Multivariate Rational Interpolation of Scattered Data

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Abstract. Rational data fitting has proved extremely useful in a number of scientific applications. We refer among others to its use in some network problems [6, 7, 15, 16], to the modelling of electro-magnetic components [20, 13], to model reduction of linear shift-invariant systems [2, 3, 8] and so on.
When computing a rational interpolant in one variable, all existing techniques deliver the same rational function, because all rational functions that satisfy the interpolation conditions reduce to the same unique irreducible form. When switching from one to many variables, the situation is entirely different. Not only does one have a large choice of multivariate rational functions, but moreover, different algorithms yield different rational interpolants and apply to different situations.
The rational interpolation of function values that are given at a set of points lying on a multidimensional grid, has extensively been dealt with in [11, 10, 5]. The case where the interpolation data are scattered in the multivariate space, is far less discussed and is the subject of this paper. We present a fast solver for the linear block Cauchy-Vandermonde system that translates the interpolation conditions, and combine it with an interval arithmetic verification step.

1 Introduction

In one variable the rational interpolation problem can be solved using the recursive technique developed by Bulirsch-Stoer, or a fast solver for the solution of the structured linear system defining the coefficients. The rational interpolant can also be obtained as the convergent of a Thiele interpolating continued fraction with inverse differences in the partial denominators. For multivariate generalizations of the Thiele interpolating continued fraction approach we refer to [21, 22, 19, 12]. For a multivariate generalization of the Bulirsch-Stoer algorithm we refer to [9]. The structured linear system solver, which is developed here, delivers the coefficients of the rational interpolant, and hence an explicit representation of the rational function.

Let the value of the univariate function $f(x)$ be given in the interpolation points $\{x_0, x_1, x_2, \ldots\}$, which are non-coinciding. The rational interpolation problem of order (n, m) for f consists in finding polynomials

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$$p(x) = \sum_{i=0}^{n} a_i x^i, \qquad q(x) = \sum_{i=0}^{m} b_i x^i,$$

with $p(x)/q(x)$ irreducible and such that

$$f(x_i) = \frac{p}{q}(x_i), \qquad i = 0, \ldots, n+m \ . \tag{1}$$

In order to solve (1) we rewrite it as

$$f(x_i)q(x_i) - p(x_i) = 0, \qquad i = 0, \ldots, n+m \ . \tag{2}$$

Condition (2) is a homogeneous system of $n+m+1$ linear equations in the $n+m+2$ unknown coefficients a_i and b_i of p and q and hence it has at least one nontrivial solution. It is well-known that all the solutions of (2) have the same irreducible form and we shall therefore denote by

$$r_{n,m}(x) = \frac{p^\star}{q^\star}(x)$$

the irreducible form of p/q with p and q satisfying (2) where $q^\star$ is normalized according to a chosen normalization. We say that $r_{n,m}$ "interpolates" the given function and by this we mean that $p^\star$ and $q^\star$ satisfy some of the interpolation conditions (1). This does not imply that $r_{n,m}$ actually interpolates the given function at all the data because, by constructing the irreducible form, a common factor and hence some interpolation conditions may be cancelled in the polynomials p and q that provide $r_{n,m}$. Since $r_{n,m}$ is the irreducible form, the rational functions p/q with p and q satisfying (2) are called "equivalent". If the rank of the linear system (2) is maximal then $r_{n,m} = p^\star/q^\star = p/q$.

Let us take a closer look at the linear system of equations (2), defining the numerator and denominator coefficients a_i and b_i. In the sequel we assume, for simplicity but without loss of generality, that this $(n+m+1) \times (n+m+2)$ homogeneous linear system of equations can be solved for the choice $b_0 = 1$.

