Centrum voor Wiskunde en Informatica
REPORT*RAPPORT*

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Modelling, Analysis and Simulation (MAS)

MAS-R9705 February 28, 1997

Report MAS-R9705
ISSN 1386-3703

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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 obvious interest in numerical mathematics and scientific modeling. Following a brief discussion of the pertinent analytical background, Lipschitz global optimization (LGO) is applied to determine –i.e., to numerically approximate– Fekete point configurations. Next to the 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.

1991 Mathematics Subject Classification: 65K10, 90C05, 90C31, 65L05.
Keywords and Phrases: Elliptic Fekete points; Lipschitz global optimization; LGO program system; DAE solvers; IVP algorithms, numerical examples; prospective applications.
Note: Work partially carried out under the projects 'Circuit simulation' (no. MAS2.2) and 'Modelling of processes in Chemistry' (no. MAS2.6).

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)

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

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

$$f_n(x(n)) = \prod_{1 \leq i < j \leq n} \|x_i - x_j\| \ , \qquad x_i \in S^2 \ , \tag{1.1}$$

where $\|\ \|$ 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

$$f_n^* = f_n(x^*(n)) = \max_{x(n)} f_n(x(n)) \ , \qquad x_i \in S^2, \quad (i = 1, \ldots, n) \ , \tag{1.2}$$

is called elliptic Fekete points of order n (Fekete, 1923). We shall name (1.2) the Fekete (global optimization) problem.

Let us note first of all that –by the classical theorem of Weierstrass– the optimization problem (1.2) has globally optimal solution(s). Second, although –for obvious reasons of symmetry– there are

infinitely many vector sets $x^*(n)$ which satisfy (1.2), 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 has been of great theoretical interest for several decades: consult the original references Fekete (1923); Szegö (1921,1924); or, more recently, for instance, Hille (1962); Tsuji (1959); Shub and Smale (1993). Apparently, it also represents a longstanding numerical challenge: Pardalos (1995) states it as an open problem. Additionally, because of the direct relation of the formulation (1.2) to models in potential theory (Tsuji, 1959), 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, Shub and Smale mentioned above.

Let D be a bounded closed set in $\mathbb{R}^3$ which contains infinitely many points. Taking n vectors $z_1, ..., z_n$ from D, define (cf. (1.1)) $z(n) = \{z_1, \ldots, z_n\}$,

$$V_n(z(n)) := \prod_{1 \le i < j \le n} \|z_i - z_j\| \ , \tag{2.1}$$

and

$$V_n^* := V_n(z^*(n)) := \max_{z(n)} V_n(z(n)) \ . \tag{2.2}$$

Define now the normalized value of V_n^* by

$$d_n := d_n(D) \quad := \quad \sqrt[\binom{n}{2}]{V_n^*} \ > \ 0 \ ; \tag{2.3}$$

then the following general result –due to Fekete (1923)– is valid.

Theorem 2.1 $d_{n+1} \le d_n$; therefore $\tau(D) = \lim_{n \to \infty} d_n$ exists.

Proof: See Tsuji (1959), p. 71.

Definition 2.1 The quantity $\tau(D)$ is called the *transfinite diameter* of the set 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, Phillips, and Sarnak (1986), as cited by Shub and Smale. 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 2.1 bears direct relevance to such problems, under very general conditions.

Shub and Smale (1993, p. 9) remark –citing Tsuji's work– that the transfinite diameter of the sphere of radius $\frac{1}{2}$ equals $\mathrm{e}^{-\frac{1}{2}}$. This directly leads to the estimate (recall (1.2))

$$d_n(S^2) \quad = \quad \sqrt[\binom{n}{2}]{f_n^*} \approx 2\mathrm{e}^{-\frac{1}{2}} = 1.21306132... \ , \tag{2.4}$$

the approximation is valid for sufficiently large n. Theorem 2.1 immediately provides also a lower bound for the solution of the maximization problem in (1.2):

$$f_n^* \geq \left(2\mathrm{e}^{-\frac{1}{2}}\right)^{\binom{n}{2}} \ . \tag{2.5}$$

