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Energy Minimization of Point Charges on a Sphere with a Spectral Projected Gradient Method

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Abstract— Thomson problem, which is one of the problems concerning of optimal configuration on the sphere, is defined. A Nonmonotone Spectral Projected Gradient Method that has been intensively used in many applications is presented. Numerical results that indicate the effectiveness of this method to tackle the Thomson problem are reported.

Index Terms—Energy-minimizing point configurations on spheres, Nonmonotone Spectral Projected Gradient Method, Thomson problem.

1 Introduction

The problem of finding how identical charges optimally distribute themselves on the sphere, generally referred to as the Thomson problem, is a largely unsolved problem. It has attracted the attention of researchers in many areas such as chemistry, physics and crystallography [1],[2],[3],[4],[5],[6]. Thomson problem has been ranked 7 in the famous list of Smal's 18 problems for our Century [7]. Recently Birgin et al. [8] have developed the spectral projected gradient method (SPG) that a fast and global technique for convex constrained optimization, and they showed the performance of the SPG on a set of large-scale box-constrained problems.

In this paper we give a mathematic modeling of the Thomson problem, which is consisting in minimizing a continuously differentiable function with simple bounds. We also present an overview of the SPG method that we adapt to Thomson problem, and then we give some implementation details and numerical results. Finally, we conclude by a perspective of research.

2 Problem Formulation

Given N identical point charges placed at $p_1, p_2, \dots, p_N$ in the surface of the unit sphere, the electrostatic potential energy between them is, up to a constant:

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

Thomson problem is to determine the configuration of those points that minimizes the quantity "(1)".

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

The point $p_i \in S^2$ can be expressed with its three Cartesian coordinates, but if we consider spherical system $(\overrightarrow{e_{\rho k}}, \overrightarrow{e_{\varphi k}}, \overrightarrow{e_{\theta k}})$, $k = 1, \dots, N$, omitting the constant sphere radius $\rho = 1$, the point can be parameterized by only two variables $\theta_i \in [0, 2\pi]$ and $\varphi_i \in [0, \pi]$.

So, we have $p_i - p_j = \overrightarrow{e_{\rho i}} - \overrightarrow{e_{\rho j}}$, and

$$\overrightarrow{e_{\rho l}} = sin\varphi_l cos\theta_l \vec{i} + sin\varphi_l sin\theta_l \vec{j} + cos\varphi_l \vec{k}$$

where $(\vec{i}, \vec{j}, \vec{k})$ is the Cartesian coordinate system.

Therefore, the distance between two point charges p_i and p_j is as the following:

$$\|p_i - p_j\| = (2 - 2sin\varphi_i \, sin\varphi_j \, \cos(\theta_i - \theta_j) - 2cos\varphi_i \, cos\varphi_j)^{1/2}$$

Where θ_i denotes longitude and φ_i denotes colatitude of the i^{th} point charge.

Our problem now becomes

$$\begin{cases} \min E(\omega_N) = \displaystyle\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{\sqrt{2(1 - sin\varphi_i sin\varphi_j \cos(\theta_i - \theta_j) - cos\varphi_i cos\varphi_j)}} \\ \varphi_i \in [0, \pi], \theta_i \in [0\ 2\pi], \qquad i = 1, \dots, N \end{cases}$$

The objective function is infinitely differentiable and has an exponential number of local minimizers.

The number of unknowns is 2N. And in order to avoid the congruent solutions, which can be caused by an arbitrary rotation, we may assume without loss of generality that the longitude of point p_1 can be fixed:

$$\theta_1 = 0$$

Moreover, the point charge N can also be fixed at the North Pole,

$$\varphi_N = 0, \qquad \theta_N = 0.$$

In this manner, the actual number of unknowns has dropped to 2N-3.

3 Nonmonotone Spectral Projected Gradient Method on Convex Sets

The spectral projected gradient method SPG is an algorithm for large-scale bound-constrained optimization introduced recently by Birgin, Martínez, and Raydan [8]. It is based on the Raydan[9] unconstrained generalization of the Barzilai-Borwein method for quadratics[10].

In this method the authors combine the projected gradient method that maintain feasibility of the iterates by frequently

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projecting trial steps on the feasible convex set, with the technique of nonmonotone line search, such a method has received many successful applications in unconstrained optimization. And they associate the spectral steplength to speed the convergence of gradient method.

The SPG method applies to problems of the form

$$min\, f(x)\ subject\ to\ x \in \Omega,$$

where Ω is a closed convex set in R^n, and f is a differentiable function.

