i, y_i) > 0$.

For given segments S_n and given sets N_ℓ and D_m, we are concerned with the problem of determining whether

$$\mathcal{R}_{\ell,m}(S_n) \neq \emptyset. \tag{6}$$

We call this *the existence problem*. In addition to the existence problem, finding a representation for $\mathcal{R}_{\ell,m}(S_n)$ is referred to as *the representation problem*. Whereas in classical rational interpolation ℓ and m are chosen so that $\ell + m + 1 = n + 1$, here we pursue $\ell + m \ll n$.

A problem similar to (5) and (6) has already been studied in [7]. Instead of considering rational models $r_{\ell,m}(x, y)$ in (5), the authors consider models which are linear in the unknown coefficients. Although we solve a linearized version of (5) and (6), our problem does not reduce to the one described in [7] since our solution set is unbounded while the solution set in [7] is bounded. We discuss the connection of [7] with our work in more detail in Section 3.

Without the intent of being exhaustive, we also mention the interval approach of Markov [5, 6]. This approach applies only to a special case of the problem (5) and (6), where instead of multivariate rational functions $r_{\ell,m}(x, y)$, univariate polynomials are considered to approximate univariate data. The method is based on the interval Lagrange representation of the interpolating polynomial. An algorithm is given that reliably solves the existence problem after performing a number of interval intersections which is combinatorial in the number of data points. With respect to the representation problem, piecewise upper and lowerbounds are provided for the univariate polynomials which satisfy the special case of (5) and (6). These are found after yet another combinatorial number of interval intersections. Due to its computational complexity, this approach is limited to low degree polynomials and small datasets.

Least squares approximation is the conventional way to model noisy or uncertain data. For non-linear models in general and rational models in particular, the least squares problem may have many local minima and the quality of the computed model therefore highly depends on the provided starting value. This is illustrated numerically in Section 4. In contrast, we prove in Section 3 that the existence and representation problem (5) and (6) reduce to solving a quadratic programming problem of which the objective function is strictly convex. Hence our problem has a unique solution, if it exists.

2 Linearization

The interpolation conditions

$$r_{\ell,m}(x_i, y_i) \in F_i \qquad i = 0, \ldots, n, \tag{7}$$

in (5) amount to

$$\underline{f}_i \le \frac{p(x_i, y_i)}{q(x_i, y_i)} \le \overline{f}_i, \; i = 0, \ldots, n.$$

Under the assumption that $q(x_i, y_i) > 0$, $i = 0, \ldots, n$, we obtain the following homogeneous system of linear inequalities after linearization

$$\begin{cases} -p(x_i, y_i) + \overline{f}_i q(x_i, y_i) \ge 0 \\ \;\; p(x_i, y_i) - \underline{f}_i q(x_i, y_i) \ge 0 \end{cases}, \quad i = 0, \ldots, n. \tag{8}$$

There is no loss of generality in assuming that $q(x, y)$ is positive in the interpolation points: the interpolation conditions (7) can be linearized for arbitrary non-zero $q(x_i, y_i)$, without changing the nature of the problem.

For ease of notation, let $\lambda = (a_0, \ldots, a_\ell, b_0, \ldots, b_m)^T$ and $k = \ell + m + 2$. We denote by U the $(2n + 2) \times k$ matrix

$$U = \begin{pmatrix} -x_0^{i_0} y_0^{j_0} & \ldots & -x_0^{i_\ell} y_0^{j_\ell} & \overline{f}_0 x_0^{d_0} y_0^{e_0} & \ldots & \overline{f}_0 x_0^{d_m} y_0^{e_m} \\ \vdots & & \vdots & \vdots & & \vdots \\ -x_n^{i_0} y_n^{j_0} & \ldots & -x_n^{i_\ell} y_n^{j_\ell} & \overline{f}_n x_n^{d_0} y_n^{e_0} & \ldots & \overline{f}_n x_n^{d_m} y_0^{e_m} \\ x_0^{i_0} y_0^{j_0} & \ldots & x_0^{i_\ell} y_0^{j_\ell} & -\underline{f}_0 x_0^{d_0} y_0^{e_0} & \ldots & -\underline{f}_0 x_0^{d_m} y_0^{e_m} \\ \vdots & & \vdots & \vdots & & \vdots \\ x_n^{i_0} y_n^{j_0} & \ldots & x_n^{i_\ell} y_n^{j_\ell} & -\underline{f}_n x_n^{d_0} y_n^{e_0} & \ldots & -\underline{f}_n x_n^{d_m} y_0^{e_m} \end{pmatrix}.$$