The concept of displacement rank was first introduced in [18]. We use the definition given in [14] where the displacement rank α of an $(n+m+1)\times(n+m+1)$ matrix A is defined as the rank of the matrix $LA - AR$ with L and R being so-called left and right displacement operators. If A is a Cauchy-Vandermonde matrix, as in (2) after choosing $b_0 = 1$, and if all $x_i \neq 0$ and all $|x_i| \neq 1$, then suitable displacement operators are given by $L = \mathrm{diag}\,(1/x_i)_{i=0,\ldots,n+m}$ and $R^T = Z_m^{(1)} \oplus Z_{n+1}^{(1)}$ with

$$Z_k^{(w)} = \begin{pmatrix} 0 & \ldots & & 0 & w \\ 1 & 0 & \ldots & & 0 \\ 0 & 1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & 1 & 0 \end{pmatrix}_{k\times k} .$$

The resulting matrix $LA - AR$ then takes the form

$$LA - AR = \begin{pmatrix} f_0(1 - x_0^m) & 0 \dots 0 & -(1/x_0 - x_0^n) & 0 \dots 0 \\ \vdots & & \vdots & \\ f_{n+m}(1 - x_{n+m}^m) & 0 \dots 0 & -(1/x_{n+m} - x_{n+m}^n) & 0 \dots 0 \end{pmatrix} .$$

Hence the displacement rank α of A equals $\alpha = 2$. When a factorization [14]

$$LA - AR = GB, \qquad G \in \mathbb{C}^{(n+m+1)\times\alpha}, \qquad B \in \mathbb{C}^{\alpha\times(n+m+1)},$$

is known, then an LU factorization of the Cauchy-like matrix $\hat{A} = A(Q_{1,m}^H \oplus Q_{1,n+1}^H)$ (the superscript ^{H} denotes complex conjugation and transposition) where the columns of the matrices $Q_{1,m}$ and $Q_{1,n+1}$ contain the eigenvectors of R^T, for which explicit formulas are known, can be obtained from [14] with order of complexity $O(2(n+m+1)^2)$.

2 Multivariate Rational Interpolation

Although the situation between one and more variables is substantially different, there is no loss in generality by describing the bivariate case instead of the general higher-dimensional case. Let the bivariate function $f(x, y)$ be given in the set of points $\{(x_k, y_k) \mid 0 \leq k \leq n+m\}$ and let us assume that none of the points (x_k, y_k) coincide. Let N and D be two finite subsets of $\mathbb{N}^2$ with which we associate the bivariate polynomials

$$p(x, y) = \sum_{(i,j)\in N} a_{ij} x^i y^j, \qquad \#N = n+1, \qquad N \text{ from "numerator"},$$

$$q(x, y) = \sum_{(i,j)\in D} b_{ij} x^i y^j, \qquad \#D = m+1, \qquad D \text{ from "denominator"} .$$

The multivariate rational interpolation problem consists in finding polynomials $p(x, y)$ and $q(x, y)$ with $p(x, y)/q(x, y)$ irreducible such that

$$f(x_k, y_k) = \frac{p}{q}(x_k, y_k), \qquad k = 0, \dots, n+m .$$

In applications where adaptive sampling is used and data points are placed at optimally located positions, it is an exception rather than the rule that some data points have the same x- or y-coordinates. Hence techniques available for a grid-like set of data points, such as in $[21, 5, 10, 22, 19, 4]$ cannot be used. In the sequel we shall deal with the more general and less-studied multivariate situation where the dataset is not necessarily grid-structured. We do however require that the sets N and D satisfy the inclusion property, which is not a serious restriction. The problem of interpolating the data by $p(x, y)/q(x, y)$ is reformulated as

$$f(x_k, y_k) \left(\sum_{(i,j)\in D} b_{ij} x_k^i y_k^j \right) - \left(\sum_{(i,j)\in N} a_{ij} x_k^i y_k^j \right) = 0, \qquad k = 0, \dots, n+m . \tag{3}$$

The set of polynomial tuples (p, q) satisfying (3) is denoted by $[N/D]_{n+m}$.

3 Fast Block Cauchy-Vandermonde Solver

Let us introduce the notations

$$\begin{aligned} I^{(N)} &= \max\{i \mid (i,j) \in N\}, \\ J^{(N)} &= \max\{j \mid (i,j) \in N\}, \\ I^{(D)} &= \max\{i \mid (i,j) \in D\}, \\ J^{(D)} &= \max\{j \mid (i,j) \in D\} \ . \end{aligned}$$

