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Finding elliptic Fekete points sets: two numerical solution approaches

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Abstract

The objective of this work is to provide a methodology for approximating globally optimal Fekete point configurations. This problem is of interest in numerical mathematics and scientific modeling. Following a brief discussion of the analytical background, Lipschitz global optimization (LGO) is applied to determine – i.e., to numerically approximate – Fekete point configurations. Next to this optimization approach, an alternative strategy by formulating a set of differential-algebraic equations (DAEs) of index 2 will be considered. The steady states of the DAEs coincide with the optima of the function to be minimized. Illustrative numerical results – with configurations of up to 150 Fekete points – are presented, to show the viability of both approaches.

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Keywords: Elliptic Fekete points; Lipschitz global optimization; LGO program system; DAE solvers; IVP algorithms; Numerical examples

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1. Introduction

We shall consider the following classical problem: given the unit sphere (ball) B in the Euclidean real space $\mathbb{R}^3$, and a positive integer n, find the n-tuple of points (unit length vectors)

$$x(n) = \{x_i,\ i = 1,\ldots,n\}, \quad x_i = (x_{i1}, x_{i2}, x_{i3})$$

on the surface S^2 of B, which maximizes the product of distances between all possible pairs $\{x_i, x_j\}$, $1 \leqslant i < j \leqslant n$. In other words, we are interested in finding the global maximum of the function

$$f_n(x(n)) = \prod_{1 \leqslant i < j \leqslant n} \|x_i - x_j\|, \quad x_i \in S^2, \tag{1}$$

where $\|\cdot\|$ indicates the Euclidean norm. A set of vectors $x^*(n) = \{x_i^*,\ i = 1,\ldots,n\}$, where $x_i^* \in S^2$, which satisfies the relations

$$f_n^* = f_n(x^*(n)) = \max_{x(n)} f_n(x(n)), \quad x_i \in S^2,\ (i = 1,\ldots,n), \tag{2}$$

is called elliptic Fekete points of order n [2]. We shall refer to (2) as the Fekete (global optimization) problem.

Let us note first of all that – by the classical theorem of Weierstrass – the optimization problem (2) has globally optimal solution(s). Second, although – for obvious reasons of symmetry – there are infinitely many vector sets $x^*(n)$ which satisfy (2), the solution can easily be made unambiguous (as will be seen in Section 3). Consequently, we shall analyze the problem of finding $x^*(n)$, and the corresponding function value $f_n^* := f_n(x^*(n))$.

The analysis and determination of elliptic Fekete point sets have been of great theoretical interest for several decades: consult, e.g., [2,12]. Apparently, it also represents a longstanding numerical challenge: Pardalos [8] states it as an open problem. Additionally, because of the direct relation of formulation (2) to models in potential theory [13], the solution of the Fekete problem (and its possible modifications) has also important practical aspects: we shall return to this point later.

We will start with a short overview of some analytical results concerning Fekete points and related topics, followed by a description of the chosen parametrization of Fekete point sets. In Sections 4 and 5 the Lipschitzian global optimization (LGO) approach and the formulation in terms of differential-algebraic equations (DAEs) will be discussed, respectively. We also give a summary of the numerical results and the corresponding performances of both approaches in Section 6. The last section presents some concluding remarks and future perspectives.

2. A brief review of some analytical background

The following notes are largely based on the works of Tsuji [13], and Shub and Smale [12]. Let D be a bounded closed set in $\mathbb{R}^3$ which contains infinitely many points. Taking n vectors $z_1,\ldots,z_n$ from D, define (cf. (1)) $z(n) = \{z_1,\ldots,z_n\}$,

$$V_n(z(n)) := \prod_{1 \leqslant i < j \leqslant n} \|z_i - z_j\|, \tag{3}$$

and

$$V_n^* := V_n(z^*(n)) := \max_{z(n)} V_n(z(n)). \tag{4}$$

Define now the normalized value of V_n^* by

$$d_n := d_n(D) := \sqrt[\binom{n}{2}]{V_n^*} > 0, \tag{5}$$

then the following general result – due to Fekete [2] – is valid.