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 $d_{n+1} \leq d_n$, which directly leads to

$$f_{n+1}^* \leq (f_n^*)^{\frac{n+1}{n-1}} \ . \tag{2.6}$$

The pair of relations (2.5)-(2.6) provides valid lower and upper bounds; (2.6) 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 (2.5)– 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 introducing 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

$$\begin{array}{rcl} x_{i1} & = & \cos(\alpha_i)\cos(\beta_i) \ , \\ x_{i2} & = & \sin(\alpha_i)\cos(\beta_i) \ , \\ x_{i3} & = & \sin(\beta_i) \ . \end{array} \qquad \left(\begin{array}{rcl} 0 \leq & \alpha_i & < 2\pi \\ -\pi/2 \leq & \beta_i & \leq \pi/2 \end{array} \right) \tag{3.1}$$

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

$$\begin{array}{rcl} 0 \leq & \alpha_i & < 2\pi \ , \\ -1 \leq & \xi_i & \leq 1 \ ; \end{array} \qquad (-\pi/2 \leq \beta_i := \arcsin(\xi_i) \leq \pi/2) \ . \tag{3.2}$$

This results in replacing the calculation of x_{i3} in (3.1) 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 important for a random search as it is used throughout the global search phase of LGO.

In order to eliminate rotational symmetries, one can select and fix three angles in the spherical representation (3.1) of $x(n)$. We choose

$$\alpha_1 = \beta_1 = \beta_2 = 0 \qquad \text{(i.e., } \alpha_1 = \xi_1 = \xi_2 = 0) \ . \tag{3.3}$$

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 (1.2) is continuously differentiable, it is also Lipschitz-continuous on $S^2 \times S^2 \times \ldots \times S^2 = \left(S^2\right)^n$. 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 $x(n),\ \widetilde{x}(n)$ from $\left(S^2\right)^n$ we have

$$|f_n(x(n)) - f_n(\widetilde{x}(n))| \leq L \|x(n) - \widetilde{x}(n)\|_\Sigma \tag{4.1}$$

the norm, $\|x(n) - \widetilde{x}(n)\|_\Sigma$ on $\left(S^2\right)^n$, is a sum of Euclidean norms.

As mentioned earlier, the function f_n is expected to become very 'steep' in certain neighborhoods in $\left(S^2\right)^n$, 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 (1.2) 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 (3.1)-(3.2).

The underlying global convergence theory of Lipschitz optimization algorithms is discussed in detail by Hansen and Jaumard (1995), Horst and Tuy (1996), and Pintér (1996a), 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 Optimization– 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 Pintér (1995, 1996b, 1997).

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. (1989) or Hairer et al. (1996a). 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 (1.1). 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 i-th 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 particles are restricted in such a way that they will stay on 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

$$F_{ij} = \frac{x_i - x_j}{\|x_i - x_j\|^\gamma} \ . \tag{5.1}$$

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 $x(t) = \{x_1(t), \ldots, x_n(t)\}$, Lagrangian mechanics tells us that $x(t)$ satisfies the following system of differential-algebraic equations:

$$x' = q, \tag{5.2}$$
$$q' = g(x,q) + G^T(x)\lambda, \tag{5.3}$$
$$0 = \phi(x), \tag{5.4}$$

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 (5.1). 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. Without this adhesion force, the particles would not stop moving, because the system would preserve its energy. The term $G^T(x)\lambda$ in (5.3) represents the normal force which keeps the particles on S^2.

Let us denote the final configuration by $\widehat{x} = \{\widehat{x}_i, i = 1, \ldots, n\}$. Since we know that the speed of this final configuration is 0, we can substitute $q = 0$ and $x = \widehat{x}$ in formula (5.3), thus arriving at

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

which is equal to

$$\sum_{i \neq j} \frac{\widehat{x}_i - \widehat{x}_j}{\|\widehat{x}_i - \widehat{x}_j\|^\gamma} = -2\lambda_i \widehat{x}_i \ . \tag{5.5}$$

If we, on the other hand, take the logarithm (which is a monotonous function) of $f_n(x(n))$ in (1.1) 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

$$\nabla_i \log(f_n(x)) \ = \sum_{i \neq j} \frac{x_i - x_j}{\|x_i - x_j\|^2} = \zeta_i x_i \ . \tag{5.6}$$

Here, ζ_i is the Lagrange multiplier. Comparing (5.6) and (5.5) tells us that computing $\widehat{x}$ for $\gamma = 2$ gives the (local) optima of the function f_n. In principle by solving the system (5.2) - (5.4) 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 $n \leq 150$, even with a constant κ and a fixed strategy for choosing the initial values, one obtains values for f_n that satisfy the conditions (2.5)-(2.6) and are at least as large as those obtained by the LGO implementation. (This will be shown in Section 6.)

