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Distinctive Computational Approaches for Solution of Energy Optimization of Particles

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Abstract

The "Thomson problem' is used to determine the minimum energy configuration of electrons on the sphere's surface. We turned this difficulty into an optimization problem, which we addressed with the help of intelligent computational techniques like Particle Swarm Optimization (PSO) and Quantum Particle Swarm Optimization (QPSO). To enhance the system's global searching ability, a Quantum behaved Particle Swarm Optimization algorithm is designed. The Thomson's problem is investigated and appraised, and has fewer parameters to govern, according to simulation data. In this work QPSO is extremely effective and successful at delivering near- optimal results, as we compared the results with Genetic Algorithm and PSO.

Keywords: Thomson's problem optimization, Minimum Energy configuration, Optimization problem, particle swarm optimization (PSO), Quantum particle swarm

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Introduction:

Finding the best way for electrons to spread themselves on a sphere is a well- known and tough problem. The behavior of the system is extremely nonlinear, and structure grows exponentially with the number of electrons. A computer assisted solution for only a few occurrences of minimal energy layouts with smaller N have been rigorously identified. When there are two points, the best configuration is antipodal points. The minimum energy configuration for N=3 is three equidistant spots on a great circle . In the case of four points, the vertices of a regular tetrahedron minimize the energy. Yudin, the vertices of a regular tetrahedron minimize the energy in the case of four points. N. N Andreev gives a way for proving that in the situation of 12 vertices, the regular icosahedron's vertex set provides a solution. Although there are different methods in science and

technology, use of Genetic Algorithm is promising approach to solve combinatorial and other optimization. The population- based algorithm which is most popular is Particle Swarm Optimization by which promising results obtained. Therefore, in the Quantum- behaved Particle Swarm Optimization method is a global convergence guaranteed search strategy that outperforms the PSO. To increase PSO performance, QPSO is proposed by integrating the classical PSO philosophy with quantum mechanics. QPSO is extremely efficient and successful at delivering near- optimal results in a matter of minutes. Next section formulates the mathematical description of Thomson's problem. In section 2, an overview of intelligent computational techniques is presented.

Intelligent Computational Techniques:

Following computational techniques have been used to find the Optimized solution of number of particles

Genetic Algorithms (GA):

Genetic Algorithms (GAs) are named after natural evolution's genetic processes. Holland created it in the mid-1960's, and they have been successfully used as a nonlinear search methodology in huge regions such as, control engineering, the design of neural and fuzzy network, and other science and engineering applications are only a few examples. To search the solution space, GA employs a population, which is basically a collection of chromosomes. There genetic operators, selection, crossover, and mutation are applied to the population during each generation. The least fit members of the preceding population are replaced with created children. The algorithm is repeated until the objective function is optimized satisfactorily. The first version of GA was in binary format. When the variables are continuous, it is more sensible to use floating- points numbers to represent them.

Particle Swarm Optimization (PSO):

Particle swarm optimization is a unique technique to find the minimum energy configuration was developed and utilized. To come up with the best solution each particle is considered as a point in an N-dimensional space that changes its "flying" based on its own and on other particles' s previous experience. Each particle keeps track of its coordinates in the solution space, which are related with the particle's best solution (fitness) so far. Personal best, or best, is the name given to

this number when the particle updates its velocity and position equations after finding the two optimal values.

$$v_k^{i+1} = \varphi v_k^i + \alpha_1 \gamma_{1k}(p_k^i - x_k^i) + +\alpha_2 \gamma_{2k}(g^i - x_k^i) \quad \ldots\ldots \quad (1)$$

$$x_k^{i+1} = x_k^i + v_k^{i+1} \quad \ldots\ldots \quad (2)$$

Where k is the particle index, α_1 is the iteration index, v is the particle' s velocity, x is its position, p is the particle's pbest and g is the gbest. Where$\alpha_1$and α_2 are random values in the range [0,1].

To stochastically, two independent random numbers are employed α_1 and α_2 are the acceleration constant used to scale the contribution of cognitive and social variable, commonly known as learning factors, and is the inertia function in equation (1). The parameter is crucial in defining the type of trajectory followed by the particle. A big inertia weight makes global exploration easier, but a smaller one makes the particle more suited to local exploration. The balancing values are provided by an appropriate selection of inertia weight. According to the results of the experiment, it is preferable to set the inertia to a value at first and then progressively reduce it to reach the refined solution. The particle reached to the next position after the velocity is applied for a specific time- step. The alternation of a particle' s seeking point is shown in **fig 1.**