Let $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)}) = J^{(D)}$ and let us introduce the shorthand notations $\nu = I^{(N)}$ and $\delta = I^{(D)}$. Since both N and D satisfy the inclusion property, we can decompose the sets as follows:

$$N = N^{(0)} \cup \cdots \cup N^{(\nu)},$$
$$N^{(i)} = \{(i,j) \mid 0 \le j \le M_i^{(N)}\}, \qquad M_i^{(N)} = \max\{j \mid (i,j) \in N\},$$

$$D = D^{(0)} \cup \cdots \cup D^{(\delta)},$$
$$D^{(i)} = \{(i,j) \mid 0 \le j \le M_i^{(D)}\}, \qquad M_i^{(D)} = \max\{j \mid (i,j) \in D\} \ .$$

If $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)}) = J^{(N)}$ we proceed analogously. If $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ is attained in the i-direction instead of in the j-direction, then the sets N and D are decomposed horizontally instead of vertically. We point out to the reader at this point that the sequel does not apply if both the sets N and D are not decomposed in the same way, either both horizontally or both vertically.

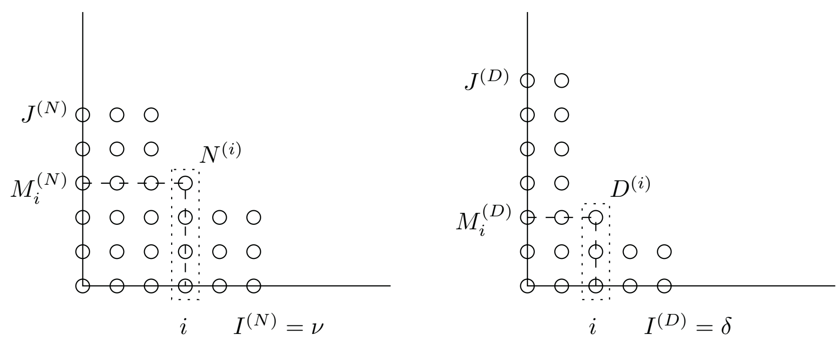

Fig. 1. Breaking up N and D

Using these notations, we arrange the unknown coefficients a_{ij} and b_{ij} as

$$\begin{aligned} \mathcal{B}^T &= \left(b_{00}, \ldots, b_{0,M_0^{(D)}} \mid b_{10}, \ldots, b_{1,M_1^{(D)}} \mid \ldots \mid b_{\delta 0}, \ldots, b_{\delta,M_\delta^{(D)}}\right), \\ \mathcal{A}^T &= \left(a_{00}, \ldots, a_{0,M_0^{(N)}} \mid a_{10}, \ldots, a_{1,M_1^{(N)}} \mid \ldots \mid a_{\nu 0}, \ldots, b_{\nu,M_\nu^{(N)}}\right) \ . \end{aligned}$$

Introducing the matrices $C_i^{(D)}$ of size $(n+m+1)\times(M_i^{(D)}+1)$ and the matrices $C_i^{(N)}$ of dimension $(n+m+1)\times(M_i^{(N)}+1)$, respectively given by

$$C_i^{(D)} = \left(f_k x_k^i \; f_k x_k^i y_k \; \ldots \; f_k x_k^i y_k^{M_i^{(D)}}\right)_{k=0,\ldots,n+m},$$
$$C_i^{(N)} = \left(-x_k^i \; -x_k^i y_k \; \ldots \; -x_k^i y_k^{M_i^{(N)}}\right)_{k=0,\ldots,n+m},$$

the system of interpolation conditions (3) looks like

$$\left(C_0^{(D)} \ldots C_\delta^{(D)} \; C_0^{(N)} \ldots C_\nu^{(N)}\right)\begin{pmatrix}\mathcal{B}\\ \mathcal{A}\end{pmatrix} = 0 \; .$$

Let all $x_i y_j \neq 0$. Again, without loss of generality, we solve this system with b_{00} normalized to 1. We denote by A the coefficient matrix of the square inhomogeneous linear system, which results from removing the first unknown from $\mathcal{B}$ and the first column from $C_0^{(D)}$. In order to generalize the fast Cauchy-Vandermonde solver, we choose a $v \neq 1$ if any of the $|y_k|$ is equal to one in case $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ is either $J^{(D)}$ or $J^{(N)}$, or any of the $|x_k|$ is equal to one in case $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ is either $I^{(D)}$ or $I^{(N)}$, and introduce

$$\tilde{Z}_k^{(v)} = \begin{pmatrix} 0 & \ldots & & 0 & 1 \\ v & 0 & \ldots & & 0 \\ 0 & v & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & v & 0 \end{pmatrix}_{k\times k} .$$