In the sequel, we abbreviate (8) to $U\lambda \geq 0$ and denote

$$\mathcal{L}_{\ell,m}(S_n) = \{ \lambda \in \mathbb{R}^k \mid U\lambda \geq 0 \}. \tag{9}$$

Geometrically, the set (9) is the intersection of a finite number of closed half spaces, whose boundary hyperplanes pass through the origin in $\mathbb{R}^k$. We assume that U has full column rank k, such that $\mathcal{L}_{\ell,m}(S_n)$ is a pointed polyhedral convex cone with apex in the origin [3, 4]. A property of polyhedra that is important for the sequel is full-dimensionality. A polyhedron $P \subseteq \mathbb{R}^k$ is said to be full-dimensional if it contains $k+1$ points $x_0, \ldots, x_k$ such that the vectors $x_1 - x_0, x_2 - x_0, \ldots, x_k - x_0$ are linearly independent. A polyhedron $P \subseteq \mathbb{R}^k$ determined by the linear inequalities $U\lambda \geq 0$ is full-dimensional if and only if it contains a point λ for which $U\lambda > 0$. Such a point is called an interior point. It follows immediately that if the linear inequalities determining the polyhedron do not contain any (implicit) equality constraints, then the polyhedron is full-dimensional [9]. Hence, if any of the vertical segments F_i is such that $\underline{f}_i = \overline{f}_i$, the polyhedron $\mathcal{L}_{\ell,m}(S_n)$ is not full-dimensional. But assuming that all F_i are such that $\underline{f}_i < \overline{f}_i$, as we have done, is not enough to guarantee that $\mathcal{L}_{\ell,m}(S_n)$ is full-dimensional.

The linearized version of the existence problem (6) consists in determining whether

$$\mathcal{L}_{\ell,m}(S_n) \neq \{0\}. \tag{10}$$

Accordingly, the linearized representation problem is concerned with finding a non-zero element λ in $\mathcal{L}_{\ell,m}(S_n)$.

Two important remarks need to be made before solving the linearized existence and representation problem. First, observe that if $\lambda \in \mathcal{L}_{\ell,m}(S_n)$, then also $t\lambda \in \mathcal{L}_{\ell,m}(S_n)$ for any $t > 0$ and all points on the ray $t\lambda = t(a_0, \ldots, a_\ell, b_0, \ldots, b_m)^T$ lead to the same rational function. Hence finding a rational function satisfying (8) corresponds to finding a ray $t\lambda$ with $\lambda \in \mathcal{L}_{\ell,m}(S_n)$. It is clear that when solving the linearized problem, no normalization can be imposed a priori on the coefficients of the rational function. Imposing such a normalization, say $b_0 = 1$, adds an additional constraint to the system (9) which potentially causes loss of solutions. For example, if the unnormalized cone (9) lies in an orthant where $b_0 < 0$, the intersection with the hyperplane $b_0 = 1$ is empty, so that the normalized problem has no solution. Such dependence on the chosen normalization is undesirable.

Second, it is well known from the theory of rational interpolation that solutions of the linearized problem (8) not necessarily solve the original problem (7) due to the possibility that, for some $i \in \{0, \ldots, n\}$,

$$p(x_i, y_i) = 0 = q(x_i, y_i). \tag{11}$$

Such points (x_i, y_i) are called unattainable [1]. If we assume that the cone $\mathcal{L}_{\ell,m}(S_n)$ is full-dimensional, then (10) and (6) are equivalent, in other words

$$\mathcal{L}_{\ell,m}(S_n) \neq \{0\} \Leftrightarrow \mathcal{R}_{\ell,m}(S_n) \neq \emptyset.$$

Indeed, in this case, a point in the interior of $\mathcal{L}_{\ell,m}(S_n)$ exists for which the inequalities (8) are strict and hence the coefficients of the corresponding rational function are such that for none of the interpolation points (11) is satisfied. Therefore (10) implies (6). Observe that $\mathcal{R}_{\ell,m}(S_n) \neq \emptyset$ always implies $\mathcal{L}_{\ell,m}(S_n) \neq \{0\}$, even if $\mathcal{L}_{\ell,m}(S_n)$ is not full-dimensional.

In the next section, we investigate the linearized representation problem and provide an algorithm to compute a ray $t\lambda \neq 0$ with $\lambda \in \mathcal{L}_{\ell,m}(S_n)$, if such a λ exists. The computed ray is such that the corresponding rational function contains no unattainable points and satisfies certain properties that are important from the point of view of numerical stability. We assume that the cone $\mathcal{L}_{\ell,m}(S_n)$ is full-dimensional, so that (6) and (10) are equivalent.