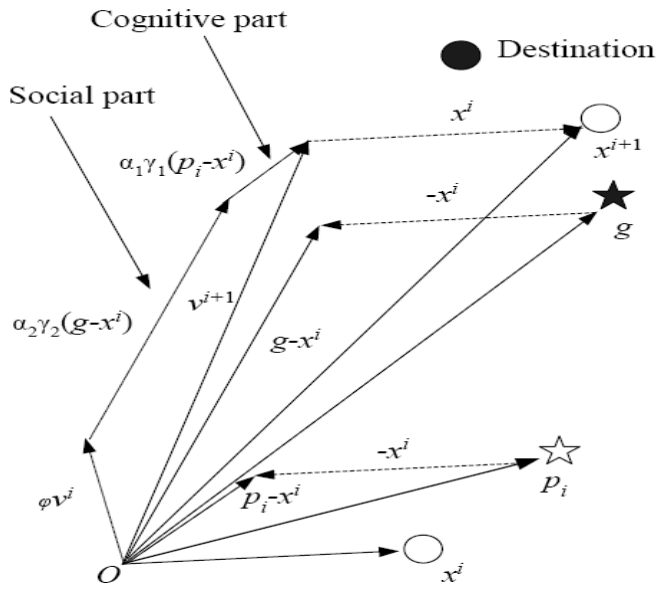

Figure 1: x_i is the current position, and x_{i+1} is the modified position. v_i is the current velocity, and v_{i+1} is modified Velocity

Since its inception, the particle optimization has gone through various stages of development and adjustments. Several researchers examined and updated the method to tackle problems in a variety of scientific and technological domains [7, 8]. Following continuous, Kennedy and Eberhart created a binary PSO [9] PSO and a neural selection mechanism, such as GAs are combined in a hybrid PSO [10, 11]. Only the gbest in PSO shares information with others. In contrast to GA, all particles in PSO tend to converge fast on the optimum solution PSO, on the other hand, has a lot in common with GA. Both PSO and GA begin with population that are generated at random. Both have fitness values that can be used to assess the populations. Random approaches are used to refresh the population and look for the best solution.

The fundamental drawback of traditional PSO is that global convergence is not guaranteed . A detailed mathematical concept and parameter control mechanism for the QPSO have also been developed. QPSO is one of the novel quantum mechanics- based optimization approaches. Each particle in the QPSO has quantum behavior. The results are much Optimized as compared to PSO and GA.

Quantum Particle Swarm Optimization (QPSO):

Only the likelihood of the particle appearing in position x can be determined using the probability density function, whose shape is determined by potential field in which the particles is located. The particles travel in accordance with the iterative equation (3).

$$x_k^{i+1} = \begin{cases} P_k^i + \beta \left| M_{best} - x_k^{i+1} \right| \ln(1/u) & if \;\; k > 0.5 \\ \\ P_k^i - \beta \left| M_{best} - x_k^{i+1} \right| \ln(1/u) & if \;\; k < 0.5 \end{cases} \qquad \ldots\ldots \; \ldots\ldots \qquad (3)$$

Where u and k are random values distributed uniformly in the range [0, 1], this is known as the expansion- contraction coefficient, and it regulate the particle's convergence speed. This is known as the contraction-expansion coefficient, and it can regulate the particle's convergence speed. The mean best values found by using the equation (4).

$$M_{best} = \frac{1}{N} \sum_{i=1}^{N} p_k^i \qquad \ldots\ldots\ldots\ldots\ldots\ldots \qquad (4)$$

for $i = 1 : iterations$
  for $k = 1 : K$
    Evaluate fitness function for k^{th} row of X
    if $(fitness(\mathbf{x}_k)) < fitness(\mathbf{p}_k)$
      $\mathbf{p}_k = \mathbf{x}_k$
  end
  if $\left(fitness(\mathbf{p}_k) \right) < fitness(\mathbf{g})$
  $\mathbf{g} = \mathbf{w}_{arg \min_{1 \le k \le S} (fitness(\mathbf{p}_k))}$
  update $\mathbf{x}$ and $\Delta\mathbf{x}$ using equations (1) and (2)
end
$\mathbf{g}$ is the solution

Figure 2. General matlab algorithm

Experiment:

System Model

Obviously, each two electrons have repelled each other with a force given below in formula and formed spherical shells is

$$F = \frac{1}{4\pi\varepsilon_0}\frac{q_e^2}{r^2} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

Where, ε_0 is the electric constant of vacuum, q_e is the charge on a single electron, and r is the distance between the two electrons. Due to these forces, each electron will strive to go far away from the others as possible. However, because they are constrained to the sphere's surface, they will optimize for a system configuration with the least amount of potential energy. For a system with N electrons, the energy is,

$$U(s) = \frac{q_e^2}{4\pi\varepsilon_0}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{1}{d_{ij}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (6)$$

Where d_{ij} is the distance between electrons i^{th} and j^{th} in the system configuration S. Any configuration with minimum potential energy is called a "ground state" of the system.

$$d_{ij} = \sqrt{2 - 2[\cos\phi_i \cos\phi_j + \sin\phi_i \sin\phi_j \cos(\theta_i - \theta_j)]} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

where $\phi_{i,} \in [-\pi/2, \pi/2]$, is the azimuth angle and $\theta_j, \theta_j \in [-\pi, \pi]$ is the elevation angle. Thus, PSO particles move in $[0,1]^{2N}$ and the location $x \in [0,1]$ of a particle decodes into a system configuration with:

$$\begin{aligned} \phi_i &= 2\pi x_{2i-1} - \pi \\ \theta_i &= \pi x_{2i} - \pi/2 \end{aligned} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (8)$$

Results and Discussions:

The studies consisted of ten separate runs with system sizes of N point charges. The method used a swarm of 50 particles in each trail, as well as social and individual learning skills 12=C=2.05.

