On Multivariate Newton Interpolation at Discrete Leja Points *

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Abstract

The basic LU factorization with row pivoting, applied to a rectangular Vandermonde-like matrix of an admissible mesh on a multidimensional compact set, extracts from the mesh the so-called Discrete Leja Points, and provides at the same time a Newton-like interpolation formula. Working on the mesh, we obtain also a good approximate estimate of the interpolation error.

1 Introduction.

In the last two years, starting from the seminal paper of Calvi and Levenberg [8], it has been recognized that the so-called "admissible meshes" play a central role in the construction of multivariate polynomial approximation processes on compact sets. This concept is essentially a matter of polynomial inequalities.

Indeed, we recall that an *admissible mesh* is a sequence of finite discrete subsets $\mathcal{A}_n$ of a compact set $K \subset \mathbb{R}^d$ (or $K \subset \mathbb{C}^d$), such that the polynomial inequality

$$\|p\|_K \leq C\|p\|_{\mathcal{A}_n} \ , \ \ \forall p \in \mathbb{P}_n^d(K) \tag{1}$$

holds for some constant $C > 0$, with $\mathrm{card}(\mathcal{A}_n)$ that grows at most polynomially in n. Here and below, $\|f\|_X = \sup_{x\in X} |f(x)|$ for f bounded on X, and $\mathbb{P}_n^d(K)$ denotes the space of d-variate polynomials of total degree at most n, restricted to K. Among their properties, it is worth recalling that admissible meshes are preserved by affine mapping, and can be extended by finite union and product.

These sets and inequalities are known also under different names in various contexts: (L^∞) discrete norming sets, Marcinkiewicz-Zygmund inequalities (especially for the sphere), and recently "stability inequalities" in more general functional settings [14].

In [8, Thm.1] it was shown that the uniform error of the n-degree *discrete least squares* polynomial approximation to a given continuous function at an

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admissible mesh is essentially within a factor $C\sqrt{\mathrm{card}(\mathcal{A}_n)}$ from the best polynomial approximation. On the other hand, *Fekete Points* (points that maximize the absolute value of the Vandermonde determinant) extracted from an admissible mesh have a Lebesgue constant

$$\Lambda_n \leq CN \ , \quad N := \dim(\mathbb{P}_n^d) \tag{2}$$

that is within a factor C from the theoretical bound for the continuous Fekete Points. Moreover, they distribute asymptotically as the continuous Fekete Points, namely the corresponding discrete measure converges weak-$*$ to the pluripotential theoretic equilibrium measure of the compact set (cf. [4]).

In principle, following [8, Thm.5], it is always possible to construct an admissible mesh on a *Markov compact*, i.e., a compact set which satisfies a Markov polynomial inequality, $\|\nabla p\|_K \leq Mn^r \|p\|_K$ for every $p \in \mathbb{P}_n^d(K)$, where $\|\nabla p\|_K = \max_{x\in K} \|\nabla p(x)\|_2$. This can be done essentially by a uniform discretization of the compact set (or even only of its boundary in the complex case) with $\mathcal{O}(n^{-r})$ spacing, but the resulting mesh has then $\mathcal{O}(n^{rd})$ cardinality for real compacts and, in general, $\mathcal{O}(n^{2rd})$ for complex compacts. Since $r = 2$ for many compacts, for example real convex compacts, the computational use of such admissible meshes becomes difficult or even impossible for $d = 2, 3$ already at moderate degrees.

On the other hand, it has been recently shown that *optimal admissible meshes*, i.e., admissible meshes with $\mathcal{O}(n^d)$ cardinality, can be constructed for important classes of compact sets, such as convex polytopes and star-like domains with smooth boundary (cf. [7, 10]). Moreover, admissible meshes whose cardinality is within a logarithmic factor from the optimal one, termed near optimal admissible meshes, exist on compact sets that are obtained from the above classes by analytic transformations (cf. [10, 12]).

An alternative way of producing good low cardinality meshes for polynomial approximation, is to look for the so-called *weakly admissible meshes*, which satisfy (1) with a non constant $C = C_n$ which increases however at most polynomially in n, cf. [8]. For example, weakly admissible meshes with $C_n = \mathcal{O}(\log^2 n)$ have been constructed on several standard 2-dimensional compact sets, such as triangles, quadrangles and disks (cf. [6] and references therein).

