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Energy Minimization of Point Charges on a Sphere with a Hybrid Approach

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Abstract

We study a method for minimizing the energy of N point charges on a sphere. It is estimated that the number of distinct local minima of the energy function grows exponentially with N, and they have energies very close to the global minimum. In this paper, we present a hybrid approach for tackling this problem, knowing as Thomson problem, by using an evolutionary algorithm and a nonmonotone spectral gradient method.

Keywords: Distributing points on a sphere, Thomson problem, Spectral gradient methods, Evolutionary algorithm

1 Introduction

The problem of finding how electrons optimally distribute themselves on the sphere is a well-known and unsolved one. It is called the Thomson problem, after the physicist Joseph John Thomson[11], who studied a related but different arrangement of point charges in one of his investigations into atomic structure. Smale in his list of problems for the current century [21], states as Problem #7 the challenge to locate these points efficiently. Thomson problem is one of the problems concerning of Optimal Configurations on the sphere [5, 19], which have proved to be useful in many scientific and technology domains ranging from Biology to Telecommunication [18, 2, 16, 14, 12, 1]. There is a large literature on Thomson's problem, it has be analyzed via various methods such as Generalized Simulated Annealing[24], Monte Carlo approaches[6, 15], the steepest-descent and the conjugate gradient algorithm [22, 23]. This problem is an ideal benchmark of new global optimization algorithms. In view of the success of the evolutionary algorithm in solving the Thomson's problem [13, 12], we decided to tackle it by combining an evolutionary algorithm and a nonmonotone spectral gradient method[1].

The spectral projected gradient method SPG is an algorithm for large-scale bound-constrained optimization introduced recently by Birgin, Martinez, and Raydan [4]. It is based on the Raydan[17] unconstrained generalization of the Barzilai-Borwein method for quadratics[20]. In our approach we have exploited the observations given by Birgin et al. [4] in their construction of the algorithm SPG2 to adapt this one to the unconstrained optimization (SG2), given bellow. In fact we can directly utilize the algorithm (GBB) developed by Raydan [17] for unconstrained optimization, but when we have tested both algorithms, we have remarked that (SG2) gives good results rather than (GBB), especially in the speed of convergence.

In the following section we give a description of the Thomson problem. A mathematical modeling is given in section 3. In section 4 we present our approach for tackling this problem and we give our numerical results in section 5. The paper is concluded in section 6.

[1]We have already tackled this problem by SPG2[4] in our Communication presented in the 10th IMACS Conference in Marrakech in morocco, and by a genetic algorithm combined with SPG2 in another Communication presented in the Mamern11 Conference in Saidia in morocco. The results found overthere motivate us to continue in this process.

2 Point charges on the sphere

The electrostatic potential energy required to assemble a collection of N identical point charges at $p_1, p_2, ..., p_N$ in $\mathbb{R}^3$ is, up to a constant,

$$\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{\|p_i - p_j\|} \tag{1}$$

If the points $p_1, p_2, ..., p_N$ are now constrained to lie in the unit sphere, then the question of what configuration of those points minimizes the quantity in (1) is called Thomson problem.

3 Mathematical modeling of the thomson problem

We introduce some notations: we denote by S^2 the unit sphere in the Euclidean space $S^2 = \{x^3 \in \mathbb{R}^3 : \|x\| = 1\}$ and $\omega_N = \{p_1, ..., p_N\}$ the set of the point charges on S^2.

The locations of the point charges are encoded in spherical coordinates $(\overrightarrow{e}_{\rho_k}, \overrightarrow{e}_{\varphi_k}, \overrightarrow{e}_{\theta_k})$, $k = 1, ..., N$, omitting the constant sphere radius $r = 1$.

The potential energy function is defined as $E(\omega_N) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{\|p_i - p_j\|}$.

We have $p_i - p_j = \overrightarrow{e}_{\rho_i} - \overrightarrow{e}_{\rho_j}$ and $\overrightarrow{e}_{\rho_i} = \sin\varphi_i \cos\theta_i \overrightarrow{i} + \sin\varphi_i \sin\theta_i \overrightarrow{j} + \cos\varphi_i \overrightarrow{k}$, where $(\overrightarrow{i}, \overrightarrow{j}, \overrightarrow{k})$ is the Cartesian coordinate system.

Therefore, the distance between two point charges p_i and p_j is given by: $d_{ij}(\varphi_i, \theta_i, \varphi_j, \theta_j) = \sqrt{2(1 - \sin\varphi_i \sin\varphi_j \cos(\theta_i - \theta_j) - \cos\varphi_i \cos\varphi_j)}$

where φ_i and θ_i denote respectively the colatitude and the longitude of the i^{th} point charge, for $i = 1, 2, ..., N$.

