ENERGY MINIMIZATION OF POINT CHARGES ON A SPHERE WITH PARTICLE SWARMS*

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In this paper we present a method to study the Thomson problem of finding the lowest energy configuration of N point charges constrained to the surface of a unit sphere. The behavior of the system is highly nonlinear and the number of metastable structures grows exponentially with N. This makes it extremely difficult to locate a global minimum. We tackle the problem of minimizing the energy of the system with Particle Swarm Optimization (PSO), a population-based stochastic optimization technique inspired by the social behavior of bird flocking. We present the Thomson problem and the basic principles of the PSO metaheuristic, together with experimental results that confirm the effectiveness of the PSO approach.

Key words: point charges, Thomson problem, particle swarm optimization.

1. INTRODUCTION

Finding the minimum energy configuration of N repulsive point charges constrained to the surface of a 2-sphere is a long standing problem, ranked 7 in Stephen Smale's famous list [1] of 18 unsolved mathematical problems to be solved in the 21st century. A configuration with global minimum energy is also referred to as ground state. The problem is named the Thomson problem after the British physicist J.J. Thomson, who first posed it in 1904 as part of the development of the plum pudding model of the atom [2]. In his model, the repulsive point charges were electrons which formed spherical shells, repelling each other with a force given by Coulomb's law. Thus, the potential energy of the system is:

$$U = \frac{q_e^2}{4\pi\varepsilon_0} \sum_{j=1}^{N-1} \sum_{i=j+1}^{N} \frac{1}{r_{ij}} \tag{1}$$

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where q_e is the electron charge, ε_0 is the permittivity of space, and r_{ij} is the distance between particles i and j.

Over the years, various generalizations of the Thomson problem have also been studied from different aspects. The most common generalization involves interactions between particles with arbitrary potentials. Bowick *et al* [3] studied a system of particles constrained to a sphere and interacting by a $1/r^{\gamma}$ potential, with $0 < \gamma < 2$. Travesset [4] studied the interactions of the particles on topologies other than the 2-sphere. Levin and Arenzon [5] studied the interactions in a N particle system with $N-1$ particles confined on the sphere and 1 particle fixed in the centre of the sphere.

Apart from its physical implications [3, 6, 7, 8, 9, 10], the Thomson problem arises in many other fields, both in classical and generalized form. In biology, it appears as the problem of determining the arrangements of the protein subunits which comprise the shells of spherical viruses [11] (e.g. adenoviruses). In structural chemistry, it appears as the problem of finding regular arrangements for proteins S-layers [10, 12] (e.g. archaea protein). It also appears frequently in other fields, like mathematics (e.g. in coding theory), telecommunications (e.g. the Iridium LEO satellite constellation, radio relays locations, cell access points for mobile phones), economy, sociology, etc.

From an optimization point of view, the Thomson problem is of great interest to computer scientists also, because it provides an excellent test bed for new optimization algorithms, due to the exponential growth of the number of configurations with local minimum energy and to their characteristics.

The problem can be tackled with various methods. For small values of N, exact solutions are known; however, for most values of $N \geq 9$, exact solutions are not known. For such cases, numerical simulations provide the best known solutions for a wide range of particle numbers. The configurations found display a great variety of geometrical structures [13].

Giomi *et al.* [14] analyzed the structure of a two-dimensional paraboloidal crystal as a specific realization of the class of crystalline structures on two-dimensional Riemannian manifold and provided a numerical analysis of a system of classical particles interacting via a Coulomb potential on the surface. In [15], the authors found, using numerical arguments, a tetrahedral configuration for $N = 306$ and a dihedral configuration for $N = 542$ to have global minimum energy. They also provide results that confirm the theory of Dodgson and Moore [16] that as N grows, dislocation defects can lower the lattice strain of symmetric configurations along with the energy.

Because of the complexity of the problem landscape and the exponential growth of the number of local minimum energy configurations, the Thomson problem is considered a good test problem for optimization algorithms, heuristics and metaheuristics. Carlson *et al.* [17] used quantum Monte Carlo simulations in a

related problem – calculations of superfluid Fermi gases with short-range two-body attractive interactions with infinite scattering length. Morris *et al.* [18] applied a genetic algorithm to the Thomson problem that proved very efficient in exploring the low energy configurations, giving competitive results even for large systems. Pérez-Garrido *et al.* [19] used a numerical algorithm based on the consideration of simultaneous many-particle transitions in order to reduce the characteristic slowing down of numerical algorithms when applied to complex systems.

Other analytical, numerical and simulation-based approaches have also been used on the Thomson problem or related problems with various results (e.g. Iterated Local Search [20], Differential Evolution [14], etc.). To the best of the authors' knowledge, this paper is the first to tackle the Thomson problem with Particle Swarm Optimization. Many studies indicate PSO to be a worthy opponent on numerical optimization problems for the previously mentioned algorithms.

