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## Computing Fekete and Lebesgue points: Simplex, square, disk\*

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#### ABSTRACT

We have computed point sets with maximal absolute value of the Vandermonde determinant (Fekete points) or minimal Lebesgue constant (Lebesgue points) on three basic bidimensional compact sets: the simplex, the square, and the disk. Using routines of the Matlab Optimization Toolbox, we have obtained some of the best bivariate interpolation sets known so far.

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#### 1. Introduction

An important and challenging topic of approximation theory is to provide, for a fixed degree n, good point sets  $\xi$  for polynomial interpolation over multivariate compact domains  $K \subset \mathbb{R}^d$ . Given a basis  $\{\phi_j\}$  of the finite dimensional vector space  $\mathbb{P}_n^d$  of d-variate polynomials of degree not greater than n, a first issue consists in finding  $\xi = \{\xi_1, \ldots, \xi_N\}$  that are unisolvent, i.e., the cardinality N of  $\xi$  is equal to the dimension of  $\mathbb{P}_n^d$  and  $det(V_n(\xi)) \neq 0$ , where

$$V_n(\xi) = [v_{ij}] = [\phi_j(\xi_i)], \quad 1 \le i, \ j \le N = \dim(\mathbb{P}_n^d)$$
(1)

is the Vandermonde matrix. It is well-known that if K is a bounded interval [a, b], then any set of N = n + 1 distinct points of K is unisolvent, but the problem is much more difficult for multivariate settings (cf., e.g., [1]). Moreover, as it has been clear since the discovery of the Runge phenomenon, unisolvence does not ensure that the set has good interpolation properties. From this point of view, one searches for unisolvent sets  $\xi = \{\xi_i\}$  with low Lebesgue constant

$$\Lambda_n(\xi) = \max_{x \in K} \sum_{i=1}^N |\ell_i(x)| \tag{2}$$

where

$$\ell_i(x) = \frac{V_n(\xi_1, \dots, \xi_{i-1}, x, \xi_{i+1}, \dots, \xi_N)}{V_n(\xi_1, \dots, \xi_N)}$$
(3)

is the i-th Lagrange polynomial w.r.t. the points  $\xi$ . It is not difficult to see that for any continuous function f in the compact domain K

$$||f - I_n f||_{\infty} \le (1 + \Lambda_n(\xi))||f - f_n^*||_{\infty} \tag{4}$$

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where  $I_n f$  is the polynomial that interpolates f in  $\xi$  and  $f_n^* \in \mathbb{P}_n$  is the polynomial of best approximation to f in the  $\infty$ -norm. The sets  $\xi$  with minimal  $\Lambda_n(\xi)$  are known as Lebesgue points. From (4), it stems that low Lebesgue constants  $\Lambda_n(\xi)$  provide sets whose interpolation error  $\|f - I_n f\|_{\infty}$  is expected to be as close as possible to that of the best interpolant  $\|f - f_n^*\|_{\infty}$ . In general, it is not easy to find these sets theoretically (Lebesgue points are not known even for the interval [2]). On the other hand, the so called Fekete points, i.e., those sets  $\xi$  maximizing the absolute value of the Vandermonde determinant (w.r.t. any polynomial basis), possess Lebesgue constants growing at most as the dimension N of the polynomial space  $\mathbb{P}_n$  since  $\|\ell_i\|_{\infty}=1$  by construction (but in practice can perform much better). They are analytically known only in few cases: the interval (Legendre–Gauss–Lobatto points) where  $\Lambda_n=O(\log n)$ , and the cube (tensor-product of Legendre–Gauss–Lobatto points) for tensorial interpolation where  $\Lambda_n=O(\log^d n)$ ; cf. [3,4].