Given $x \in R^n$ we define $P(x)$ the projection on Ω. We denote $g(x) = \nabla f(x)$. The algorithm starts with $x_0 \in \Omega$ and use an integer $M \geq 1$; 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. Given $x_k \in \Omega$ and $\alpha_k \in [\alpha_{min}, \alpha_{max}]$, the following algorithm describes how to obtain x_{k+1} and α_{k+1}, and when to terminate the process.

Algorithm (SPG)

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 $d_k = P(x_k - \alpha_k g(x_k)) - x_k$. Set $\lambda = 1$

Step 2.2. Set $\tilde{x} = x_k + \lambda d_k$

Step 2.3. If

$$f(\tilde{x}) \leq \max_{0 \leq j \leq \min\{k,M\}} f\left(x_{k-j}\right) + \gamma\lambda < g(x_k), d_k > \quad (2)$$

then define $\lambda_k = \lambda$, $x_{k+1} = \tilde{x}$, $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g(x_k) - g(x_{k-1})$, and go to **Step 3.**

If "(2)"does not hold, define

$$\lambda_{new} \in [\sigma_1, \sigma_2 \lambda] \quad (3)$$

set $\lambda = \lambda_{new}$ and go to **Step 2.2**.

Step 3.

Compute $b_k =< s_k, y_k >$.

If $b_k \leq 0$, set $\alpha_{k+1} = \alpha_{max}$, else, compute $a_k =< s_k, s_k >$ and

$$\alpha_{k+1} = \min\{\alpha_{max}, \max\{\alpha_{min}, a_k / b_k\}\}$$

The algorithm is fully described in [8],[11].

Remark 1. The projection of any $x \in R^n$ onto the set Ω, where $\Omega = [l_1, u_1] \times \ldots \times [l_n, u_n]$ is an n-dimensional box, is given, for $i = 1,..,n$ by

$$(P(x))_i = \begin{cases} l_i \text{ if } x_i < l_i \\ x_i \text{ if } l_i \leq x_i \leq u_i \\ u_i \text{ if } x_i > u_i \end{cases}$$

But before projecting, we prefer to exploit the fact that our objective function is periodic of period 2π.

4 Computational Results

The variable of our problem has the form $x = (\varphi_1, \varphi_2, \ldots, \varphi_{N-1}, \theta_2, \theta_3, \ldots, \theta_{N-1})$, where N represents the number of points to distribute in the surface of the sphere. $\varphi_N, \theta_1$and θ_N have been fixed at zero.

We implement the algorithm SPG in MatLab with the parameters described in [8]:
$\alpha_{min} = 10^{-30}, \alpha_{max} = 10^{30}, \sigma_1 = 0.1, \sigma_2 = 0.9, \gamma = 10^{-4}$, $\alpha_0 = \|\nabla f\|_\infty^{-1}$ and $M = 5$.

We stopped the execution of the SPG algorithm when the criterion $\|\nabla f\|_\infty \leq 10^{-5}$ was satisfied or when 5000 were completed without achieving convergence.

In the TABLE 1, N indicates system size and SPG presents the minimum energy of the solution found with the SPG method for this system size.

TABLE 1.Minimum energies found in experiments

N	SPG	Smallest known Known
3	1.732050808	1.732050808
4	3.674234614	3.674234614
5	6.474691495	6.474691495
6	9.985281374	9.985281374
7	14.452977434	14.452997414
8	19.675287861	19.675287861
9	25.759986531	25.759986531
10	32.716949461	32.716949461
11	40.596450508	40.596450510
12	49.165253058	49.165253058
13	58.853230612	58.853230612
14	69.306363297	69.306363297
15	80.670244114	80.670244114
16	92.911655303	92.911655302
17	106.050404829	106.050404829
18	120.084467448	120.084467447
19	135.089467588	135.089467557
20	150.881568334	150.881568334
21	167.641622410	167.641622399
22	185.287536150	185.287536149
23	203.930190663	203.930190663
24	223.347074052	223.347074052
25	243.812760301	243.812760299
26	265.133326318	265.133326317
27	287.302615033	287.302615033
28	310.491542358	310.491542358
29	334.634439921	334.634439920
30	359.603945908	359.603945904
31	385.530838063	385.530838063
32	412.261274651	412.261274651
33	440.204057462	440.204057448
34	468.904853281	468.904853281
35	498.569872492	498.569872491
36	529.122408407	529.122408375
37	560.618887746	560.618887731
38	593.038503566	593.038503566
39	626.389009017	626.389009017
40	660.675278835	660.675278835
41	695.916744342	695.916744342
42	732.078107544	732.078107544
43	769.190846502	769.190846459
44	807.174263087	807.174263085
45	846.188401070	846.188401061
46	886.167113644	886.167113639
47	927.059270681	927.059270680
48	968.713455344	968.713455344
49	1011.557182654	1011.557182654
50	1055.182314726	1055.182314726

From the results presented in TABLE 1, we observe that in most values of N the SPG method finds the same minimum energies as given in the literature [12], and it gives good approximations for the other values of N. For N=11 we have successfully improved the minimum energy, in the TABLE 2 we give the spherical coordinates of the solution that gives this minimum.