Theorem 1. *$d_{n+1} \leqslant d_n$; therefore $\tau(D) = \lim_{n\to\infty} d_n$ exists.*

Proof. See Tsuji [13, p. 71].

Definition 2. For a set D, the quantity $\tau(D)$ is called the *transfinite diameter* of D.

The apparent connection of Fekete's transfinite diameter with certain problems of packing – i.e., 'find a set of points in D which are located so that no two are very close together' – is discussed, e.g., by Lubotzky et al. [7]. In this context, they also refer briefly to the connection of the transfinite diameter and the so-called elliptic capacity. In problems of finding electrostatic equilibria, the resulting point configurations – modeling repellent bodies – are located on a corresponding equipotential surface. Obviously, physically stable, minimal energy configurations are of great importance also in other areas of natural sciences, most notably, in physics and chemistry. Although both the topology of the potential surface in question and the functional form (the underlying analytical description) of characterizing the 'goodness' of point configurations may vary, the result described by Theorem 1 bears direct relevance to such problems, under very general conditions.

Shub and Smale [12, p. 9] remark that the transfinite diameter of the sphere of radius $\frac{1}{2}$ equals $e^{-1/2}$. This directly leads to the estimate (recall (2))

$$d_n(S^2) = \sqrt[\binom{n}{2}]{f_n^*} \approx 2e^{-1/2} = 1.21306132\ldots, \tag{6}$$

the approximation is valid for sufficiently large n. Theorem 1 also provides a lower bound for the solution of the maximization problem in (2):

$$f_n^* \geqslant (2e^{-1/2})^{\binom{n}{2}}. \tag{7}$$

This estimate shows the rate of increase of the global optimum value, as a function of the number of Fekete points in the optimal configuration. One can also use the estimate $d_{n+1} \leqslant d_n$, which directly leads to

$$f_{n+1}^* \leqslant (f_n^*)^{(n+1)/(n-1)}. \tag{8}$$

The pair of relations (7)–(8) provides valid lower and upper bounds; (8) also bounds the rate of increase of subsequent optimal function values in the Fekete problem.

Concluding this brief review of some essential analytical background, let us note finally that Shub and Smale also refer to the apparently significant numerical difficulty of finding the globally optimal configuration $x^*(n)$, for a given – not too small – n. Difficulties arise due to several reasons: viz., the above mentioned various symmetries of the function f_n, and – more essentially – its inherent multiextremality. Obviously, $f_n(x(n))$ equals zero, whenever (at least) two points x_i coincide. Furthermore – (see (7) – its maximal value very rapidly increases as a function of n. These properties

together lead to functions f_n which tend to change in an extremely 'abrupt' manner, making any perceivable numerical solution procedure inherently tedious.

In the following two sections, first we shall introduce a suitable problem representation, and then consider a global optimization approach to solving Fekete problems (approximately), in a robust and numerically viable sense.

3. Unique parametric representation of n-tuple point configurations on S^2

It is a natural approach to represent arbitrary point configurations on the surface S^2 by spherical coordinates. Let us denote the three unit vectors in the usual Cartesian coordinate setting by e_1, e_2, and e_3. Furthermore, for $x_i \in S^2$, let β_i denote the angle between x_i and its projection onto the plane defined by e_1 and e_2; and α_i denote the angle between this projection and e_1. Then the n-tuple $x(n)$ – consisting of corresponding unit length vectors x_i, $i = 1,\ldots,n$ – is described by

$$\begin{aligned} x_{i1} &= \cos(\alpha_i)\cos(\beta_i), \\ x_{i2} &= \sin(\alpha_i)\cos(\beta_i), \quad \begin{pmatrix} 0 \leqslant \alpha_i < 2\pi \\ -\pi/2 \leqslant \beta_i \leqslant \pi/2 \end{pmatrix}, \\ x_{i3} &= \sin(\beta_i). \end{aligned} \tag{9}$$