2. PARTICLE SWARM OPTIMIZATION

Particle Swarm Optimization (PSO) is a metaheuristic inspired by the social behavior of bird flocking [21]. It is based on the evolutionary cultural model of Boyd and Richerson [23] which states that in social environments individuals have two learning sources: individual learning and cultural transmission. Individual learning is an important feature in homogeneous environments; cultural transmission is an essential characteristic in heterogeneous environments. Successful individuals combine both these sources to increase their gain in knowledge. In a similar fashion, PSO solves optimization problems by using a set of potential solutions, called swarm of particles, which gather and share information about the problem landscape [22]. Therefore the driving force of PSO is the collective swarm intelligence. The problem landscape is determined by a function that maps candidate solutions for the problem at hand to rewards. Similar to birds foraging, the particles "fly", at certain speeds, over the problem landscape searching locations with higher rewards. They also exchange information about these locations with their neighbors, thus improving the "quality of life" of the swarm. In the rest of the paper, we will use the term "point charges" to refer to the repelling particles on the sphere, in order to avoid confusion with particles – the candidate solutions of the PSO algorithm.

In order to apply PSO to the Thomson problem, the position of each particle in the problem space encodes the distribution of the N point charges on the unit sphere. The PSO algorithm begins with a swarm of particles randomly scattered around the search space. This generic initialization method can be replaced with a problem specific one (e.g. spherical initialization) which might determine better results.

After the initialization phase, an iterative process, called flight, begins. During each iteration of the flight, each particle updates its speed vector according

to its own past experience (i.e. individual learning) and information from its neighbors (i.e. cultural transmission) using the formula:

$$v_t = \max\left(-v_{\max}, \min\left(v_{\max}, \omega v_{t-1} + \phi_1 c_1 \left(p_p - p_{t-1}\right) + \phi_2 c_2 \left(p_g - p_{t-1}\right)\right)\right) \quad (2)$$

where v_t is the speed of the particle on iteration t, ω is the inertia factor of the particle, p_t is the position of the particle on iteration t, p_p is the best position found by the particle until iteration t, and p_g is the best position found in the neighborhood of the particle until iteration t.

Because the problem landscape is unknown, the importance of individual learning and cultural transmission is unknown. Thus, these factors are weighted by random constants ϕ_i. An undesirable result of this approach is that, without proper control, the particle's trajectory can expand into wider and wider cycles through the problem space, eventually approaching infinity. To prevent this kind of behavior, the speed is bounded by a maximum speed parameter ($v_{\max}$). Using the updated speeds, the positions of the particles are computed with (3) (usually for $\Delta t = 1$ iteration):

$$p_t = p_{t-1} + v_t \Delta t \quad (3)$$

An important aspect when engaging optimization problems with PSO or other nature inspired metaheuristics is the definition of a fitness function to map candidate solutions to rewards. The fitness function we defined for the Thomson problem is a simplified version of (1):

$$F(p) = \sum_{j=1}^{N-1} \sum_{i=j+1}^{N} \frac{1}{d_{ij}^p} \quad (4)$$

where d_{ij}^p denotes the Euclidian distance between point charges i and j encoded by the particle p.

In order to reduce the problem space and to save computation time, the locations of the point charges are encoded in spherical coordinates, omitting the constant sphere radius $r = 1$. Therefore, the distance between two point charges is computed with:

$$d_{ij}^p = \sqrt{2 - 2\left(\cos\left(\phi_i^p\right)\cos\left(\phi_j^p\right) + \sin\left(\phi_i^p\right)\sin\left(\phi_j^p\right)\cos\left(\theta_i^p - \theta_j^p\right)\right)} \quad (5)$$

where $\phi_i^p \in [-\pi, \pi]$ and $\theta_i^p \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ denote the azimuth and elevation angles of the i^{th} point charge according to the solution encoded in the particle p.

3. EXPERIMENTAL RESULTS

The experiments consisted in 10 independent runs performed for system sizes of $N \in \{2,\ldots,50\}$ point charges. In each experiment, the algorithm used a swarm of 50 particles with an inertia factor of $\omega = 0.9$, social and individual learning skills $c_1 = c_2 = 2.05$. The values of these parameters were as recommended in the literature, but fine tuning them may lead to better results. The algorithm performed flights of 500 iterations using global neighborhoods, which means that each particle interacted with all the other particles in the swarm.

