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Rational Interpolation and Its Ill-conditioned Property

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Abstract. A rational interpolation is obtained by solving a system of linear equations. However, when the system is solved by floating point arithmetic, there appears a pathological feature such as undesired zeros and poles. In this paper, a method is described with the help from computer assisted proof to eliminate the feature.

Keywords. Approximate GCD, rational interpolation, ill conditioned property.

1. Introduction

A rational interpolation approximates a given function to a rational function, which is defined as a ratio of numerator and denominator polynomials as

$$r_{m,n}(x) = \frac{p_m(x)}{q_n(x)} = \frac{a_0 + a_1 x + \cdots + a_m x^m}{1 + b_1 x + \cdots + b_n x^n}. \tag{1.1}$$

This interpolates a function $f(x)$ or a set of discrete data on a range $[\alpha, \beta]$. For any given points $\alpha < x_0 < x_1 < \cdots < x_{m+n} < \beta$ we have

$$r_{m,n}(x_k) = f(x_k) := f_k, \quad \text{for} \quad k = 0, \ldots, m+n.$$

Then we obtain the linearized equations

$$\sum_{i=0}^{m} a_i x_k^i - f_k \sum_{j=1}^{n} b_j x_k^j = f_k. \tag{1.2}$$

The unknown coefficients a_i, b_j can be determined by solving the Equ. (1.2) by Gaussian elimination.

However, when the linearized equations are solved by floating point arithmetic, there appears a pathological feature such as undesired zeros and poles [6]. A reason of the appearance of undesired zeros and poles is highly ill-conditioned property of the Equ. (1.2) [4, 5].

For the well-conditioned case, there are modern fast algorithms for rational interpolation (see, e.g., [8]). When we consider only the ill-conditioned case, the naïve method such as Gaussian elimination may be investigated.

In this paper, the reason of the appearance of undesired zeros and poles is stated more precisely. A method to eliminate the pathological feature is presented using computer assisted proof.

2. Undesired Zeros and Poles

Suppose that the system Equ. (1.2) is $Ay = B$. Here, the coefficients a_i, b_j are represented by a vector $y \in R^{m+n+1}$ as $y = (a_0, \ldots, a_m, b_1, \ldots, b_n)^T$. Then the matrix $A \in R^{(m+n+1)\times(m+n+1)}$ and the vector $B \in R^{m+n+1}$ are represented as follows:

$$A = \begin{pmatrix} 1 & x_0 & \cdots & x_0^m & -f_0 x_0 & \cdots & -f_0 x_0^n \\ 1 & x_1 & \cdots & x_1^m & -f_1 x_1 & \cdots & -f_1 x_1^n \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m+n} & \cdots & x_{m+n}^m & -f_{m+n} x_{m+n} & \cdots & -f_{m+n} x_{m+n}^n \end{pmatrix}, \tag{2.1}$$

$$B = (f_0, f_1, \ldots, f_{m+n})^T . \tag{2.2}$$

The matrix A containing two column blocks of Krylov matrix is known as ill-conditioned matrix [1]. The ill-conditioned property of the system gives the pathological feature such as the appearance of approximate common factors. The approximate common factors cause undesired zeros and poles in the rational interpolants. We analyze the system in the following two cases:

1. the matrix A is a singular matrix,
2. the matrix A is an ill-conditioned matrix.

2.1. Case 1: A Is a Singular Matrix

Suppose that the given function $f(x)$ is a rational function $r_{M,N}(x) = p_M(x)/q_N(x)$, where $M < m$ and $N < n$; then the matrix A will be singular. In order to show this, we need the following property of the rational interpolation.