3 Solution of the existence and representation problem

Throughout this section, we denote by u_j the jth row ($j = 1, \ldots, 2n+2$) of U. Unless specifically mentioned otherwise, the norm $\|\cdot\|$ is Euclidean.

The algorithm we develop, simultaneously solves the linearized existence problem (10) and, if a solution exists, computes a non-zero $\lambda \in \mathcal{L}_{\ell,m}(S_n)$ in such a way that λ satisfies certain essential properties, which we discuss next.

From the point of view of numerical stability, a rational function passing closely through the centers of the intervals F_i is more appropriate. Computing rational functions with this property is also consistent with the maximum likelihood assumption of standard regression techniques that the noise is normally distributed with zero mean (see for example chapter 13 of [8] and section 15.1 of [10]). Adopting this view, we need to avoid points λ which are not interior points of $\mathcal{L}_{\ell,m}(S_n)$. Indeed, for any non-interior point λ, the corresponding rational function exactly fits at least one of the bounds of the interval data.

Another consideration are unattainable points. Because unattainable points necessarily imply that the corresponding inequalities in (8) are equalities, they must occur on a boundary hyperplane of the polyhedral cone. In order to avoid solutions λ yielding unattainable points, we again look for rays that lie strictly in the interior of the polyhedral cone. The ray (or direction) that we aim for has maximal *depth*. Such a ray is called a Chebyshev direction. In what follows, we state precisely what that means and show how such a ray can be computed.

Denote the Euclidean ball of radius r and center λ by

$$B(\lambda, r) = \{\lambda + h \quad | \quad \|h\| \leq r\}.$$

Let $P \subset \mathbb{R}^k$ be a bounded polyhedron (a polytope) and let $\lambda \in P$. We recall from [11] that the depth of λ with respect to P is defined by

$$\begin{aligned} \text{depth}(\lambda, P) &= \text{dist}(\lambda, \mathbb{R}^k \setminus P) \\ &= \inf_{z \in \mathbb{R}^k \setminus P} \|\lambda - z\| \\ &= \max_{B(\lambda, r) \subset P} r, \end{aligned} \tag{12}$$

and that a Chebyshev center [11] of a polytope $P \subset \mathbb{R}^k$ is given by

$$\lambda_c = \underset{\lambda \in P}{\text{argmax}}\, \text{depth}(\lambda, P) \tag{13}$$

In words, a Chebyshev center of a polytope P is every point $\lambda_c \in P$ for which the distance to the exterior of P is maximal. It is also the center of a largest inscribed ball. In analogy, let $C \subset \mathbb{R}^k$ be a pointed polyhedral convex cone with apex in the origin. We define the depth of a non-zero point $\lambda \in C$ with respect to C as follows

$$\begin{aligned} \text{depth}(\lambda, C) &= \text{dist}\left(\frac{\lambda}{\|\lambda\|}, \mathbb{R}^k \setminus C\right) \\ &= \inf_{z \in \mathbb{R}^k \setminus C} \left\| \frac{\lambda}{\|\lambda\|} - z \right\|. \end{aligned} \tag{14}$$

The $\text{depth}(\lambda, C)$ is the distance of the normalized vector $\lambda / \|\lambda\|$ to the exterior of C. Due to the normalization, $\text{depth}(\lambda, C)$ is bounded. We then call λ_c a Chebyshev direction of $C \subset \mathbb{R}^k$ if and only if

$$\lambda_c = \underset{\lambda \in C}{\text{argmax}}\, \text{depth}(\lambda, C). \tag{15}$$

Since $\text{depth}(\lambda, C)$ is equal for all λ that make up the same direction, (15) can be reformulated as

$$\begin{aligned} \lambda_c &= t \underset{\lambda \in C, \|\lambda\| = \gamma}{\text{argmax}}\, \text{depth}(\lambda, C) \qquad t, \gamma > 0, \\ &= t \underset{\lambda \in C, \|\lambda\| = \gamma}{\text{argmax}}\, \frac{\text{dist}(\lambda, \mathbb{R}^k \setminus C)}{\gamma} \qquad t, \gamma > 0. \end{aligned} \tag{16}$$