Even when low cardinality admissible meshes are at hand, extracting good interpolation points from them is a large-scale computational problem.

Indeed, consider the so-called Fekete points. These are defined as follows. Suppose that $\boldsymbol{z} = (z_i)_{1\leq i\leq N}$ is an array of points restricted to lie in a compact subset $\widetilde{K} \subset K$ and that $\boldsymbol{p} = (p_j)_{1\leq i\leq N}$ is an array of basis polynomials for $\mathbb{P}_n^d$ (both ordered in some manner). We may form the Vandermonde matrix

$$V(\boldsymbol{z};\boldsymbol{p}) = V(z_1,\ldots,z_N;p_1,\ldots,p_N) = [p_j(z_i)] \in \mathbb{C}^{N\times N}.$$

The Fekete points of K of degree n, associated to $\widetilde{K}$, are those which maximize $\det(V(\boldsymbol{z};\boldsymbol{p}))$ over $\boldsymbol{z} \in \widetilde{K}^N$. For $\widetilde{K} = K$ these *continuous* Fekete points are well-known to be good interpolation points for any compact K. However, computing them is a difficult optimization problem.

Closely related to the Fekete points are the so-called Leja points; the main difference being that the Leja points are a sequence while the Fekete points in general are completely different for each order. Specifically, the Leja points associated to $\widetilde{K}$ are defined as follows. The first point ξ_1 is defined as

$$\xi_1 = \arg\max_{x\in\widetilde{K}} |p_1(x)|.$$

Then, supposing that $\xi_1, \xi_2, \cdots, \xi_{k-1}$ have already been defined, the next point is defined to be

$$\xi_k = \arg\max_{x\in\widetilde{K}} \det|V(\xi_1, \ldots, \xi_{k-1}, x; p_1, \ldots, p_k)|.$$

In case of non-uniqueness it can be chosen arbitrarily among the various max points.

A less computationally expensive way of obtaining good points is to use $\widetilde{K} = \mathcal{A}_n$, an admissible mesh, with n sufficiently large to serve as a reasonable discrete model of K resulting in *discrete* Fekete or Leja points. Specifically, we form the rectangular Vandermonde-like matrix associated to $\mathcal{A}_n$

$$V(\boldsymbol{a}; \boldsymbol{p}) = V(a_1, \ldots, a_M; p_1, \ldots, p_N) = [p_j(a_i)] \in \mathbb{C}^{M\times N} \tag{3}$$

where $\boldsymbol{a} = (a_i)$ is the array of the points of $\mathcal{A}_n$, and $\boldsymbol{p} = (p_j)$ is again the array of basis polynomials for $\mathbb{P}_n^d$ (both ordered in some manner). For convenience, we shall consider $\boldsymbol{p}$ as a column vector $\boldsymbol{p} = (p_1, \ldots, p_N)^t$. Since the rows of the rectangular Vandermonde matrix $V(\boldsymbol{a}; \boldsymbol{p})$ correspond to the mesh points and the columns to the basis elements, computing the Fekete Points of an admissible mesh amounts to selecting N rows of $V(\boldsymbol{a}; \boldsymbol{p})$ such that the volume generated by these rows, i.e., the absolute value of the determinant of the resulting $N \times N$ submatrix, is maximum.

This problem is known to be NP-hard, so heuristic or stochastic algorithms are mandatory; cf. [9] for the notion of volume generated by a set of vectors (which generalizes the geometric concept related to parallelograms and parallelepipeds), and an analysis of the problem from a computational complexity point of view.

Almost surprisingly, good approximate solutions, called *Discrete Extremal Sets*, can be given by basic procedures of numerical linear algebra. The first, which gives the *Approximate Fekete Points*, corresponds to a greedy maximization of submatrix volumes, and can be implemented by the *QR factorization with column pivoting* (Businger and Golub 1965) of the transposed Vandermonde matrix. This factorization is what is used by Matlab for the solution of underdetermined systems by the "backslash" operator.

The second, which gives the *Discrete Leja Points*, corresponds to a greedy maximization of nested square submatrix determinants, can be implemented by the standard *LU factorization with row pivoting.* See [4, 5, 17] and the references therein for a complete discussion of these two approaches.