Lemma 2.1. *Suppose that $r_{m,n}(x)$ is a rational interpolant of the rational function $r_{M,N}(x)$. Then*

$$r_{m,n}(x) \sim r_{M,N}(x). \tag{2.3}$$

Proof. If we assume $r_{m,n}(x) \neq r_{M,N}(x)$, then the number of intersection of these functions is up to $\max\{M + n, N + m\}$. However we have $m + n + 1$ points to interpolate $r_{M,N}(x)$. This leads to contradiction of the assumption $r_{m,n}(x) \neq r_{M,N}(x)$. □

Lemma 2.1 implies that $r_{m,n}(x)$ is represented by the following equation:

$$r_{m,n}(x) = \frac{g(x)p_M(x)}{g(x)q_N(x)}, \tag{2.4}$$

where $g(x)$ is a polynomial and the degree is $\gamma := \min\{m - M, n - N\}$. From this observation, the number of the unknown coefficients for this problem is reduced to $m + n + 1 - \gamma$. Thus, the following property holds immediately.

Corollary 2.2. *The matrix A is singular and its rank is $m + n + 1 - \gamma$.*

Suppose that $\hat{A}y = \hat{B}$ is a triangularized system by Gaussian elimination of $Ay = B$. The last γ rows of $\hat{A}$ and $\hat{B}$ will be all zero. We may substitute symbols $t_1, \ldots, t_\gamma$ in the solution to have a unique solution, such as $b_n = t_\gamma, \ldots, b_{n-\gamma-1} = t_1$. Then, we have the following form:

$$r_{m,n}(x) = \frac{p_0(x) + t_1 p_1(x) + \cdots + t_\gamma p_\gamma(x)}{q_0(x) + t_1 q_1(x) + \cdots + t_\gamma q_\gamma(x)}. \tag{2.5}$$

Since $r_{M,N}(x)$ is free from the symbols $t_1, \ldots, t_\gamma$, $p_M(x) = p_0(x)$ and $q_N(x) = q_0(x)$. From Lemma 2.1, $p_i(x) = v_i(x)p_0(x)$ and $q_i(x) = v_i(x)q_0(x)$ must be allowed as well, where $v_i(x)$ are polynomials. Hence, the following property holds.

Theorem 2.3 (Murakami et al. [5]). *If A is singular (has the rank $m+n+1-\gamma$), then $r_{m,n}(x)$ may be represented as follows:*

$$r_{m,n}(x) = \frac{g(x)p_M(x)}{g(x)q_N(x)}, \tag{2.6}$$

$$g(x) = \begin{cases} 1 + \sum_{i=1}^{\gamma} t_i v_i(x) & \text{for } \gamma > 0, \\ 1 & \text{for } \gamma = 0. \end{cases} \tag{2.7}$$

The converse may also hold.

Example. For $\gamma = 1$, if $r_{M,N}(x)$ is represented as

$$r_{M,N}(x) = \frac{a_0 + \cdots + a_M x^M}{1 + b_1 x + \cdots + b_N x^N}, \tag{2.8}$$

then Theorem 2.3 shows that $g(x) = 1 + t_1 v_1(x)$, where $v_1(x) = x/b_M$ by easy derivation.

The rational interpolant $r_{m,n}(x)$ may be computed in floating point arithmetic, but the symbols t_i will be substituted by rounding errors. This computation will raise an approximate GCD in $r_{m,n}(x)$.

2.2. Case 2: A Is an Ill-conditioned Matrix

If the given function $f(x)$ is not a rational function, the matrix A is not singular in general. But, there are undesired zeros and poles in the rational interpolant, as we have observed experimentally in [3] and [6]. As is well-known in numerical computation, if the condition number of A is large, then the matrix A is numerically singular.

Example. We compute a rational interpolant $r_{4,4}(x)$ for the function $f(x) = \log(x+2)$ in $x \in [0,1]$. By using the similar procedures discussed in the previous section, $\hat{A}$ and $\hat{B}$ are obtained after Gaussian elimination as