Now we describe how the DAE system given by the equations (5.2) - (5.4) and $\gamma = 2$ can be solved numerically. Since (5.4) 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 Brenan et al. (1989), p. 153) by replacing (5.2) by

$$x' = q + G^T(p)\mu, \tag{5.7}$$

where $\mu \in I\!R^n$, and appending the differentiated constraint

$$0 = G(x)q. \tag{5.8}$$

The system (5.7), (5.3), (5.4), (5.8) 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

$$M\frac{dy}{dt} = w(y), \quad y(0) = y_0, \tag{5.9}$$

with

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

where I_{6n} is the identity matrix of dimension $6n$,

$$\begin{aligned} & & y \in I\!R^{8n}, & \qquad 0 \le t \le t_{\text{end}}\ , \\ y = (x, q, \lambda, \mu)^T \text{ and } w(y) = w(x, q, \lambda, \mu) &= & (q + G^T\mu, g + G^T\lambda, \phi, Gq)^T\ . & \end{aligned}$$

Here, t_{end} is chosen such that

$$|q_i(t_{\text{end}})| < 10^{-14}, \qquad \forall\, i \in \{1, 2, \ldots, n\}. \tag{5.10}$$

Numerical experiments show that if $t_{\text{end}} = 1000$, then (5.10) holds for $n \le 150$.

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 (1.1) 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 (1996b), 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 (1996a). RADAU5 can integrate problems of the form (5.9) up to index 3.

As an example, Figure 1 depicts the solution obtained by RADAU5 for $n = 20$, the same solution in the $\{\alpha, \beta\}$-plane (cf. (3.1)) –after a rotation such that (3.3) is fulfilled– is shown in Figure 2.

Remark: for $n = 20$ the DAE formulation of the Fekete problem is included in the Test Set for IVP Solvers (see Lioen et al. (1996)).

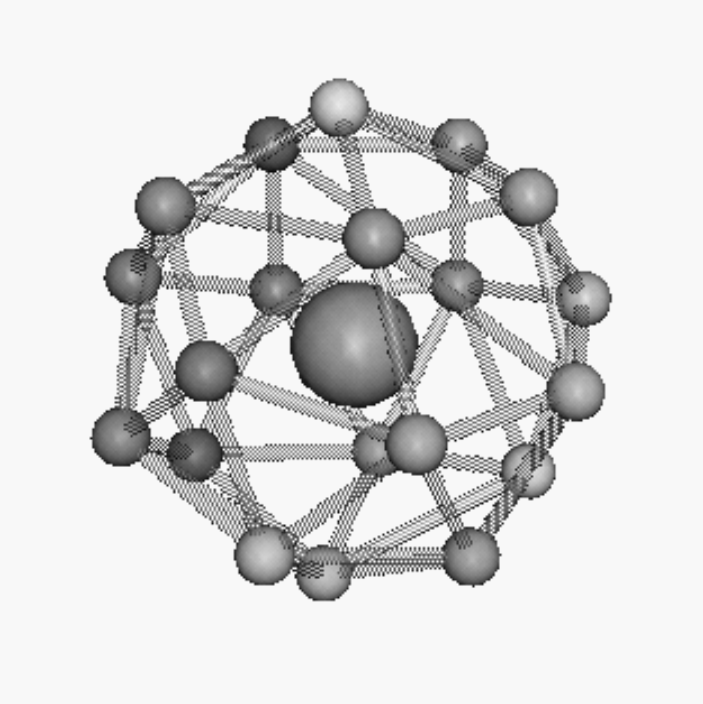

Figure 1: Final configuration obtained with RADAU5 for $n = 20$. The large ball is centered at the origin and only added to facilitate the 3-D perception.