In words, among all vectors λ with $\|\lambda\| = \gamma$, a Chebyshev direction of C maximizes the distance from λ to the exterior of the polyhedral cone C. Since $\text{depth}(\lambda, C) = \text{dist}(\lambda, \mathbb{R}^k \setminus C)/\|\lambda\|$, a Chebyshev direction is also a direction that, among all vectors λ with distance δ to the exterior of C, minimizes the norm of λ:

$$\begin{aligned}\lambda_c &= t \operatorname*{argmax}_{\lambda \in C, \mathrm{dist}(\lambda, \mathbb{R}^k \setminus C) = \delta} \mathrm{depth}(\lambda, C) \qquad t, \delta > 0, \\ &= t \operatorname*{argmax}_{\lambda \in C, \mathrm{dist}(\lambda, \mathbb{R}^k \setminus C) = \delta} \frac{\delta}{\|\lambda\|} \qquad t, \delta > 0. \end{aligned} \tag{17}$$

Analogous to a Chebyshev center, a Chebyshev direction corresponds to the axis of a largest cone inscribed in the pointed polyhedral cone C.

The main result of this section is the following.

Theorem 1 *Let $\mathcal{L}_{\ell,m}(S_n)$ be the polyhedral cone (9). Then $\mathcal{L}_{\ell,m}(S_n)$ is full-dimensional and $\mathcal{R}_{\ell,m}(S_n) \neq \emptyset$ if and only if, for some $\delta > 0$, the quadratic programming problem*

$$\begin{aligned} &\operatorname*{argmin}_{\lambda \in \mathbb{R}^{\ell+m+2}} \|\lambda\|^2 \\ &s.t.\ \ u_j\lambda - \delta\|u_j\| \geq 0, \qquad j = 1, \ldots, 2n+2 \end{aligned} \tag{18}$$

has a solution. If (18) has a solution for some $\delta > 0$, then this solution λ_{min} is unique and the ray $t\lambda_{min}$, $t > 0$, is the unique Chebyshev direction of $\mathcal{L}_{\ell,m}(S_n)$. The corresponding rational function is an element of $\mathcal{R}_{\ell,m}(S_n)$.

Proof We start by characterizing balls inscribed in $C = \mathcal{L}_{\ell,m}(S_n)$. For a single half space $u_j\lambda \geq 0$, the ball $B(\lambda, r)$ lies in the correct half space if and only if

$$\inf_{\|h\| \leq r} u_j(\lambda + h) \geq 0.$$

We express this into a form independent of h, by noting that

$$\inf_{\|h\| \leq r} u_j(\lambda + h) \geq 0 \Leftrightarrow \inf_{\|h\| \leq r} u_j\lambda - |u_j \cdot h| \geq 0$$

and also

$$\begin{aligned}\inf_{\|h\| \leq r} u_j\lambda - |u_j \cdot h| &= u_j\lambda - \sup_{\|h\| \leq r} |u_j \cdot h| \\ &= u_j\lambda - r\|u_j\|.\end{aligned}$$

Hence, balls $B(\lambda, r)$ inscribed in the polyhedral cone $C = \mathcal{L}_{\ell,m}(S_n)$ satisfy

$$u_j\lambda - r\|u_j\| \geq 0, \qquad j = 1, \ldots, 2n+2. \tag{19}$$

If we set $r = \mathrm{dist}(\lambda, \mathbb{R}^k \setminus C)$ in (19), then $\lambda \in C = \mathcal{L}_{\ell,m}(S_n)$, if and only if

$$u_j\lambda - \mathrm{dist}(\lambda, \mathbb{R}^k \setminus C)\|u_j\| \geq 0, \qquad j = 1, \ldots, 2n+2. \tag{20}$$

It follows from (20) that there exists an interior point λ in $\mathcal{L}_{\ell,m}(S_n)$ if and only if the quadratic programming problem (18) has a solution. Hence $\mathcal{L}_{\ell,m}(S_n)$ is full-dimensional and $\mathcal{R}_{\ell,m}(S_n) \neq \emptyset$ if and only if the quadratic programming problem has a solution.

We now assume that there exists a $\lambda \neq 0$ in $\mathcal{L}_{\ell,m}(S_n)$. By combining (20) with (17), we find that λ is a Chebyshev direction of the polyhedral cone $C = \mathcal{L}_{\ell,m}(S_n)$ if and only if for some fixed $\delta > 0$,

$$\lambda_c = t \operatorname*{argmax}_{\lambda \in \mathbb{R}^k} \frac{\delta}{\|\lambda\|} \qquad t > 0$$
$$\text{s.t. } u_j\lambda - \delta\|u_j\| \geq 0, \qquad j = 1, \ldots, 2n+2, \tag{21}$$

or equivalently

$$\lambda_c = t \operatorname*{argmin}_{\lambda \in \mathbb{R}^k} \|\lambda\|^2 \qquad t > 0$$
$$\text{s.t. } u_j\lambda - \delta\|u_j\| \geq 0, \qquad j = 1, \ldots, 2n+2. \tag{22}$$

Since $\|\lambda\|^2$ is a strictly convex function, the minimizer $\lambda_{\min}$ of (18) is unique and hence the corresponding direction $t\lambda_{\min}$ is the unique Chebyshev direction of $C = \mathcal{L}_{\ell,m}(S_n)$. This concludes the proof. □

Observe that the Chebyshev direction obtained by solving (18) is independent of the choice of $\delta > 0$. How to best choose δ is discussed in Section 4.