$$\begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & & 1 & -1.1 & -1.1 & -1.1 & -1.1 \\ 0 & & -0.4 & 0.09 & 0.3 & 0.4 & 0.5 \\ 0 & & 0.08 & 0.004 & -0.02 & -0.06 & -0.1 \\ 0 & \vdots & -0.03 & 0.0005 & -0.002 & 0.008 & 0.04 \\ 0 & & 0 & 0.0002 & -0.00007 & 0.0002 & -0.001 \\ 0 & & 0 & 0 & -0.0000007 & 0.000006 & -0.00007 \\ 0 & & 0 & 0 & 0 & 0.2\cdot 10^{-7} & -0.7\cdot 10^{-6} \\ 0 & \cdots & 0 & 0 & 0 & 0 & 0.5\cdot 10^{-7} \end{bmatrix}$$

and

$$\left(0.7,\ 0.4,\ 0.02,\ 0.001,\ 0.0002,\ 0.000009,\ -0.00000006,\ 0.5\cdot 10^{-9},\ -0.3\cdot 10^{-9}\right)^T$$

by 9 digits floating point arithmetic. More precisely, the elements $\hat{A}_{9,9} \simeq 0.52292 \cdot 10^{-7}$ and $\hat{B}_9 \simeq -0.27990 \cdot 10^{-9}$ in the last row are very small. By a straightforward computation, we can obtain the following rational interpolant:

$$r_{4,4}(x) \simeq 4.5843 \frac{(x+11.392)(x+2.9853)(x+1.0001)(x-0.8305033948)}{(x+21.676)(x+4.4851)(x+2.3139)(x-0.8305033945)}.$$

We can observe an undesired zero and pole appearing around 0.83053 in $r_{4,4}(x)$.

Here, we eliminate the undesired zero and pole from $r_{4,4}(x)$. Then the remaining part is as follows:

$$\begin{aligned} r_{3,3}(x) &= 4.5843 \frac{(x+11.392)(x+2.9853)(x+1.0001)}{(x+21.676)(x+4.4851)(x+2.3139)} \\ &= \frac{0.69315 + 0.98608x + 0.31337x^2 + 0.020379x^3}{1 + 0.70126x + 0.12658x^2 + 0.00444539x^3}. \end{aligned}$$

In order to show that A is numerically singular, let us assume that the given function $f(x)$ is this rational function $r_{3,3}(x)$. From Theorem 2.3, since $t_1 = \hat{B}_9/\hat{A}_{9,9} = -0.27990 \cdot 10^{-9}/0.52292 \cdot 10^{-7} = -0.00535265$ and $b_3 = 0.00444539$, the GCD is constructed as follows:

$$g(x) = 1 + \frac{t_1}{b_3}x \simeq 1 + \frac{-0.00535265}{0.00444539}x = -1.20409(x - 0.830503).$$

This result agrees with the position of undesired zero and pole. This shows that the matrix A is numerically singular.

3. To Eliminate the Feature

There exists a well-known property to state how much a regular matrix is close to a singular matrix. Let P be the set of singular matrices. Let $\operatorname{dist}(A, P)$ denote the minimum distance from the matrix A to the set P. Then

$$\mathrm{dist}(A,P) = \| A^{-1} \|^{-1} = \frac{\| A \|}{\mathrm{cond}(A)},$$

where $\| \cdot \|$ denotes an arbitrary norm and $\mathrm{cond}(A)$ is the condition number of the matrix A (see, e.g., [2]).

This property indicates that we need higher digits of floating point arithmetic than the following positive integer d to eliminate the feature:

$$d = \left\lceil -\log_{10} \frac{\| A \|}{\mathrm{cond}(A)} \right\rceil .$$

In the example for $\log(x+2)$, the condition number of A is estimated as

$$\frac{||A||}{\mathrm{cond}A} = 6.974 \cdot 10^{-12}.$$

This result shows that we need $d = 12$ digits at least to have an accurate result for this problem. Thus, the matrix A is numerically singular in 9 digits floating point arithmetic and, in fact, we have an approximate GCD $g(x) = x - 0.830503$.

We can consider two methods to eliminate the pathological feature:

1. use approximate GCD and eliminate the undesired zeros and poles, or
2. compute in higher precision.

The first method is called Hybrid Rational Function Approximation (HRFA) and works well for computing a rational approximation in limited precision [3, 6]. If higher precision is available, the second method may give us an accurate rational interpolant for a function.