We shall also use the equivalent parametrization, with the auxiliary variables ξ_i

$$\begin{aligned} &0 \leqslant \alpha_i < 2\pi, \\ &-1 \leqslant \xi_i \leqslant 1 \quad (-\pi/2 \leqslant \beta_i := \arcsin(\xi_i) \leqslant \pi/2). \end{aligned} \tag{10}$$

This results in replacing the calculation of x_{i3} in (9) simply by $x_{i3} = \xi_i$. The reparametrization has the advantage that if α_i and ξ_i are taken from a uniform distribution from their domains, then the corresponding points x_i have a uniform distribution on the sphere. This is especially important in the context of randomized search strategies which are used in LGO.

In order to eliminate rotational symmetries, one can select and fix three angles in spherical representation (9) of $x(n)$. We choose

$$\alpha_1 = \beta_1 = \beta_2 = 0 \quad (\text{i.e., } \alpha_1 = \xi_1 = \xi_2 = 0). \tag{11}$$

Geometrically, this means that the unit vector $e_1 = (1,0,0)$ is always a component of the optimized Fekete point configuration. Additionally, at least another (the second) vector in the Fekete set sought belongs to the $\{e_1, e_2\}$-plane. This convention effectively reduces the number of unknown parameters in $x(n)$ to $2n-3$.

4. Applying LGO approach

Since S^2 is bounded and closed, and the objective function $f_n(x(n))$ in (2) is continuously differentiable, it is also Lipschitz-continuous on $S^2 \times S^2 \times \cdots \times S^2 = (S^2)^n$. In other words, for any given n and corresponding f_n, there exists a Lipschitz-constant $L = L(n)$ such that for all possible pairs $x(n), \tilde{x}(n)$ from $(S^2)^n$ we have

$$|f_n(x(n)) - f_n(\tilde{x}(n))| \leqslant L\|x(n) - \tilde{x}(n)\|_\Sigma. \tag{12}$$

The norm $\|x(n) - \tilde{x}(n)\|_\Sigma$, defined on $(S^2)^n$, is the sum of the componentwise Euclidean norms.

As mentioned earlier, the function f_n is expected to become very 'steep' in certain neighborhoods in $(S^2)^n$, especially when n becomes large. The complicated structure of function f_n can also be simply visualized, observing that the derivative of f_n has a non-polynomially increasing number of zeros – as a function of n – indicating local minima, maxima and saddle points. Consequently, we shall consider the Fekete problem (2) as an instance from the broad category of Lipschitz global optimization problems, without further – more narrow, and algorithmically exploitable – specification. Note additionally that only simple lower and upper bound ('box') constraints are explicitly stated by the parametrization (9)–(10).

The underlying global convergence theory of Lipschitz optimization algorithms is discussed in detail by Horst and Tuy [5], and Pintér [10], with numerous references therein. The latter monograph also presents details on implementing algorithms for continuous and Lipschitz global optimization, and reviews a number of prospective applications and case studies.

The numerical results obtained on the basis of a program system called LGO – abbreviating Lipschitz Global Optimizer – are given in Section 6 and compared with the results obtained via an alternative approach which will be described in the next section. For more details on LGO, consult [11].

5. Formulation for DAE approach

As already mentioned, we have used two approaches to approximate Fekete point sets numerically. The previous section dealt briefly with a global optimization approach. Another way to approximate Fekete point sets is based upon the numerical solution of an index 2 system of differential-algebraic equations (DAEs). For more details on DAEs see Brenan et al. [1] or Hairer et al. [4]. This section starts with a derivation of the DAE formulation. We will show that the stable steady states of these DAEs coincide with the optima of the function f_n in (1). Some practical remarks concerning the numerical implementation of this approach are also highlighted.