In this paper we show that the computational process that produces the Discrete Leja Points also naturally provides a multivariate version of Newton interpolation, and a good numerical estimate of the interpolation error.

2 Multivariate Newton-like Interpolation.

The computation of Discrete Leja Points is based on the following algorithm, that performs a greedy maximization of subdeterminants of the Vandermonde matrix at an admissible mesh. We use the notation $V_0([i_1,\dots,i_k],[j_1,\dots,j_k])$ to indicate the square submatrix of V_0 corresponding to the row indices $i_1,\dots,i_k$ and the column indices $j_1,\dots,j_k$.

greedy algorithm (Discrete Leja Points):
- $V_0 = V(\boldsymbol{a};\boldsymbol{p})$; $\boldsymbol{i} = [\,]$;
- `for` $k = 1 : N$
  "select i_k to maximize $|\det V_0([\boldsymbol{i}, i_k],[1,\dots,k])|$"; $\boldsymbol{i} = [\boldsymbol{i}, i_k]$;
  `end`
- $\boldsymbol{\xi} = \boldsymbol{a}(i_1,\dots,i_N)$

Observe that the selected points depend not only on the basis (as is also the case with the Approximate Fekete Points), but also on its ordering. This does not happen with the continuous Fekete Points, which are independent of the polynomial basis. In the univariate case with the standard monomial basis, it is not difficult to see that the selected points are indeed the Leja points extracted from the mesh, i.e., given $\xi_1 \in \mathcal{A}_n$, the point $z = \xi_k \in \mathcal{A}_n$ is chosen in such a way that $\prod_{j=1}^{k-1} |z - \xi_j|$ is a maximum, $k = 2, 3, \dots, N = n + 1$ (cf. [1, 15] and references therein).

The greedy algorithm above can be immediately implemented by the LU factorization with standard row pivoting, as is sketched in the following Matlab-like script:

algorithm DLP (Discrete Leja Points):
- $V_0 = V(\boldsymbol{a};\boldsymbol{p})$; $\boldsymbol{i} = (1,\dots,M)^t$;
- $[P_0, L_0, U_0] = \mathtt{LU}(V_0)$; $\boldsymbol{i} = P_0\,\boldsymbol{i}$;
- $\boldsymbol{\xi} = \boldsymbol{a}(i_1,\dots,i_N)$

This works since the effect of Gaussian elimination with row pivoting is exactly that of iteratively seeking the maximum, keeping invariant the absolute value of the relevant subdeterminants (see [5] for a full discussion of the computational process). Observe that $P_0V_0 = L_0U_0$, where P_0 is an $M \times M$ permutation matrix, L_0 is $M \times N$ lower "triangular" with ones on the diagonal, and U_0 is $N \times N$ upper triangular.

An important feature is that Discrete Leja Points form a *sequence*, i.e., the first $m_1 = \dim(\boldsymbol{q}_1)$ computed for an ordered basis $\{\boldsymbol{q}_1, \boldsymbol{q}_2\}$ are exactly the Discrete Leja Points for $\boldsymbol{q}_1$. Hence, if the basis $\boldsymbol{p}$ is such that

$$\mathrm{span}(p_1,\dots,p_{N_\nu}) = \mathbb{P}_\nu^d\ ,\quad N_\nu := \dim(\mathbb{P}_\nu^d)\ ,\quad 0 \le \nu \le n \tag{4}$$

then the first N_ν Discrete Leja Points are a unisolvent set for interpolation in $\mathbb{P}_\nu^d$ for $0 \le \nu \le n$. Moreover, it has been proved in [5, Thm.6.2] that, under assumption (4), Discrete Leja Points have the same asymptotic behavior of continuous Fekete Points (and of Approximate Fekete Points, cf. [4]), namely the corresponding discrete measures converge weak-$*$ to the pluripotential theoretic equilibrium measure of the compact set.

We show now that the same computational process that gives the Discrete Leja Points also naturally provides a *Newton-like interpolation formula*. The connection between the LU factorization of Vandermonde matrices and Newton-like interpolation was originally recognized by de Boor (see pages 865–866 of [3] and also page 888 of [2] for the univariate case), and recently reconsidered in a more general functional framework by Schaback et al. [11, 16].