The value of the parameter was as advised in the literature, although fine adjusting it could result in better out comes. The initial trail was done with PSObest, a free PSO toolbox for Matlab that can be found at http: psotoolbox.sourceforge.net/. With this script, the results in Table 1 were achieved. The average runtime required by all techniques on a machine with a Pentium 4 microprocessor running at 3 GHz and 512MB RAM (Random Access Memory) is shown in the fourth column**.**

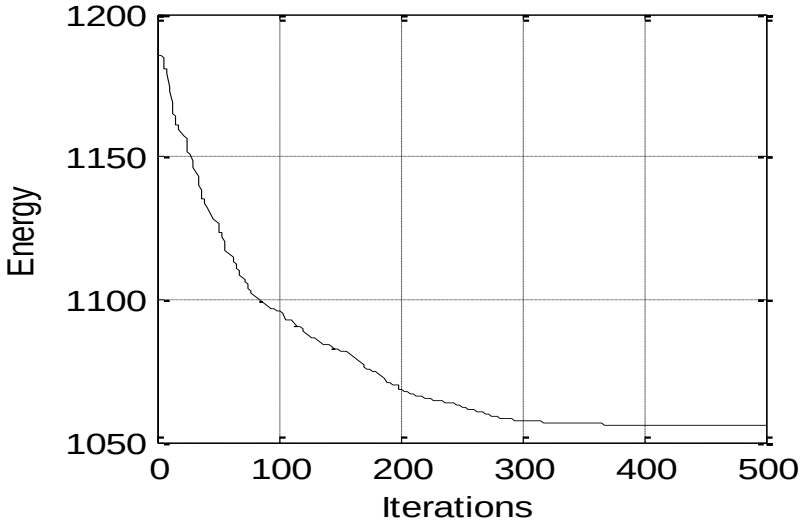

Figure 2: Minimum Energies found with number of iterations.

Table 1. Minimum Energies found in simulations.

Iteration	**Energy solutions found with GA**	**Energy solutions found with PSO**	**Energy found by QPSO**	**Energy of ground states reported in [15, 16]**
2	0.50000000	0.50000000	0.500000000	0.500000000
3	1.73205708	1.732050808	1.732050808	1.732050808
4	3.67426527	3.674234614	3.674234614	3.674234614
5	6.47742357	6.474691495	6.474691495	6.474691495

6	9.98563494	9.985281374	9.985281374	9.985281374
7	14.4579365	14.452997414	14.45297741	14.452997414
8	19.6933923	19.675287861	19.67528786	19.675287861
9	25.7841371	25.759986531	25.75998653	25.759986531
10	32.7459927	40.596450549	32.71694946	32.716949460
11	40.6137292	40.596450549	40.59645051	40.596450510
12	49.3960962	49.165253067	49.16525306	49.165253058
13	58.9555378	58.853326485	58.85325241	58.853230612
14	69.4043658	69.306461333	69.30636330	69.306363297
15	80.7273665	80.670617827	80.67024413	80.670244114
16	93.0505831	92.917369707	92.91165640	92.911655300
17	106.192773	106.050606097	106.0504118	106.050404829
18	120.379950	120.087059280	120.0845281	120.084467447

19	135.248331	135.096210250	135.0898471	35.089467557
20	151.107682	150.894135172	150.8821874	150.881568334
21	167.879864	167.660869512	167.6417572	167.641622399
22	185.671837	185.320722913	185.2887766	185.287536149
23	204.269089	203.955672783	203.9410667	203.930190663
24	223.925889	223.433627450	223.3488802	223.347074052
25	244.236818	243.856156962	243.8135930	243.812760299
26	265.610747	265.301652244	265.1345905	265.133326317
27	287.866900	287.429529418	287.3049550	287.302615033
28	310.993947	310.648071055	310.5054477	310.491542358
29	335.096314	334.831687736	334.6401816	334.634439920
30	360.396697	359.860169140	359.6266774	359.603945904

35	499.876013	499.019259674	498.6226150	498.569872491
40	662.434294	661.056373164	660.9162530	660.675278835
45	848.813056	846.860299001	846.7600190	846.188401061
50	1059.148465	1056.45945968	1055.630892	1055.68231472

Conclusion:

To estimate the ground state of several cases of the Thomson problem, we used a GA, PSO, and QPSO algorithm. Preliminary results are promising, especially because this approach may readily be scaled up to bigger systems because to the algorithm's underlying correspondence. More research into the ideal setting for the PSO algorithm, as well as more problem- specific initialization methods, is required. We predicted that QPSO will play a key role in discovering numerical solutions to this and other Statistical physics problems. Because the results we have obtained using QPSO are extremely superior.

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