Let us consider a set of n repellent particles on the unit sphere. The coordinates of the ith particle are denoted by x_i. Due to the dynamic behavior of the particles, these coordinates will be parametrized by a time variable, t. The movement of the particles is restricted in such a way that they will stay on the surface of the the unit sphere in $\mathbb{R}^3$; $x_i(t) \in S^2$. We define the repulsive force on particle i caused by particle j by

$$F_{ij} = \frac{x_i - x_j}{\|x_i - x_j\|^\gamma}. \tag{13}$$

Note that the choice $\gamma = 3$ can be interpreted as an electrical force affecting particles with unit charge. Furthermore, we imply an adhesion force on the particles, due to which the particles will stop moving after some time. Denoting the configuration of the particles at time t by $x(t) = \{x_1(t), \ldots, x_n(t)\}$, Lagrange mechanics states that $x(t)$ satisfies the following system of differential-algebraic equations:

$$x' = q, \tag{14}$$

$$q' = g(x, q) + G^{\mathrm{T}}(x)\lambda, \tag{15}$$

$$0 = \phi(x), \tag{16}$$

where q is the velocity vector, $G = \partial\phi/\partial x$ and $\lambda \in \mathbb{R}^n$. The function $\phi : \mathbb{R}^{3n} \to \mathbb{R}^n$ is the constraint, which states that the particles cannot leave the unit sphere:

$$\phi_i(x) = x_{i,1}^2 + x_{i,2}^2 + x_{i,3}^2 - 1.$$

The function $g : \mathbb{R}^{6n} \to \mathbb{R}^{3n}$ is given by $g = (g_i)$, $i = 1, \ldots, n$, where

$$g_i(x, q) = \sum_{j \neq i} F_{ij}(x) + A_i(q),$$

where F_{ij} is given by (13). The function A_i is the adhesion force affecting particle i and is given by the formula

$$A_i = -\kappa q_i.$$

Here, κ is set to 0.5. The term $G^{\mathrm{T}}(x)\lambda$ in (15) represents the normal force which keeps the particles on S^2.

Let us denote the final configuration by $\hat{x} \in \mathbb{R}^{3n}$. Since we know that the speed of this final configuration is 0, we can substitute $q = 0$ and $x = \hat{x}$ in (15), thus arriving at

$$0 = \sum_{j \neq i} F_{ij}(\hat{x}) + G^{\mathrm{T}}(\hat{x})\lambda$$

which is equal to

$$\sum_{i \neq j} \frac{\hat{x}_i - \hat{x}_j}{\|\hat{x}_i - \hat{x}_j\|^{\gamma}} = -2\lambda_i \hat{x}_i. \tag{17}$$

Let us now take the logarithm (which is a monotonous function) of $f_n(x(n))$ in (1) and differentiate $\log(f_n(x(n)))$ with respect to x_i. Then, by applying the method of Lagrange multipliers, we know that f_n has a (local) maximum at x, where x satisfies

$$\nabla_i \log(f_n(x)) = \sum_{i \neq j} \frac{x_i - x_j}{\|x_i - x_j\|^2} = \zeta_i x_i. \tag{18}$$

Here, ζ_i is the Lagrange multiplier. Comparison of (18) and (17) tells us that computing $\hat{x}$ for $\gamma = 2$ gives the (local) optima of the function f_n. In principle, by solving system (14)–(16), it is possible to arrive at the global maximum by varying the initial values and the adhesion parameter κ. However, numerical experiments show that for $n \leqslant 150$, even with a constant κ and a fixed strategy for choosing the initial values, one obtains values for f_n that satisfy conditions (7) and (8) and are at least as good as those obtained by the LGO implementation (available at CWI since 1995). This will be shown in Section 6.