Consider the square Vandermonde matrix in the basis $\boldsymbol{p}$ at the Discrete Leja Points $\boldsymbol{\xi}$, where we assume (4). We have

$$V = V(\boldsymbol{\xi};\boldsymbol{p}) = (P_0 V_0)_{1\leq i,j\leq N} = LU \tag{5}$$

where $L = (L_0)_{1\leq i,j\leq N}$ and $U = U_0$. The polynomial interpolating a function f at $\boldsymbol{\xi}$, with the notation $\boldsymbol{f} = f(\boldsymbol{\xi}) \in \mathbb{C}^N$, can be written as

$$\mathcal{L}_n f(x) = \boldsymbol{c}^t \boldsymbol{p}(x) = (V^{-1}\boldsymbol{f})^t \boldsymbol{p}(x) = (U^{-1}L^{-1}\boldsymbol{f})^t \boldsymbol{p}(x) = \boldsymbol{d}^t \boldsymbol{\phi}(x) \tag{6}$$

where

$$\boldsymbol{d}^t = (L^{-1}\boldsymbol{f})^t \ , \ \ \boldsymbol{\phi}(x) = U^{-t}\boldsymbol{p}(x) \ . \tag{7}$$

Since U^{-t} is lower triangular, by (4) the basis $\boldsymbol{\phi}$ is such that $\mathrm{span}(\phi_1,\dots,\phi_{N_\nu}) = \mathbb{P}^d_\nu$, $0\leq \nu\leq n$, which shows that (6) is a type of Newton interpolation formula. Moreover, if we consider the Vandermonde matrix at the Discrete Leja Points in this basis, we get

$$V(\boldsymbol{\xi};\boldsymbol{\phi}) = V(\boldsymbol{\xi};\boldsymbol{p})U^{-1} = LUU^{-1} = L \ ,$$

a lower triangular matrix. Hence $\phi_j(\xi_j) = 1$ and ϕ_j vanishes at all the interpolation points from the first to the $(j-1)$-th for $j > 1$. In the univariate case, since $\phi_j \in \mathbb{P}^1_{j-1}$ by (4) and (7), this means that $\phi_1 \equiv 1$, $\phi_j(x) = \alpha_j(x - x_1)\dots(x - x_{j-1})$ for $2 \leq j \leq N = n+1$ with $\alpha_j = ((x_j - x_1)\dots(x_j - x_{j-1}))^{-1}$. This is the classical Newton basis up to multiplicative constants, and thus the $\{d_j\}$ are the classical univariate divided differences up to the multiplicative constants $\{1/\alpha_j\}$.

It is therefore reasonable, following de Boor, to say in general that (6) is a multivariate Newton-like interpolation formula, that $\boldsymbol{\phi}$ is a multivariate "Newton basis", and that $\boldsymbol{d}$ is a kind of multivariate "divided difference". Note that this would work even if we started from *any* unisolvent interpolation array $\boldsymbol{\eta}$, computing directly the LU factorization $PV = LU$. In this case $\boldsymbol{\xi} = P\boldsymbol{\eta}$ would be a *Leja reordering* of the interpolation points, that in the univariate case is known to stabilize the Newton interpolation formula, cf. [13].

2.1 Error estimate and numerical results.

Let us write the multivariate Newton interpolation formula (6) as

$$\mathcal{L}_n f(x) = \boldsymbol{d}^t \boldsymbol{\phi}(x) = \delta_0(x) + \dots + \delta_n(x) \tag{8}$$

where the polynomials $\delta_\nu \in \mathbb{P}^d_\nu$, $0 \leq \nu \leq n$, are defined as

$$\delta_\nu = (\boldsymbol{d})^t_{j\in\Delta_\nu}(\boldsymbol{\phi})_{j\in\Delta_\nu} \ , \ \ \Delta_\nu = \{N_{\nu-1}+1,\dots,N_\nu\} \ . \tag{9}$$