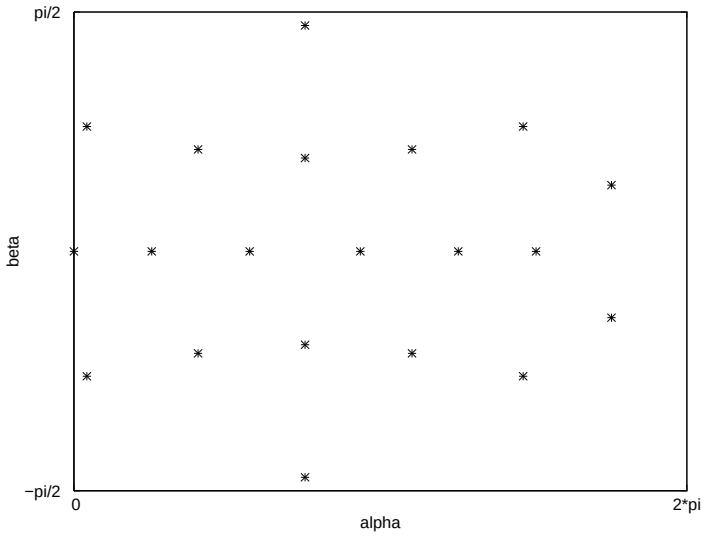

Figure 2: Final configuration, as in Figure 1, where the Fekete points are given in the $\{\alpha, \beta\}$-plane. A rotation has been applied such that (3.3) is fulfilled.

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 4 194 Mhz R10010SC processors, start with a few seconds for both approaches up to 15 points and lead to CPU times between 2 and 17 hours for n in the range of 100 to 150 Fekete points. Even a powerful personal computer is too slow for such a task, 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 MB, while the LGO approach comes up with an executable of 0.1 MB 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 $2 \cdot 10^3 n^2$ 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 $n \geq 50$– 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, 4 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) ten thousand 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 1 serves to summarize the results obtained on a workstation using the LGO version described in Pintér (1995) and the DAE approach.

Concerning the the results, several additional points should be mentioned; see also the notes provided in the table.

- For almost all cases the DAE approach gives a slightly better solution, although the differences are not that big. 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 can not be obtained with a DAE solver and a more general, e.g. LGO style, solver is indispensable.

- 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.

- Concerning 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 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.

- Concerning 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

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

n	$^{10}\log(f^*(n))^a$ (LGO vs. DAE)		$d(f^*(n))^b$	CPU^c (LGO vs. 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 (1.2)
[b] For definition see (2.3). 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 (2.4)

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 $n \geq 50$.

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

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 $\mathbb{R}^d$ $d \geq 2$, 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 $z(n) = (z_1, ..., z_n)$ such that z_i belongs to D, and the product

$$V_n(z(n)) := \prod_{1 \leq i < j \leq n} \|z_i - z_j\| \,, \tag{7.1}$$

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 nonlinear regression. From linear regression one obtains an ellipsoidal level set, which can be used as an approximation for the level set of the regression variables in the nonlinear case. 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 nonlinearity 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 (7.1), 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 (7.1) is replaced by other suitable (Lipschitzian function) models/formulae expressing the 'quality' of the configurations sought. For detailed discussions and various applications, consult, for instance the papers in special issues of the Journal of Global Optimization (1994, 1995), or Shalloway (1992), Oresiĉ and Shalloway (1994), Botina and Rabitz (1995), Botina, Rabitz and Rahman (1995), Lu and Rabitz (1995), Moré and Wu (1995a,b), Amara, Ma and Straub (1996), Andricioaei and Straub (1996), Bollweg, Maurer and Kroll (1997), Church, Oresiĉ and Shalloway (1996), Dill, Phillips and Rosen (1997), Phillips, Rosen and Valke (1996), with numerous further references.

Acknowledgements

This research has been initiated during J.D.P.'s visit at CWI, and was partially supported by the Dutch Technology Foundation (Grant No. CWI55.3638). The research leading to the LGO development has

also been supported earlier by the Hungarian Scientific Research Fund (OTKA). W.S. and J.deS. are both supported via the Dutch Technology Foundation (Grant No's. CWI22.2695 and CWI22.2703, respectively). Comments received from Claus Führer are gratefully acknowledged. We thank Robert van Liere for producing Figure 1.

Note finally that Kai Dirscherl (1996) was kind to share information with us related to his experiments to solve the Fekete problem. Using a multistart approach, he recently solved smaller size problems (configurations of up to 12 Fekete points).

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