Now we describe how the DAE system given by Eqs. (14)–(16) and $\gamma = 2$ can be solved numerically. Since (16) is a position constraint, the system is of index 3. To arrive at a more stable formulation of the problem, we stabilize the constraint (see [1, p. 153]) by replacing (14) by

$$x' = q + G^{\mathrm{T}}(p)\mu, \tag{19}$$

where $\mu \in \mathbb{R}^n$, and appending the differentiated constraint

$$0 = G(x)q. \tag{20}$$

System (19), (15), (16), (20) is now of index 2; the variables x and q are of index 1, the variables λ and μ of index 2.

We choose the initial positions $x_i(0)$ on the intersection of S^2 and the $\{e_1, e_2\}$-plane, except the first particle, which is initially in $(0,0,1)$. Choosing $q(0)=0$ yields $\mu(0)=0$ and $\phi_i'(0)=\langle 2x_i(0), q_i(0)\rangle=0$. Consequently,

$$\begin{aligned}\phi_i''(0) &= \langle 2x_i(0), q_i'(0)\rangle \\ &= \langle 2x_i(0), g_i(x(0), q(0)) + 2\lambda_i(0)x_i(0)\rangle.\end{aligned}$$

Requiring $\phi_i''(0) = 0$ gives

$$\lambda_i(0) = -\frac{\langle x_i(0), g_i(x(0), q(0))\rangle}{2\langle x_i(0), x_i(0)\rangle} = -\frac{1}{2}\langle x_i(0), g_i(p(0), q(0))\rangle.$$

The problem is now of the form

$$M\frac{\mathrm{d}y}{\mathrm{d}t} = w(y), \quad y(0) = y_0 \tag{21}$$

with

$$M = \begin{pmatrix} I_{6n} & 0 \\ 0 & 0 \end{pmatrix},$$

$$y \in \mathbb{R}^{8n}, \quad 0 \leqslant t \leqslant t_{\mathrm{end}}, \quad y = \begin{pmatrix} x \\ q \\ \lambda \\ \mu \end{pmatrix} \quad \text{and} \quad w(y) = \begin{pmatrix} q + G^{\mathrm{T}}\mu \\ g + G^{\mathrm{T}}\lambda \\ \phi \\ Gq \end{pmatrix}.$$

Here, t_{end} is chosen such that

$$\max_{i\in\{1,2,\ldots,n\}} \| q_i(t_{\mathrm{end}})\| < 10^{-14}. \tag{22}$$

Numerical experiments show that if $t_{\mathrm{end}} = 1000$, then (22) holds for $n \leqslant 150$.

Solving the problem numerically leads to a phenomenon that one might call numerical bifurcation. Assume that two particles x_i and x_j are close to each other at time t_1 with $x_{i,1}(t_1) > x_{j,1}(t_1)$. It may happen that the numerical integration method applied with finite error tolerance τ computes a new stepsize h_τ such that $x_{i,1}(t+h_\tau) > x_{j,1}(t+h_\tau)$, whereas the same method applied with error tolerance $\tilde{\tau}$ results in a stepsize $h_{\tilde{\tau}}$ for which $x_{i,1}(t+h_{\tilde{\tau}}) < x_{j,1}(t+h_{\tilde{\tau}})$. This means that for different error tolerances, the numerical integration method may compute paths of particles that differ significantly. The occurrence of this phenomenon is irrespective of the scale of the error tolerance and can happen for every value of n (although it is more probable for larger values of n). However, the quantity of interest here is (1) which is independent of the path that the particles followed to arrive at the final configuration.

To solve the DAE we use RADAU5 by Hairer and Wanner [3], which is an implementation of the 3-stage implicit Runge–Kutta method of Radau IIA type. For more information related to this code, we refer to Hairer and Wanner [4]. RADAU5 can integrate problems of form (21) up to index 3.

As an example, Fig. 1 depicts the solution obtained by RADAU5 for $n = 20$. The same solution in the $\{\alpha, \beta\}$-plane (cf. (9)) – after a rotation such that (11) is fulfilled – is shown in Fig. 2.