And hence, our goal is to resolve the following minimization problem

$$\begin{cases} \min \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{d_{ij}(\varphi_i, \theta_i, \varphi_j, \theta_j)} \\ \varphi_i \in \mathbb{R} \quad (1 \leq i \leq N) \\ \theta_i \in \mathbb{R} \quad (1 \leq i \leq N) \end{cases}$$

4 A hybrid approach for tackling the Thomson problem

In our approach an evolutionary algorithm carries out first a certain number of generations and then a spectral gradient method, is applied to refine the approximations.

The Evolutionary Algorithms (EAs) are stochastic search methods that have been successfully applied in many searches, and optimization problems. It can be summarized briefly by following cycle: Evaluate the fitness of all the individuals in the population. Create a new population by performing operations such as crossover and mutation.

A string represents a solution to the problem and is encoded as a vector of random real numbers. Each solution string is made of N genes where N is the number of the points to be distributed into the unit sphere.

$$\text{string } = ((\varphi_1, \theta_1), (\varphi_2, \theta_2), ..., (\varphi_N, \theta_N))$$

where each gene represents the coordinates of a point on the sphere.

Description of an Evolutionary Algorithms adapted for solving Thomson problem

Our evolutionary algorithm begins with a population of random string in $([0, \pi] \times [0, 2\pi])^N$, which every string is the encoded real version of a tentative solution. We consider the potential energy as the evaluation function associated to every string. Strings are ranked from the most-fit to the least-fit. And we divide the population into three sup-populations. The first third that contains the most fit strings is accepted, and unacceptable strings are discarded. Then we generate the strings of the second part applying crossover and mutation to the first part of the population. Here in the mutation we randomly select one gene, and set it equal to a random vector in the $[0, \pi] \times [0, 2\pi]$. The population is completed by random strings. This process is repeated until either a certain number of generations is reached or there is no change in the best solution found for many generations.

The solution found by the previous algorithm is, then improved by using a modified spectral gradient method (SG2).

Description of a modified spectral gradient method

The unconstrained minimization problem

$$\min_{x \in \mathbb{R}^n} f(x)$$

where $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ is a continuously differentiable function, has different iterative methods to solve it: If x_k denotes the current iterate, and if it is not a good estimator of the solution x_*, a better one, $x_{k+1} = x_k - \alpha_k g_k$ is required. Here g_k is the gradient vector of f at x_k and the scalar α_k , is the step length.

A variant of the steepest descent was proposed in [20], which referred to the 'Barzilai and Borwein' (BB) algorithm, where the step length α_k along the

steepest descent $-g_k$ is chosen as in the raliegh quotient $\alpha_k = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T y_{k-1}}$, where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$. This choice of step length requires little computational work and greatly speeds up the convergence of gradient methods. Raydan in [17] has proved a global convergence of (BB) algorithm under a non-monotone line search.

In non-monotone spectral gradient method, the iterate x_k satisfies a non-monotone Armijo line search (using sufficient decrease parameter γ over the last M steps),

$$f(x_{k+1}) \leq \max_{0 \leq j \leq \min\{k,M\}} f(x_{k-j}) + \gamma \langle g_k, x_{k+1} - x_k \rangle \tag{2}$$

Here the function values are allowed to increase at some iterations. This type of condition (2) was introduced by Grippo, Lampariello, and Lucidi [10] and successfully applied to Newton's method for a set of test functions.

As we have mentioned, we have adapted the SPG2 algorithm developed by Birgin et al [4], to the unconstrained optimization, in which the projection of the point is itself.

Algorithm SG2

The algorithm starts with $x_0 \in \mathbb{R}^n$ and use an integer $M \geq 0$; a small parameter $\alpha_{min} > 0$; a large parameter $\alpha_{max} > 0$; a sufficient decrease parameter $\gamma \in (0, 1)$ and safeguarding parameters $0 < \sigma_1 < \sigma_2 < 1$. Initially, $\alpha_0 \in [\alpha_{min}, \alpha_{max}]$ is arbitrary.

Step 1. Detect whether the current point is stationary
If $\|g(x_k)\| = 0$, stop, declaring that x_k is stationary.

Step 2. Backtracking

Step 2.1 Compute $d_k = -\alpha_k g_k$. Set $\lambda = 1$.

Step 2.2 Set $x_+ = x_k + \lambda d_k$.

Step 2.3 If

$$f(x_{k+1}) \leq \max_{0 \leq j \leq \min\{k,M\}} f(x_{k-j}) + \gamma \lambda \langle d_k, g_k \rangle \tag{3}$$

then set $\lambda_k = \lambda$, $x_{k+1} = x_+$, $s_k = x_{k+1} - x_k$, $y_k = g_{k+1} - g_k$ and go to **Step 3**, else, define $\lambda_{new} \in [\sigma_1, \sigma_2 \lambda]$. Set $\lambda = \lambda_{new}$ and go to **Step 2.2**.