Let us briefly come back to the relation between the results presented here and in [7]. Considering the representation problem for models which are linear in the unknown coefficients as in [7], rather than for rational models $r_{\ell,m}(x, y)$ as in (5), changes the nature of the problem. Indeed, for the former the problem can be reduced to the computation of a Chebyshev center of a bounded polyhedron [7]. This amounts to solving a linear programming problem. For the latter, we have shown that the problem can be reduced to the computation of a Chebyshev direction of an unbounded polyhedral set, resulting in a quadratic programming problem. Only if we add additional linear constraints to bound $\mathcal{L}_{\ell,m}(S_n)$, can we reduce the problem to the one discussed in [7]. A possible way to bound $\mathcal{L}_{\ell,m}(S_n)$ is by imposing conditions on the coefficients of the rational function. We have already indicated that a normalization where one of the coefficients is chosen a priori, e.g. $b_0 = 1$, potentially causes loss of solutions. But what happens to the solution set if we add the conditions $|\lambda_j| \leq 1$, $j = 1, \ldots, k$, where λ_j denotes the j^{th} element of the vector $\lambda = (a_0, \ldots, a_\ell, b_0, \ldots, b_m)^T$? For $L > 0$, let

$$\mathcal{BL}_{\ell,m}(S_n, L) = \{\lambda \in \mathbb{R}^k \mid U\lambda \geq 0, |\lambda_i| \leq L, i = 1, \ldots, k\}. \tag{23}$$

A Chebyshev center of this bounded polyhedron is found by solving the linear programming problem [11]

$$\begin{aligned} &\max r \\ \text{s.t. } u_j\lambda - r\|u_j\| &\geq 0, \qquad j = 1, \ldots, 2n+2, \\ \lambda_j - r &\geq -L, \qquad j = 1, \ldots, k, \\ -\lambda_j - r &\geq -L, \qquad j = 1, \ldots, k, \\ r &\geq 0. \end{aligned} \tag{24}$$

Since (24) is a linear programming problem, and (18) is a quadratic programming problem, it seems natural to solve (24) and not (18). We have reformulated the problem as a quadratic programming problem for the following important reasons. First, as is clear from Fig. 1, a Chebyshev center of the bounded polyhedron is not necessarily the Chebyshev direction of the corresponding unbounded polyhedral cone. Second, in case the bounded polyhedron $\mathcal{BL}_{\ell,m}(S_n, L)$ has different Chebyshev centers, as is the case in Fig. 1, the solution of the linear programming problem (24) is not unique. In contrast, the polyhedral cone $\mathcal{L}_{\ell,m}(S_n)$ has a unique Chebyshev direction, which is the solution of the quadratic programming problem (18). Third, as noted in [2], for linear programming problems that are highly homogeneous, such as is the case in (24), computer cycling of the simplex method is the rule rather than the exception. We have found in practice that solving the quadratic programming problem is far more accurate and faster than solving the corresponding LP problem, either by the simplex method or by an interior point method.

The following theorem summarizes the relation between the linear programming problem (24) and the quadratic programming problem (18).

Theorem 2 *Let $\mathcal{L}_{\ell,m}(S_n)$ be the polyhedral cone (9) with apex at the origin and let $\mathcal{BL}_{\ell,m}(S_n, L_1)$ be the corresponding polytope (23). Then $\mathcal{L}_{\ell,m}(S_n) \neq \{0\}$ if and only if $\mathcal{BL}_{\ell,m}(S_n, L) \neq \{0\}$ for any $L > 0$. Moreover, If λ_1 is a Chebyshev center of $\mathcal{BL}_{\ell,m}(S_n, L_1)$ with radius r_1, then there exists a $t > 0$ such that $t\lambda_1$ is a Chebyshev center of $\mathcal{BL}_{\ell,m}(S_n, L_2)$ for any $L_2 > 0$.*

Proof If $\mathcal{L}_{\ell,m}(S_n) \neq \{0\}$ then for any non-zero vector $\lambda \in \mathcal{L}_{\ell,m}(S_n)$ also $t\lambda \in \mathcal{L}_{\ell,m}(S_n)$ for all $t > 0$. Therefore $\mathcal{BL}_{\ell,m}(S_n, L) \neq \{0\}$ for any $L > 0$. Conversely, if there exists a vector $\lambda \in \mathcal{BL}_{\ell,m}(S_n, L)$ with $\lambda \neq 0$, then $U\lambda \geq 0$, hence $\lambda \in \mathcal{L}_{\ell,m}(S_n)$.