With

$$\tilde{L} = \mathrm{diag}(v/y_i)_{i=0,\ldots,n+m}, \qquad \tilde{R} = \tilde{Z}^{(v)\,T}_{M_0^{(D)}} \oplus \left(\bigoplus_{i=1}^{\delta} \tilde{Z}^{(v)\,T}_{M_i^{(D)}+1}\right) \oplus \left(\bigoplus_{i=0}^{\nu} \tilde{Z}^{(v)\,T}_{M_i^{(N)}+1}\right),$$

it is easy to see that the resulting $(n+m+1)\times(n+m+1)$ matrix $\tilde{L}A - A\tilde{R}$ can be factored as

$$\tilde{L}A - A\tilde{R} = \left(G_1 \; G_2\right) B \tag{4}$$

where the $(n+m+1)\times(\delta+1)$ and $(n+m+1)\times(\nu+1)$ submatrices G_1 and G_2 are given by

$$G_1 = f_k\left(v - y_k^{M_0^{(D)}} \;\; x_k(v/y_k - y_k^{M_1^{(D)}}) \ldots x_k^\delta(v/y_k - y_k^{M_\delta^{(D)}})\right)_{k=0,\ldots,n+m},$$
$$G_2 = \left(-x_k^0(v/y_k - y_k^{M_0^{(N)}}) \ldots -x_k^\nu(v/y_k - y_k^{M_\nu^{(N)}})\right)_{k=0,\ldots,n+m},$$

and the matrix B consists of zeroes with the exception of the following entries which equal one:

$$\begin{aligned}
\ell = 0 :& \quad \text{column number 1, row number 1,} \\
\ell = 1,\ldots,\delta :& \quad \text{column number } \sum_{i=1}^{\ell} \left(M_{i-1}^{(D)} + 1 \right), \\
& \quad \text{row number } \ell + 1, \\
\ell = 0 :& \quad \text{column number } m+1, \text{ row number } \delta + 2, \\
\ell = 1,\ldots,\nu :& \quad \text{column number } (m+1) + \sum_{i=1}^{\ell} \left(M_{i-1}^{(N)} + 1 \right), \\
& \quad \text{row number } (\delta+1) + (\ell+1) \ .
\end{aligned}$$

When $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ is either $I^{(N)}$ or $I^{(D)}$ and N and D are being decomposed horizontally, then $\tilde{L}$ is replaced by $\tilde{L} = \operatorname{diag}(v/x_i)_{i=0,\ldots,n+m}$. From the factorization (4) for $\tilde{L}A - A\tilde{R}$, and from the factorizations

$$\tilde{Z}_k^{(v)} = v\, Q_{1/v,k}^H D_{1/v,k} Q_{1/v,k} = v\, Q_{1/v,k}^H \operatorname{diag}\left(\lambda_{1,k}^{(1/v)}, \ldots, \lambda_{k,k}^{(1/v)} \right) Q_{1/v,k}$$

where the eigenvalues $\lambda_{i,k}^{(1/v)}$ are the k complex zeroes of $vz^k = 1$ and the columns of the unitary matrix $Q_{1/v,k}$ are the eigenvectors of $Z_k^{(1/v)}$, we obtain with

$$\begin{aligned}
F^H &= Q^H_{1/v, M_0^{(D)}} \oplus \left(\bigoplus_{i=1}^{\delta} Q^H_{1/v, M_i^{(D)}+1} \right) \oplus \left(\bigoplus_{i=0}^{\nu} Q^H_{1/v, M_i^{(N)}+1} \right), \\
D^H &= D^H_{1/v, M_0^{(D)}} \oplus \left(\bigoplus_{i=1}^{\delta} D^H_{1/v, M_i^{(D)}+1} \right) \oplus \left(\bigoplus_{i=0}^{\nu} D^H_{1/v, M_i^{(N)}+1} \right),
\end{aligned}$$

the factorization (the superscript ^{H} denotes transposition and complex conjugation)

$$\begin{aligned}
\tilde{L}(AF^H) - (AF^H)vD^H &= \tilde{L}(AF^H) - A\tilde{R}F^H \\
&= (\tilde{L}A - A\tilde{R})F^H \\
&= G(BF^H), \qquad G = \begin{pmatrix} G_1 & G_2 \end{pmatrix} \ . \qquad (5)
\end{aligned}$$