Step 3. Compute $b_k = \langle s_k, y_k \rangle$.
If $b_k \leq 0$, set $\alpha_{k+1} = \alpha_{max}$, else, compute $a_k = \langle s_k, s_k \rangle$ and
$\alpha_{k+1} = \min\{\alpha_{max}, \max\{\alpha_{min}, a_k/b_k\}\}$

Remark 4.1 *The computation of λ_{new} uses one-dimensional quadratic interpolation [7].*

5 Numerical results

In this section we report the numerical results obtained for the Thomson problem.

The hybrid algorithm was implemented in Matlab. Table 1 shows the parameter settings for the evolutionary algorithm.

Population Size	54
Maximum Number of Generations	500
Crossover Points	2
Crossover Rate	0.8
Mutation rate	0.08

Table 1: Parameters used in the evolutionary algorithm

We implement the Algorithm SG2 with the parameters described in [4]: $\gamma = 10^{-4},\ \alpha_{min} = 10^{-30},\ \alpha_{max} = 10^{30},\ \sigma_1 = 0.1,\ \sigma_2 = 0.9, \alpha_0 = 1/\|\nabla E\|_\infty$.

We have tested our method with $M \in \{5, 10, 15\}$, and we have decided to use $M = 5$ as the choice that gives minimal energies. We stopped the execution of SG2 when the criterion $\|\nabla E\|_\infty \leq 10^{-5}$ was satisfied or when 50000 iterations were completed without achieving convergence.

In table 2 we present the minimum energies found with our approach. The first column lists the number of point charges N. The next column shows the minimum energy of the solution found by the hybrid method EA_SG2. The energy of the presently known ground state for this system size is presented in the third column . Column 4 lists the energies found by the function `ga` of the Toolbox of Genetic Algorithms of MatLab and improved by the `fminunc` of the Toolbox of optimization of MatLab, and the last column presents the minimum energy of the solution found by PSO (Particle Swarms Optimization) presented in [1].

6 conclusion

We present a hybrid approach to solve the Thomson problem. We use evolutionary algorithm for exploring the search space and exploiting the best solutions found, and a modified nonmonotone spectral gradient method is used for improving the solutions. Our numerical experiments seem to indicate that our approach is competitive and sometimes preferable to the results given by ga_fminunc and recent implementations of the PSO.

We intend afterward to combine the (SG2) with other heuristics, PSO for example.

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N	EA_SG2	Smallest known energy	ga_fminunc	By PSO [1]
3	1.732050808	1.732050808	1.732050808	1.732050808
4	3.674234614	3.674234614	3.674234614	3.674234614
5	6.474691495	6.474691495	6.474691495	6.474691495
6	9.985281374	9.985281374	9.985281374	9.985281374
7	14.452977414	14.452997414	14.452977414	14.452977414
8	19.675287861	19.675287861	19.675287861	19.675287861
9	25.759986531	25.759986531	25.759986531	25.759986531
10	32.716949461	32.716949461	32.716949460	32.716949460
11	40.596450508	40.596450510	40.596450508	40.596450549
12	49.165253058	49.165253058	49.165253058	49.165253067
13	58.853230612	58.853230612	58.853230612	58.853326485
14	69.306363297	69.306363297	69.306363297	69.306461333
15	80.670244114	80.670244114	80.670244114	80.670617827
16	92.911655303	92.911655302	92.911655303	92.917369707
17	106.050404829	106.050404829	106.050404829	106.050606097
18	120.084467447	120.084467447	120.084467448	120.087059280
19	135.089467558	135.089467557	135.089467557	135.096210250
20	150.881568334	150.881568334	150.881568342	150.894135172
21	167.641622400	167.641622399	167.641622632	167.660869512
22	185,287536149	185.287536149	185.287536149	185.320722913
23	203.930190663	203.930190663	203.930190665	203.955672783
24	223.347074052	223,347074052	223.347074052	223.433627450
25	243,812760300	243.812760299	243.812761344	243.856156962
26	265.133326317	265.133326317	265.133340865	265.301652244
27	287.302615033	287.302615033	287.302615034	287.429529418
28	310.491542358	310.491542358	310.491543027	310.648071055
29	334.634439920	334.634439920	334.634829668	334.831687736
30	359.603945904	359.603945904	359.604047846	359.860169140
35	498.569872491	498.569872491	498.574039623	499.019259674
40	660.675278835	660.675278835	660.675288505	661.056373164
45	846.188401061	846.188401061	846.188706860	846.860299001
50	1055.182314726	1055.182314726	1055.192609989	1056.459459680

Table 2: Minimum energies found in experiments

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