TABLE 2. Spherical coordinates of the configuration of 11 points

Colatitudes	Longitude
1.401623216607999	0
2.156367100166367	1.051818698843048
1.401643107595485	3.141609960117691
2.156382696927945	4.193409334072129
1.029426696865827	4.193409959411595
1.401619226304498	2.103629335868977
2.508083140386192	5.764222507526097
2.508081713254755	2.622597499926048
1.401642195442267	5.245207974203244
1.029430235059431	1.051812594874388
0	0

5 RESEARCH PERSPECTIVE

The effectiveness of the SPG algorithm in tackling Thomson problem, motivate us afterward to combine it with a heuristic algorithm to approach global minimum.

REFERENCES

[1] R. Backofen, A. Voigt and T. Witkowski, "Particles on curved surfaces: A dynamic approach by a phase field-crystal model", Phys. Rev. E 81, 025701(R) (2010).

[2] M. Bowick, A. Cacciuto, D.R. Nelson and A. Travesset, "Crystalline Order on a Sphere and the Generalized Thomson Problem", Physical Review Letters, 89, 185502, (2002).

[3] M. Patra, M. Patriarca and M. Karttunen, "Stability of charge inversion, Thomson problem and application to electrophoresis", Phys. Rev. E 67, 031402 (2003).

[4] Kari J. Nurmela, "Stochastic Optimization Methods in Sphere Packing and Covering Problems in Discrete Geometry and Coding Theory" (1997) (Hecse 95-97).

[5] J. R. Morris, D. M. Deaven, K. M. Ho, C. Z. Wang, B. C. Pan, J. G. Wacker and D. E. Turner, "Genetic algorithm optimization of atomic clusters". 1996 Dec 31.

[6] A. Băutu and E. Băutu, "Energy Minimization of point charges on a sphere with Particle Swarm", 7th International Balkan Workshop on Applied Physics, Constantza, Jul. 2007.

[7] S. Smale, "Mathematical Problems for the Next Century, Mathematics: Frontiers and Perspectives", edited by Arnold, Atiyah, Lax, and Mazur. Providence, RI: Amer. Math. Society, (2000).

[8] E.G.Birgin, J.M.Martínez and M.Raydan, "Nonmonotone Spectral Projected Gradient Methods on Convex Sets". SIAM J. on Optimization, 10(4): 11961211, 2000.

[9] M.Raydan, "The Barzilai and Borwein gradient method for the large scale unconstrained minimization problem", SIAM J. on Optimization, 7(1): 2633, 1997.

[10] J. Barzilai and J. M. Borwein, "Two point step size gradient methods", IMA J. Numer. Anal., 8 (1988), pp. 141148.

[11] G.Birgin and M.Raydan, "SPG Software for Convex-Constrained Optimization", ACM Transactions on Mathematical Software, Vol. 27, No. 3, September 2001, Pages 340-394.

[12] Thomson problem. From wikipedia, http://en.wikipedia.org/wiki/Thomson_problem

[13] E. Saff and A. B. J. Kuijlaars, "Distributing many points on a sphere", Math. Intelligencer 19 (1997); 5 11.

[14] R. Womersley, "Distributing points on the sphere", School of Mathematics, UNSW. http://www.maths.unsw.edu.au/school/articles/me100.html

[15] J. J. Thomson, "On the Structure of the Atom", Philosophical Magazine Series 6, Vol 7 (1904) 237-265.

[16] J. Fitzpatrick, "The geometry of optimal and near optimal Riesz energy configuration", PhD thesis, Vanderbilt University (2010).

[17] J. Fliege and U. Maier, "A Two-Stage Approach for Computing Cubature Formulae for the Sphere", Mathematik 139T, Universitat Dortmund, Fachbereich Mathematik, Universitat Dortmund, 44221 (1996).

[18] D.J. Wales and S. Ulker, "Structure and Dynamics of Spherical Crystals Characterized for the Thomson Problem", Physical Review B, 74, 212101; 2006.