Notice that, whereas the existence of Fekete points for a given compact set K is trivial, since  $\det(V_n(\xi))$  is a polynomial in  $\xi \in K^N$ , the problem is more subtle concerning Lebesgue points. Indeed, the Lebesgue constant  $\Lambda_n(\xi)$  is not continuous on the whole  $K^N$ , since the denominator of the Lagrange polynomials vanishes on a subset of  $K^N$  which is an algebraic variety. Nevertheless, if K is polynomial determining, that is polynomials vanishing there vanish everywhere (this is true for example whenever K has internal points), such is  $K^N$  and thus there are points in  $K^N$  where  $\det(V_n(\xi))$  does not vanish. The Lebesgue constant is then positive, goes to infinity at the variety, and is continuous in the rest of  $K^N$ . By a suitable redefinition on the variety, the Lebesgue constant becomes lower-semicontinuous and thus has a global minimum on the compact  $K^N$ , that is taken at Lebesgue points (which, as Fekete points, are not unique, in general).

Computing Fekete and Lebesgue points requires solving a large-scale nonlinear optimization problem. Indeed, the number of variables (that are the coordinates of the optimal points) is 2N, with  $N=\dim(\mathbb{P}_n^d)$ . In dimension d=2, for example, we deal with  $2\times 66=122$  variables already at degree n=10. In order to provide a cheap numerical approximation of Fekete points, recently *Approximate Fekete Points* and *Discrete Leja Points* have been introduced, cf. [5–7]. Though they are not optimal, the absolute values of their Vandermonde determinants are significantly high and the computation requires only basic linear algebra routines (QR and LU factorizations of Vandermonde matrices). Furthermore, they provide good interpolation sets on rather general compact domains, and can be used, as is done in the present work, as starting guess for more sophisticated optimization procedures.

The main purpose of this paper is to provide Fekete and Lebesgue points on three basic bidimensional compact sets, the simplex, the square, and the disk, by solving numerically the corresponding large-scale nonlinear optimization problems up to degree n=18. Once such points have been computed in one reference set, they can be used on any triangle, parallelogram, and ellipse, by affine mapping. The results of our computational work reach and often improve those previously known. The interpolation sets and the Matlab codes are available at the webpage [8]. The codes can be easily extended to other domains, for instance simple polygons. In the case of the simplex, due to their relevance in developing spectral and high-order methods for PDEs we have also computed interpolation sets that have an assigned distribution on the sides (Legendre–Gauss–Lobatto side nodes), which appear to be better than those provided in [9,10]. Concerning the square, besides Fekete and Lebesgue points, we have computed some new sets that generalize the Padua points [11] and improve their already good quality. Very little seems to be known about Fekete and Lebesgue points for the disk (cf., e.g., [12]), and we hope that our computational results could put some insight into this topic.

#### 2. Computational aspects

For computing almost optimal points, the Matlab Optimization Toolbox (cf. [13]) is particularly appealing since we can determine the desired point sets by methods that are considered state of the art. This numerical environment provides three built-in routines, fmincon for constrained minimization and fminsearch, fminunc for unconstrained optimization. Their usage is straightforward, one has only to provide the target function F to minimize, and a good starting guess. Each of these routines computes (approximately) the minimum of F. The optimization algorithms have default options to free the user from the burden of deciding some specific parameters as the size of the derivatives, the number of iterations, .... However, we experienced that these settings were not fully tailored to our purposes. For this reason, beyond MaxIter and MatFunEvals that determine the maximum number of iterations and of function evaluations, after several trials and numerical experiments, it has been important to put RelLineSrchBnd and DiffMaxChange equal to  $10^{-3}$ . With such modifications, the methods that were erratic or too static achieved a better numerical behavior.

In the present context, for a given set of points  $\xi \subset K$ , we will consider as target functions the numerically evaluated Lebesgue constant and the absolute value of the determinant of  $V_n(\xi)$ , where the latter is the Vandermonde matrix of degree n w.r.t. a certain polynomial basis. We point out that the sets that we obtain are not the true Fekete or Lebesgue points, but that they share with them low Lebesgue constants and high (relative to the given polynomial basis) absolute values of  $\det(V_n(\xi))$ .

In order to compute the Lebesgue constant  $\Lambda_n(\xi)$  of a particular point set  $\xi = \{\xi_i\}$ , usually one fixes a fine reference mesh  $X \subset K$  and evaluates the Lebesgue function

$$\lambda_n(x;\xi) = \sum_{i=1}^N |\ell_i(x)|, \quad x \in X.$$
 (5)

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