Since the matrix AF^H is a Cauchy-like matrix, the technique proposed in [14] can be applied. It incorporates partial pivoting while its complexity of $O((\delta + \nu + 2)(n+m+1)^2)$ is noticeably smaller than that of the classical Gaussian elimination. The latter is achieved because the technique exploits the structure of the coefficient matrix AF^H by constructing the LU factorization of AF^H from the knowledge of the matrix factors G and B in the factorization (5).

4 Complexity, Stability and Reliability

The procedure to compute the LU factorization of AF^H directly from the matrix factors G and B is detailed in [14]. Roughly speaking all entries in the LU

factors can be computed from the scalar products of the rows in G and the columns in B, and the differences of the entries in the left and right displacement operators $\tilde{L}$ and vD^H. Having the LU decomposition of AF^H at our disposal, an approximate inverse W of A can be computed (remember that $FF^H = I$) and the following interval arithmetic verification step can easily be performed. We again for simplicity assume that the system of interpolation conditions (3) can be solved with the choice $b_{00} = 1$. We denote the coefficient matrix resulting from the choice $b_{00} = 1$ by A, the righthand side of the square inhomogeneous linear system by c and the computed floating-point solution of $(AF^H)Fx = c$ by means of the fast technique described in [14] by $F\tilde{x}$. The fixpoint of the iteration function

$$f(e) = W(c - A\tilde{x}) + (I - WA)e$$

is the defect vector $e = \hat{x} - \tilde{x}$ where $\hat{x}$ is the exact solution of $Ax = c$ [17]. If $\mathcal{F}(E)$ denotes its interval extension and if for some interval E,

$$\mathcal{F}(E) \subset \breve{E}$$

where $\breve{E}$ denotes the interior of the interval E, then the linear system $Ax = c$ has one and only one solution in the interval $\tilde{x} + \breve{E}$.

For classical Gaussian elimination with partial pivoting performed on the full matrix A instead of on the factors G and B of AF^H, the error in $\tilde{x}$, say the width of $\breve{E}$, is typically of the order of the product of the condition number of A and the machine epsilon $\frac{1}{2}\beta^{-t+1}$ where β and t respectively denote the radix and precision of the floating-point system in use. In Table 1 we illustrate that the fast Gaussian elimination with partial pivoting performed on the factors G and B enjoys the same property, under the condition that (6) is not too small. This is in fact an optimal result for a fast linear system solver. In Table 1 the value diam(E) with $E = (E_1, \ldots, E_{n+m+1})$ is defined by

$$\mathrm{diam}(E) = \sqrt{\sum_{i=1}^{n+m+1} \mathrm{diam}\,(E_i)^2}$$

Let us denote the matrix elements in the factors G and B of (5) by $G = (\gamma_{ij})$ and $B = (\beta_{ij})$. According to [1], instabilities can occur if the size of the matrix elements $\left|\sum_{k=1}^{\delta+\nu+2} \gamma_{ik}\beta_{kj}\right|$ is small compared to that of the elements $\sum_{k=1}^{\delta+\nu+2} |\gamma_{ik}| \cdot |\beta_{kj}|$. Therefore, in the Tables 3 and 4, the value

$$\min_{i,j=1,\ldots,n+m+1} \frac{\left|\sum_{k=1}^{\delta+\nu+2} \gamma_{ik}\beta_{kj}\right|}{\sum_{k=1}^{\delta+\nu+2} |\gamma_{ik}| \cdot |\beta_{kj}|} \qquad (6)$$

is tabulated together with the evaluations of each scattered rational interpolant, the norms of the residue r and normalized residue r_{norm}, and the ℓ_2 condition number $\kappa_2(A)$ of the square matrix A.