If λ_1 is a Chebyshev center of $\mathcal{BL}_{\ell,m}(S_n, L_1)$ with radius r_1, it satisfies (24) with $L = L_1$ and $r = r_1$. It follows immediately that for any $L_2 > 0$, $L_2\lambda/L_1$ is a Chebyshev center of $\mathcal{BL}_{\ell,m}(S_n, L_2)$ with radius $L_2 r_1/L_1$. This concludes the proof. □

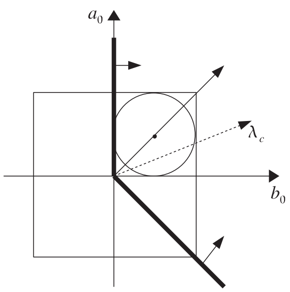


Fig. 1 The *boldface lines* denote the boundary of the polyhedral cone $\mathcal{L}_{\ell,m}(S_n)$, and λ_c denotes its Chebyshev direction. The *center of the disk* is a Chebyshev *center* of $\mathcal{BL}_{\ell,m}(S_n, 1)$

It follows from Theorem 2 that if the bounded polyhedron has a unique Chebyshev center, the rational function that corresponds to the solution λ of (24) is independent of the constant L. If the Chebyshev center of the bounded polyhedron is not unique, solving (24) for different values of L may yield Chebyshev centra which are not on the same ray through the origin and hence different rational functions.

4 Algorithmic aspects and numerical examples

In this section we discuss a number of aspects related to the solution of the representation problem for (5):

– Given $n+1$ vertical segments, how do we determine the numerator and denominator degrees of the rational function to fit these data?
– How do we choose δ in (18)?

We then illustrate our technique with some numerical examples.

First, the complexity of a rational function is determined by its degree sets N_ℓ and D_m. As ℓ and m increase, so does the complexity of the rational function $r_{\ell,m}(x, y)$. For $\ell = 0, 1, \ldots$ and $m = 0, 1, \ldots$, we organize the rational functions $r_{\ell,m}(x, y)$ in a two-dimensional table as indicated in Table 1. In order to determine the rational model of lowest complexity for which $\mathcal{R}_{\ell,m}(S_n) \neq \emptyset$, we enumerate over the upward sloping diagonals of Table 1, each time solving the quadratic programming problem (18). The following pseudocode summarizes the algorithm.

```
solution= ∅
for d = 0, 1, 2, ...
  for ℓ = d, ..., 0
     solve (18) for numerator degree set N_ℓ
               and denominator degree set D_{d−ℓ}
     if (18) has the unique solution λ_min
         let r_{ℓ,d−ℓ}(x, y) be the irreducible rational function
               derived from the coefficients in λ_min
         solution:= solution ∪{r_{ℓ,d−ℓ}(x, y)}
     endif
  endfor
if solution≠ ∅ return solution
endfor
```

Table 1 Table of rational interpolants

$r_{0,0}(x, y)$	$r_{0,1}(x, y)$	$r_{0,2}(x, y)$	$\cdots$
$r_{1,0}(x, y)$	$r_{1,1}(x, y)$	$r_{1,2}(x, y)$	$\cdots$
$r_{2,0}(x, y)$	$r_{2,1}(x, y)$	$r_{2,2}(x, y)$	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\ddots$

We call the rational functions $r_{\ell,m}(x, y)$ in `solution` the rational functions of minimal complexity satisfying the interpolation conditions (7). We remark that there may exist a rational function $r_{\nu,\mu}(x, y)$ with $\nu + \mu < \ell + m$ and such that $r_{\nu,\mu}(x_i, y_i) \in F_i$, $i = 0, \ldots, n$. Indeed, we recall from Theorem 1 that the quadratic programming problem has a solution if and only if $\mathcal{L}_{\nu,\mu}(S_n)$ is full-dimensional. If this is not the case, this does not imply $\mathcal{L}_{\nu,\mu}(S_n) = \{0\}$. However, for any non-zero element in $\mathcal{L}_{\nu,\mu}(S_n)$, the corresponding rational function then exactly fits at least one of the bounds of the interval data and may have unattainable points, which is not desirable.