This is clearly a multivariate version of the incremental form of the Newton interpolation formula, where each new degree comes into play as a block of summands. In the case of the continuum Leja Points, if f is sufficiently regular to ensure uniform convergence of the interpolating polynomials, i.e.,

$$f(x) = \sum_{k=0}^{\infty} \delta_k(x) \ ,$$

then

$$f(x) - \mathcal{L}_{\nu-1} f(x) = \sum_{k=\nu}^{\infty} \delta_k(x)$$

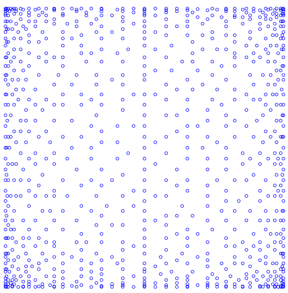
and we may obtain an estimate, or at least an indication, of the error from the norm of the first neglected term in the series, i.e.,

$$\|\mathcal{L}_{\nu-1} f - f\|_K \approx \|\delta_\nu\|_K \leq C \|\delta_\nu\|_{\mathcal{A}_n} \;, \quad \nu \leq n \;. \tag{10}$$

By analogy, we may apply (10) also in the case of the Discrete Leja Points. We caution the reader however that although, for simplicity's sake we have written δ_k, this quantity is related to points extracted from $\mathcal{A}_n$ and hence also depends on n. The idea is to choose a fixed n sufficiently large so that $\mathcal{A}_n$ is a sufficiently good model (for all practical purposes) of the underlying compact set K.

While the first approximation in (10) is quite heuristic, its bound is rigorous, being based on the fact that the error indicator δ_ν is a polynomial, and that we have at hand the admissible mesh from which we extract the Discrete Leja Points (observe that if $\mathcal{A}_n$ is an admissible mesh for degree n on K then property (1) holds for any degree $\nu \leq n$). To our knowledge, this is the first time that admissible meshes are used to numerically estimate polynomial approximation errors.

In Figures 1-2 below, we show some numerical results concerning the square $K = [-1, 1]^2$. At each degree, the points are extracted from a $(2n+1) \times (2n+1)$ Chebyshev-Lobatto grid, which is an admissible mesh with $C = 2$ as proved in [7], applying algorithm DLP to the corresponding rectangular Vandermonde matrix in the Chebyshev product basis. The interpolation errors (for two functions of different regularity) have been computed on a 100×100 uniform control grid. Though the (numerically estimated) Lebesgue constant exhibits an irregular behavior, as it is usual with Leja-like points, it is below the theoretical overestimate (2). For both test functions, (10) turns out to be a good estimate of the interpolation error, especially for higher degrees.



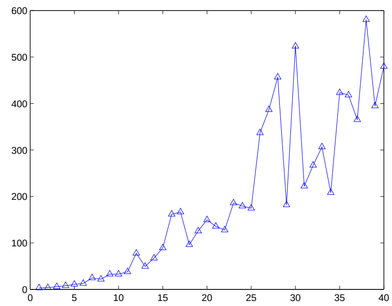


Figure 1: Left: $N = 861$ Discrete Leja Points for degree $n = 40$ on the square, extracted from an 81×81 Chebyshev-Lobatto grid; Right: Lebesgue constants of Discrete Leja Points on the square for $n = 1, \ldots, 40$.

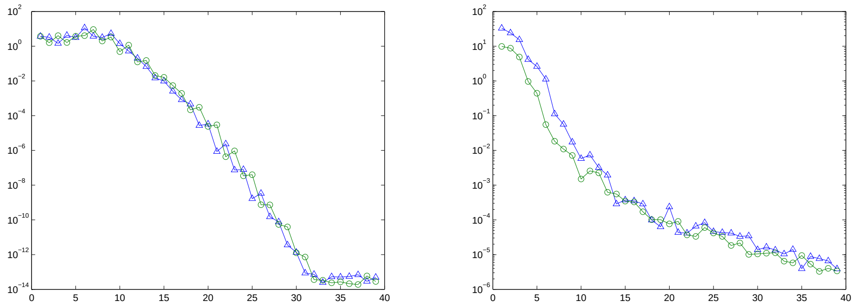


Figure 2: Uniform error (circles) and estimate (10) (triangles) of Newton interpolation at Discrete Leja Points on the square for $\nu = 2, \ldots, 40$; Left: $f(x_1, x_2) = \cos(5(x_1 + x_2))$; Right: $f(x_1, x_2) = [(x_1 - 1/3)^2 + (x_2 - 1/3)^2]^{5/2}$.

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