Table 1. Conditioning and stability (IEEE standard double precision)

k	dim(A)	$\kappa_2(A)$	diam(E)
1	6	1.4e+02	2.3e−13
5	24	3.8e+03	9.6e−12
9	58	1.9e+06	7.2e−09
13	105	1.2e+09	3.5e−06

Table 2. Exact values of the Beta function

$x\backslash y$	-0.75	-0.25	+0.25	+0.75
-0.75	+9.88839827894	+0.00000000000	+4.94419913947	+0.00000000000
-0.25	+0.00000000000	−6.77770467835	+0.00000000000	−3.38885233918
+0.25	+4.94419913947	+0.00000000000	+7.41629870921	+4.44288293816
+0.75	+0.00000000000	−3.38885233918	+4.44288293816	+1.69442616959

Table 3. Scattered interpolant $[N_{11}/D]_{I_{11}}$

k	(6)	$\|r\|_2$	$\|r_{\text{norm}}\|_2$	$\kappa_2(V)$
11	1.0e+00	2.8e-14	2.7e-15	6.2e+08
$x\backslash y$	-0.75	-0.25	+0.25	+0.75
-0.75	+9.88685119987	+0.00224594375	+4.94385076491	+0.00009350063
-0.25	−0.00098402596	−6.77769745504	+0.00001290232	−3.38885282711
+0.25	+4.94390538464	−0.00000679165	+7.41629926989	+4.44288258156
+0.75	+0.00030912310	−3.38885313920	+4.44288082939	+1.69442607545

Table 4. Scattered interpolant $[N_{15}/D]_{I_{15}}$

k	(6)	$\|r\|_2$	$\|r_{\text{norm}}\|_2$	$\kappa_2(V)$
15	1.0e+00	2.3e-13	1.6e-14	3.2e+11
$x\backslash y$	-0.75	-0.25	+0.25	+0.75
-0.75	+9.88838464368	+0.00000158653	+4.94419901680	−0.00000021220
-0.25	+0.00000233463	−6.77770469003	−0.00000000786	−3.38885234732
+0.25	+4.94419930347	+0.00000000528	+7.41629870926	+4.44288293815
+0.75	−0.00000220603	−3.38885234095	+4.44288293796	+1.69442616960

As an illustration of the technique, we apply the structured Cauchy-Vandermonde solver to the computation of some bivariate rational interpolants from scattered data obtained from the Beta-function

$$B(x,y) = \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x+y)}$$

where Γ denotes the Gamma function. The Beta function is an interesting example because of its meromorphy. By means of the recurrence formulas

$$\Gamma(x+1) = x\,\Gamma(x), \qquad \Gamma(y+1) = y\,\Gamma(y),$$

for the Gamma function, we can write

$$B(x,y) = \frac{1 + (x-1)(y-1)f(x-1,y-1)}{xy} \ . \tag{7}$$

If we approximate the function $f(x-1, y-1)$ by a rational interpolant $[N/D]_I(x,y)$ and plug this approximant into (7), we obtain a rational approximant for $B(x,y)$. Because of the location of the poles of $B(x,y)$ at $x = -k$ and $y = -k$ for $k = 1, 2, \ldots$ and its zeroes at $x+y = -\ell$ for $\ell = 0, 1, 2, \ldots$, we choose

$$\begin{aligned} D &= \{(0,0),(1,0),(0,1),(1,1)\}, \\ N_k &= \{(i,j) \mid 0 \le i+j \le k\}, \qquad k = 1,2,\ldots, \\ \#I_k &= (k+1)(k+2)/2 + 3 \ . \end{aligned}$$

With this choice of index sets, $\max(I^{(N_k)}, J^{(N_k)}, I^{(D)}, J^{(D)}) = I^{(N_k)} = J^{(N_k)}$ and $\delta = 1, m+1 = 4, \nu = k, n+1 = (k+1)(k+2)/2$. For the interpolation points indexed by I_k we choose randomly generated tuples in the domain $[-1,1]\times[-1,1]$. The displacement rank of AF^H equals $\delta+\nu+2 = k+3$. Since $n \approx \nu^2/2 \approx k^2/2$, the technique described in Sect. 3 significantly reduces the complexity when k is larger.

All rational interpolants are evaluated in the 16 points

$$\{-0.75, -0.25, 0.25, 0.75\} \times \{-0.75, -0.25, 0.25, 0.75\} \ .$$

The exact value of the Beta function in these 16 points can be found in Table 2.

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