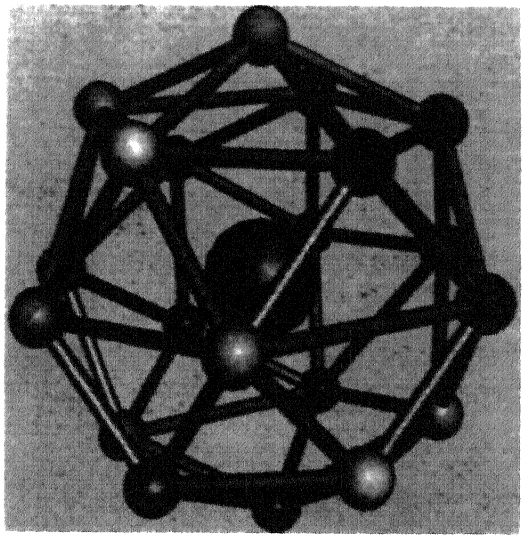

Fig. 1. Final configuration obtained with RADAU5 for $n = 20$. The large ball is centered at the origin and only added to facilitate the 3-D perception.

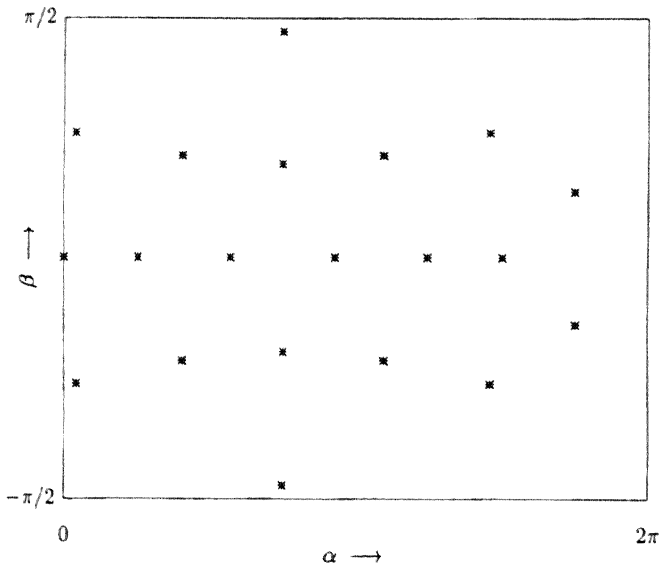

Fig. 2. Final configuration, as in Fig. 1, where the Fekete points are given in the $\{\alpha, \beta\}$-plane. A rotation has been applied such that (11) is fulfilled.

Remark 3. For $n = 20$ the code for the DAE formulation of the Fekete problem can be obtained via [6].

6. Numerical results and discussion

From the previous exposition it should be clear that the numerical determination of Fekete point sets leads to rapidly growing computational demands which can easily become prohibitive. Therefore – although 'precise' globally optimal solutions have been sought – the results reported in this section should be considered as numerical approximations obtained with a reasonable computational effort, for the purposes of this exploratory study. The individual solution times on a SGI workstation, Indy with 4194 Mhz R10010SC processors, start with a few seconds for both approaches up to 15 points and lead to CPU times between 2 and 17 h for n in the range of 100–150 Fekete points. Even a more powerful computer can become inadequate for such a task.

In addition, memory limitations will become a serious drawback for the DAE approach in case of increasing n. To give an impression: the size of the executable file for the DAE approach with 150 points was already 50 MByte, while the LGO approach comes up with an executable of 0.1 MByte for the same number of Fekete points. The highest-order term of the storage required by RADAU5 is $4(8n)^2$ real numbers. This means that using double precision, we need about $2 \times 10^3 n^2$ bytes of memory. For $n = 150$ this is about 45 MByte, which can be a severe restriction on small computer systems. Concerning this comparison of the sizes – especially for $n \geqslant 50$ – the LGO approach is favorite.