Second, it follows from Theorem 1 that solving the representation problem for (5), amounts to computing the solution of the quadratic programming problem (18) for some $\delta > 0$. It seems natural to set $\delta = 1$. Instead of this obvious choice, it is better, from a numerical point of view, to determine δ differently and take into account the condition number of the matrix U in (9). If the matrix U in (9) is almost rank deficient, then the depth of any point λ strictly in the interior of the cone determined by $U\lambda \geq 0$ is close to zero. Since

$$\text{depth}(\lambda, C) = \frac{\text{dist}(\lambda, C)}{\|\lambda\|} = \frac{\delta}{\|\lambda\|}$$

the choice $\delta = 1$ implies that the norm of λ obtained from (18) is large. In order to avoid explosive growth of the elements of λ, we need to choose δ much smaller when U is ill-conditioned. Therefore, we set $\delta = 1/\kappa(U)$, where $\kappa(U)$ is the condition number of the matrix U defined by

$$\kappa(U) = \frac{\sigma_{max}(U)}{\sigma_{min}(U)}, \tag{25}$$

and $\sigma_{max}(U)$ and $\sigma_{min}(U)$ are, respectively, the largest and the smallest singular value of U.

We next illustrate our technique for several datasets. To improve the numerical conditioning of the problem, the independent variables x_i, y_i are each rescaled to the interval $[-1, 1]$ and products of Chebyshev polynomials $T_i(x)$ and $T_j(y)$ of the first kind are used as basis functions. The coefficients of $p(x, y)$ and $q(x, y)$ with respect to these basis functions are denoted by $\tilde{\lambda} = (\tilde{a}_0, \ldots, \tilde{a}_\ell, \tilde{b}_0, \ldots, \tilde{b}_m)^T$. The quadratic programming problem (18) is solved using the optimization toolbox of Matlab Release 2006*a*.

A first univariate illustration is the Kirby2 dataset, part of the NIST Statistical Reference Datasets.[1] There are 151 observations (x_i, f_i). From the NIST Statistical Reference Datasets website we find an indication that an error margin on the f_i values is of the order of

$$F_i = [f_i - 2\sigma, f_i + 2\sigma]$$

with $\sigma = 0.16354535131$[1]. For the vertical segments $S_{150} = \{(x_i, F_i) | i = 1, \ldots, 151\}$, our algorithm returns `solution`$= \{r_{2,2}(x)\}$. The rational function $r_{2,2}(x)$

[1] http://www.itl.nist.gov/div898/strd/index.html

has coefficients $\tilde{a}_0 = 31.82, \tilde{a}_1 = 43.55, \tilde{a}_2 = 11.83, \tilde{b}_0 = 0.53, \tilde{b}_1 = 0.32, \tilde{b}_2 = 0.11$ and is plotted in Fig. 2a.

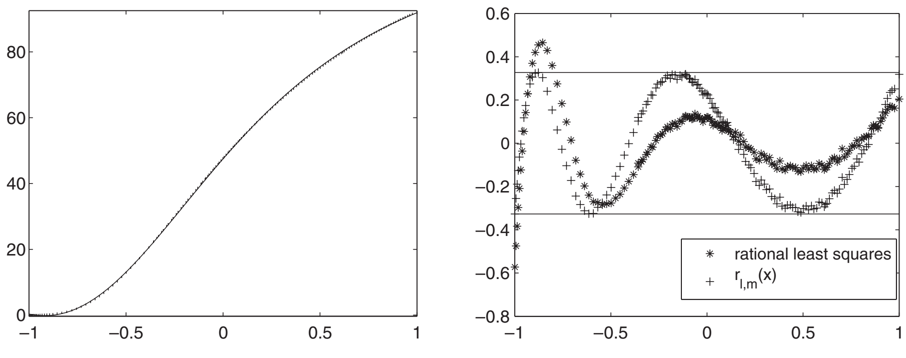
For the same data set, we also compute the rational least squares model $r^{\text{rls}}_{2,2}(x)$ of degree 2 in numerator and denominator with the `nlinfit` function of the Statistics Toolbox for Matlab. In rational least squares, the coefficients of the regression model $r(x)$ are estimated by minimizing the least squares criterion