To verify the solutions of the linear equations $Ay = B$, we refer to Algorithm 3.1 in [7]. It can verify nonsingularity of A, after an approximate inverse matrix of A is computed. If the verification is successful, then the result is guaranteed to be accurate.

However, if the condition number of A is large, the verification may fail. We use, therefore, iterative increment of the precision of floating point arithmetic. The following method is derived:

Algorithm 1 (Rational interpolation using computer assisted proof)

1. Set initial digits to the number d.
2. Solve the linear equations $Ay = B$ by Gaussian elimination and obtain an approximate solution $\tilde{y}$ and an approximate inverse matrix R of A.
3. Verify the solution using Algorithm 3.1 in [7].
4. If nonsingularity of A is verified, then output the result. Otherwise, increase the digits (for example, twice) and go to step 2.

This method should work well. In the example for $\log(x+2)$, starting from $d = 8$, the verification succeeds at precision $d = 16$. This gives us an accurate rational interpolant successfully as follows:

$$r_{4,4}(x) = 5.0787 \frac{(x+19.851)(x+4.8602)(x+2.4752)(x+1)}{(x+35.346)(x+7.0401)(x+3.2192)(x+2.1843)}.$$

Table 1. The error of rational approximations by HRFA

Interpolation $r_{m,n}(x)$	HRFA $\tilde{r}_{m,n}(x)$	Error E_{Ave}
$(7,7)$	$(6,6)$	$2.13 \cdot 10^{-6}$
$(8,8)$	$(4,4)$	$1.05 \cdot 10^{-5}$
$(9,9)$	$(6,6)$	$1.51 \cdot 10^{-4}$

Table 2. The error of rational interpolants by Algorithm 1

Interpolation $r_{m,n}(x)$	Precision d	Error E_{Ave}
$(7,7)$	32	$1.12 \cdot 10^{-24}$
$(8,8)$	32	$1.12 \cdot 10^{-28}$
$(9,9)$	64	$9.20 \cdot 10^{-33}$

Tables 1 and 2 show numerical comparisons between the error of the approximation by HRFA and Algorithm 1.

The function $f(x) = e^{x+2}$, $x \in [0,1]$ is approximated with the equidistant points from 0 to 1. The error of a rational approximation is estimated by the following expression

$$E_{\text{Ave}} := \frac{\sum_{i=1}^{100}(f(x_i) - r_{m,n}(x_i))/f(x_i)}{100},$$

where $x_i = (i-1)/99$.

The results by HRFA are shown in Table 1. Here, naïve rational interpolants are computed at precision $d = 8$, and we denote the degree of the rational function $r_{m,n}(x)$ by (m,n). For example, $r_{7,7}(x)$ has an undesired pole in the range $x \in [0,1]$. HRFA gives a reduced rational approximation $\tilde{r}_{6,6}(x)$ after eliminating the undesired pole, where the approximate GCD is computed by QRGCD in Maple 10 with parameter $\epsilon = 10^{-4}$. The results in Table 1 show that HRFA gives accurate approximations at the fixed precision.

The results by Algorithm 1 are shown in Table 2. For the computation of the rational interpolants $r_{7,7}(x)$, $r_{8,8}(x)$ and $r_{9,9}(x)$, starting at precision $d = 8$, the verification succeeds at precision $d = 32$, $d = 32$ and $d = 64$, respectively. Table 2 shows that, if multiple precision arithmetic is available, then we have accurate rational interpolants by Algorithm 1.

4. Conclusion

As already shown by M.-T. Noda and the author, hybrid rational function approximation (HRFA) works well for naïve rational function approximations. HRFA gives accurate approximation for given functions. One of the remaining problems is to consider a reason for the appearance of undesired zeros and poles. In this paper, we discuss the problem and show that it depends on the ill-conditioned property of the system of linear equations, which determines the coefficients of the rational interpolants. A straihgtforward method to eliminate the feature may be useful to give an accurate rational interpolant for a given data set.

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