Later on in this section we show a more thorough comparison of the two approaches. Numerical tests can be performed for smaller number of points on a personal computer or a workstation, but in order to give an overall comparison we did all the computations on the above-mentioned, powerful, four processor workstation. Faster machines are useful – and are even available right now – of course, but the essential computational complexity of the Fekete problem remains exponential. Applying a similar global (exhaustive) search methodology to that of LGO, even on a (say) 10 000 times faster machine, the hardware limitations could be easily reached. For this reason, different heuristic solution strategies need to play a role in solving Fekete problems for large values of n.

Table 1serves to summarize the results obtained on a workstation using the LGO version described in [9] and the DAE approach.

Several additional points should be mentioned; see also the notes provided in the table.

(1) For almost all cases the DAE approach gives a slightly better solution, although the differences are marginal. Except for the above-mentioned computer memory limitations, the DAE approach performs somewhat better than the LGO approach (according to their given implementations). It should be mentioned here that this optimization problem is special because it can be rewritten as a set of DAEs, for more general optimization problems the solution cannot be obtained with a DAE solver and a more general, e.g. LGO style, solver is indispensable.

(2) For the values $n = 2, 3, 4$ and 6, the exact analytical solution is trivial, or can be easily verified; with the exception of $n=2$, however, all values in the tables resulted from numerical calculations. Consequently, all entries are approximate values, except when stated otherwise.

(3) A note regarding the LGO approach: since the function value f_n^* grows very rapidly as n increases, and the resulting (overall) Lipschitzian problem characteristics are also rapidly

Table 1
Summary of the numerical results obtained with LGO and DAE approach

n	$^{10}\log(f^*(n))$[a]		$d(f^*(n))$[b]	CPU[c]	
	For LGO	For DAE		For LGO	For DAE
3	0.71568197[d]	0.715681882	1.732050808	0.32	0.02
4	1.27790594[e]	1.277906197	1.632993162	0.81	0.03
5	1.91980124	1.915913829	1.555894423	1.72	0.06
6	2.70926213[f]	2.709269961	1.515716566	3.11	0.17
7	3.55244136	3.553605389	1.476451904	5.51	0.29
8	4.52830887	4.528830580	1.451255736	8.29	0.49
9	5.59671545	5.597079893	1.430455795	11.24	0.49
10	6.75809669	6.758978609	1.413186645	14.85	0.60
11	7.99809456	7.999912697	1.397825498	22.15	0.83
12	9.38208294	9.383429649	1.387308913	29.05	1.08
13	10.79686832	10.799480094	1.375481878	37.04	1.44
14	12.33009911	12.337356433	1.366392109	46.61	1.68
15	13.95238304	13.961645275	1.358213523	57.78	2.15
16	15.67958355	15.680702647	1.351053423	70.17	4.67
17	17.47670937	17.490362341	1.344638697	84.72	3.49
18	19.38352394	19.391373372	1.338877991	101.07	4.49
19	21.35863686	21.367241420	1.333382123	119.02	5.06
20	23.43731117	23.456734617	1.328790449	139.12	6.07
25	35.16385269	35.176771046	1.309953572	273.17	16.52
30	49.09183884	49.114039625	1.296898053	476.75	32.42
35	65.15724182	65.227582124	1.287141190	757.61	58.50
40	83.40406036	83.531197391	1.279650229	1012.75	138.31
45	103.83299255	103.993419796	1.273631696	1614.29	169.41
50	126.39979553	126.609262581	1.268687030	2222.95	224.81
60	178.03697205	178.291893702	1.261042964	3850.51	586.50
70	238.21658325	238.547125801	1.255385990	5949.21	1573.90
80	306.96221924	307.343814269	1.251009768	9102.11	3380.64
90	384.40673828	384.668442639	1.247518664	11950.35	5511.98
100	470.00125122	470.493394133	1.244655523	17919.00	8844.01
125	721.47052002	722.227981483	1.239340686	33587.70	23703.40
150	1026.29870605	1026.946736740	1.235653773	59967.91	55152.32
∞	∞	∞	1.213061394[g]		