$$\sum_{i=0}^{n} (f_i - r(x_i))^2 \tag{26}$$

over all rational functions $r(x)$ of fixed numerator and denominator degree. As already pointed out, the solution of non-linear least squares approximation problems depends on the starting values, since the objective function (26) may have many local minima. With the starting values $\tilde{a}_0 = \tilde{a}_1 = \tilde{a}_2 = \tilde{b}_0 = \tilde{b}_1 = \tilde{b}_2 = 1$, the procedure to minimize (26) over all rational functions of degree 2 in numerator and denominator stops with an objective function value of $1.333 * 10^5$, while the global minimum is 3.905! If we choose as starting values the coefficients of $r_{2,2}(x)$, normalized such that $b_0 = 1$, then the optimization procedure does converge to the global minimum. This is not surprising: evaluating (26) for $r(x) = r_{2,2}(x)$ gives the value 7.418, while the optimal value obtained for $r(x) = r^{\text{rls}}_{2,2}(x)$ is 3.905. In Fig. 2b, the absolute error of $r_{2,2}(x)$ is compared with that of $r^{\text{rls}}_{2,2}(x)$. From this plot one can see that $r_{2,2}(x)$ stays within the required bound $2\sigma \approx 0.32709$ of the point data.

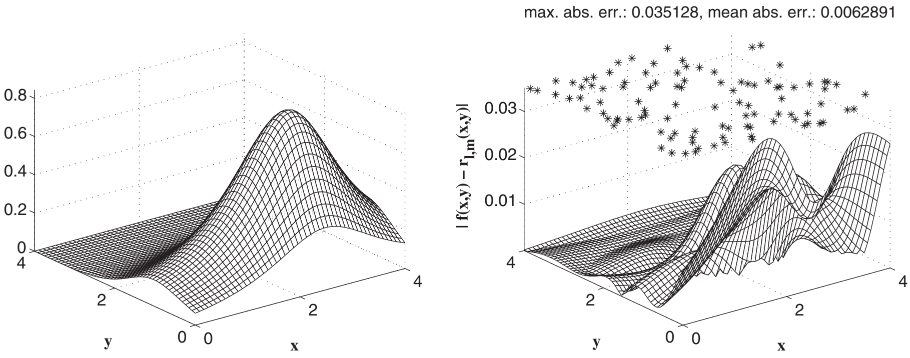
The second example is another benchmark problem, the bivariate Kotancheck function

$$f(x, y) = \frac{e^{-(y-1)^2}}{1.2 + (x - 2.5)^2}. \tag{27}$$



a Fitted versus observed values **b** Absolute error

Fig. 2 Kirby2 dataset. **a** shows the *vertical* data segments and $r_{2,2}(x)$, which is the rational model of minimal complexity satisfying the interpolation conditions. **b** shows the *absolute error* of $r_{2,2}(x)$ (*plus*) and of the rational least squares model of degree 2 in numerator and denominator (*star*). The *two lines* represent the boundaries $\pm 2\sigma$



a [6/12] rational model **b** Absolute error

Fig. 3 Kotancheck function. **a** shows $r_{6,12}(x, y)$ which is the rational model of minimal complexity satisfying the interpolation conditions. **b** shows the *absolute error* over the entire interval. Also the location of the 100 scattered data points is indicated

There are 100 scattered samples (x_i, y_i, f_i), selected from the interval $[0, 4] \times [0, 4]$. Each observation has been corrupted by random noise in $[-0.0252, 0.0252]$, to generate vertical segments of different width enclosing the function value. If we enumerate $\mathbb{N}^2$ along downward sloping diagonals to construct the numerator and denominator index sets N_ℓ and D_m for increasing values of ℓ and m, then the algorithm returns `solution=` $\{r_{6,12}(x, y)\}$, where the numerator and denominator degree sets are respectively given by

$$N_6 = \{(0,0), (0,1), (1,0), (0,2), (1,1), (2,0), (0,3)\}$$
$$D_{12} = \{(0,0), (0,1), (1,0), (0,2), (1,1), (2,0), (0,3), (1,2), (2,1), (3,0), (0,4), (1,3), (2,2)\}$$

and where $r_{6,12}(x, y)$ is plotted in Fig. 3. To evaluate the goodness of fit of $r_{6,12}(x, y)$, we also plot the absolute error $|r_{6,12}(x, y) - f(x, y)|$ in Fig. 3b, and observe that it is much smaller than the maximum width of the vertical segments over the entire interval.

5 Conclusion and future work

A very natural way to deal with uncertainty in data is by means of an uncertainty interval. Here, we have assumed that the uncertainty in the independent variable is negligible and that for each observation, an uncertainty interval can be given which contains the (unknown) exact value. We have presented an approach to compute rational functions intersecting the interval data and shown that the problem reduces to a quadratic programming problem, which has a unique solution and which is easy to solve by standard methods. In the future, we intend to investigate the behaviour of the poles of the approximating rational function. In none of the examples we have run, did the approximating rational function have poles in the domain of interest.

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