The initial experiments were carried out using the `psotb`, a PSO toolbox for Matlab freely available from http://psotoolbox.sourceforge.net/. Although this toolbox provides a highly optimized PSO implementation, it does not implement some of the recent developments in the PSO field, especially the dynamic update of the swarm leader [22]. Due to these limitations, the initial results obtained were not very competitive, especially on large systems. Therefore, we implemented a simplified version of the PSO algorithm, less optimized, but which uses the dynamic update of the swarm leader. The Matlab script for this algorithm is presented in Figure 1. The results reported in Table 1 were obtained with this script.

```
function [fs,s] = pso_thomson(charges, swarmsize, maxiter)
if nargin < 2; swarmsize = 50; end;
if nargin < 3; maxiter = 500; end;
vmax = 0.1; omega = 0.9; chi = 0.729844;
partsize = charges * 2;
x = rand(swarmsize,partsize);
fx = zeros(swarmsize,1);
v = (rand(swarmsize,partsize) * 2 -1) * vmax;
fs = inf;
for i = 1:swarmsize
   fx(i) = fitness(x(i,:));
   if fx(i) < fs
      s = x(i,:);
      fs = fx(i);
   end
end
b = x; fb = fx;
for it = 1:maxiter
   for i = 1:swarmsize
      [fxmin, g] = min(fb);
      v(i,:) = v(i,:) * omega;
      v(i,:) = v(i,:) + rand(1, partsize) .* (b(i,:) - x(i,:));
      v(i,:) = v(i,:) + rand(1, partsize) .* (b(g,:) - x(i,:));
      v(i,:) = v(i,:) * chi;
      v(i,:) = min(vmax, max(-vmax, v(i,:)));
      x(i,:) = x(i,:) + v(i,:);
      x(i,:) = min(1, max(0, x(i,:)));
      fx(i) = fitness(x(i,:));
      if fx(i) < fb(i)
         fb(i) = fx(i);
         b(i,:) = x(i,:);
```

```
         if fb(i) < fs
            s = b(i,:);
            fs = fb(i);
         end
      end
   end
end

function fit = fitness(ind)
fit = 0;
dim = size(ind, 2);
for i = 1:2:dim
   phi1 = 2 * (ind(i) - 0.5) * pi;
   theta1 = (ind(i+1) - 0.5) * pi;
   for j = i+2:2:dim
      phi2 = 2 *(ind(j) - 0.5) * pi;
      theta2 = (ind(j+1) - 0.5) * pi;
      fit = fit + 1/sqrt(2 - 2 * (cos(phi1) * cos(phi2) * cos(theta1-theta2)
+ sin(phi1)*sin(phi2)));
   end
end
```

Fig. 1. – The Matlab implementation of the PSO algorithm used for the Thomson problem.

The minimum energies found with PSO are presented in Table 1. For each system size indicated in the first column, the table presents in the second column the minimum energy of the solution found by PSO. The energy of the presently known ground state for this system size is presented in the third column as reported in [13]. The fourth column presents the average runtime required by PSO on a computer with a Pentium 4 microprocessor running at 3GHz and 512MB RAM. The PSO implementation uses no parallelization techniques, although such features can be added easily. Results from Table 1 indicate that PSO is capable of finding perfect solutions for small systems and approximate solutions for larger systems.

Table 1

Minimum energies found in experiments

N	Energy of solutions found with PSO	Energy of ground states reported in [13]	Average runtime for PSO (s)
2	0.500000000	0.500000000	1
3	1.732050808	1.732050808	1
4	3.674234614	3.674234614	1
5	6.474691495	6.474691495	1
6	9.985281374	9.985281374	1
7	14.452977414	14.452997414	1
8	19.675287861	19.675287861	2
9	25.759986531	25.759986531	2
10	32.716949460	32.716949460	2
11	40.596450549	40.596450510	3
12	49.165253067	49.165253058	3
13	58.853326485	58.853230612	3

14	69.306461333	69.306363297	4
15	80.670617827	80.670244114	4
16	92.917369707	92.911655300	5
17	106.050606097	106.050404829	6
18	120.087059280	120.084467447	6
19	135.096210250	135.089467557	7
20	150.894135172	150.881568334	8
21	167.660869512	167.641622399	9
22	185.320722913	185.287536149	9
23	203.955672783	203.930190663	11
24	223.433627450	223.347074052	11
25	243.856156962	243.812760299	12
26	265.301652244	265.133326317	14
27	287.429529418	287.302615033	14
28	310.648071055	310.491542358	15
29	334.831687736	334.634439920	17
30	359.860169140	359.603945904	18
35	499.019259674	498.569872491	24
40	661.056373164	660.675278835	31
45	846.860299001	846.188401061	40
50	1056.459459680	1055.182314726	51

4. CONCLUSIONS

We have applied a PSO algorithm to estimate the ground states of various instances of the Thomson problem. Preliminary results look very promising, especially because this approach can be extended easily to larger systems, taking advantage of the implicit parallelism of the algorithm. A further investigation of optimal parameters for the PSO algorithm and more problem specific initialization methods are necessary. We expect that PSO will play an important role in finding numerical solutions for this and other related problems in Statistical Physics.

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