[a] For definition see (2).
[b] For definition see (5). The $f^*(n)$ value from the DAE approach has been used every time, except for $n = 5$.
[c] In seconds.
[d] Exact value: $^{10}\log(3\sqrt{3}) = 0.715681882\ldots$.
[e] Exact value: $^{10}\log((8/3)^3) = 1.2779061968\ldots$.
[f] Exact value: $^{10}\log(512) = 2.7092699609\ldots$.
[g] Recall (6).

becoming less favorable. Therefore, the value of $f_n(x(n))$ has been directly optimized only up to $n = 6$. Starting from $n = 7$, optimization using the original objective function form has been replaced, by applying a logarithmic transformation.

(4) In the LGO approach: 'exact' (exhaustive) search has been attempted for the 'small' values $n = 3,\ldots,15$. That is, up to $n = 15$, all entries have been calculated by fully automatic LGO

execution in which the stated global and local limits imposed on the allowed search effort did not seem to be restrictive. (In particular, the bound on the number of allowable local search steps has not ever been attained, indicating that the LGO search was completed by finding a solution 'as precise as possible' under the given LGO parametrization.) In order to avoid very excessive runtimes, in the cases $n = 50, 60, \ldots, 125, 150$ the number of global search function evaluations was – based on the analysis of detailed LGO output listings, but still somewhat arbitrarily – restricted by 250 000 to 750 000. In light of the computational effort in smaller dimensional Fekete problems, such limitations could be a bit 'optimistic', and may have stopped the global search phase somewhat prematurely. Furthermore, the local search effort (limited by 100 000 to 300 000) has also been attained, in several higher-dimensional cases. Notwithstanding these numerical limitations, all LGO runs provided 'plausible' results, conforming with the theoretical bounds and asymptotics reviewed in Section 2. The global and local search efforts were also chosen in such a way that their sum was comparable to the CPU time for the DAE approach for $n \geqslant 50$.

(5) Concerning the DAE approach: the input parameters for RADAU5 are `h0=atol=rtol=1d-4`.
(6) For both approaches the machine used: SGI workstation, *Indy* with 4 194 Mhz R10010SC processors.
(7) Compiler: FORTRAN 77 of SGI with optimization: `f77 -O`.
(8) Timing function: `ETIME`.

7. Generalizations and application perspectives

An obvious generalization of the Fekete problem – which immediately falls within the scope of the numerical solution strategy suggested – is its extension to arbitrary dimensionality, and for general compact sets. Let D be a bounded closed set in $\mathbb{R}^d$ $d \geqslant 2$, which contains infinitely many points. Then (recalling the discussion in Section 2) the generalized Fekete configuration problem consists of finding an n-tuple of points $z(n) = (z_1, \ldots, z_n)$ such that each z_i belongs to D, and the product

$$V_n(z(n)) := \prod_{1 \leqslant i < j \leqslant n} \|z_i - z_j\| \tag{23}$$

is maximized. As noted earlier, problems of this general class have relevance in diverse areas of scientific modeling.

The higher-dimensional case is also of interest in the area of non-linear regression. A linear approximation provides an ellipsoidal level set, which can be used as an estimate for the level set of the regression variables. Evaluation of the regression criterion at points which are distributed in a regular and uniform way on such an ellipse gives good insight into the non-linearity of the regression problem; the ellipsoid turns into a 'cashew nut', for example. The uniformly distributed sample points on such an ellipsoidal level set can be obtained by solving the Fekete problem (23), where D is the ellipsoidal level set and n the number of sample points.

Again, the numerical solution approach – Lipschitzian global optimization or DAE formulation – advocated by the present work is directly relevant to analyze and solve such problems. This statement remains true, of course, if the 'simple' objective function type (23) is replaced by other suitable (Lipschitzian function) models/formulae expressing the 'quality' of the configurations sought.

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