EVOLUTIONARY COMPUTATION HYBRIDS WITH MONTE CARLO METHOD FOR DIFFERENTIAL EQUATION

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Abstract. This article uses the hybrids between the evolutionary method and Monte Carlo method to solve the differential equation, for example in this article, the Schrodinger equation for atom

1. Introduction

The most common method of Monte Carlo [1] to solve the differential equation is to solve it apparently and algebraically first, and calculates the integration of the solution by Monte Carlo method. Hence Monte Carlo Method is not really to solve the equation directly, instead, it only calculates the solution in the form of integration. The real method for solving equation has not been born. This article explores this kind of real methods in two ways: fitness method and "delta recursive substitution".

2. The Character of Evolution

The character of evolution in probabilities method is recursive substitution and the divergent computation is meaningless. A evolution in computer is always a Markov Process that's described by a Transient Probabilities Matrix: M. The distribution of probabilities of all possible population (S_n) of n-th generation is like this way:

$$S_{n+1} = S_n M$$

The convergence of infinite generation is A that

$$A = AM$$

It's a stable distribution of probabilities. By easy math

$$A = A_0 \lim_{n\to\infty} M^n$$

When M has a character like e^{ia}, with a not zero, the evolution is divergent and the distribution of probabilities resembles a fluctuation, which is meaningless because even successive generations have great difference on population's probability. In this point of view, an evolution is a recursive substitution of the Transient Probabilities Matrix. We can analogs a differential equation to an evolution and hope to solve it by probabilities.

Key words and phrases. Schordinger equation, Monte Carlo Method, Evolutionary Computation.

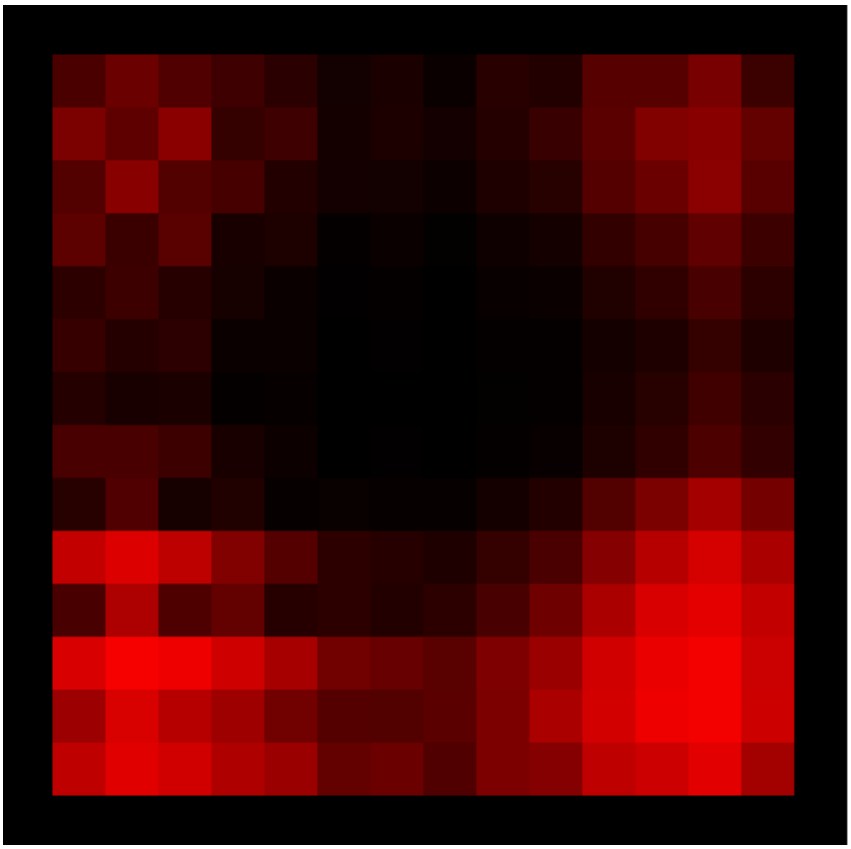

FIGURE 1. a slice of the field, brighter means greater R

3. Evolution and equation—-fitness methods

The Schrodinger equation for atom is considered

$$-iF_t = k\nabla^2 F - QF/r$$

It's derived from the Least Energy Principle that

$$E = \nabla F \cdot \nabla F^* + QFF^*/r$$

keeps the least of its sum. The real part of F:R also has the same

$$E = \nabla R \cdot \nabla R + QRR/r$$

We try to compose a program to implements this logics—randomly alters the R between a pair of point, but keeps the square sum of the two R constant, then keeps for the next evolution the one with less fitness E.

The program operates on a 16x16x16 cube with its border having zero values of R. A figure that describe the data of convergent R is like the following figures 1,2

We can guess the symmetry of the solution is the symmetry of a cube (border). The most frequented points are near the eight corners of the cube.

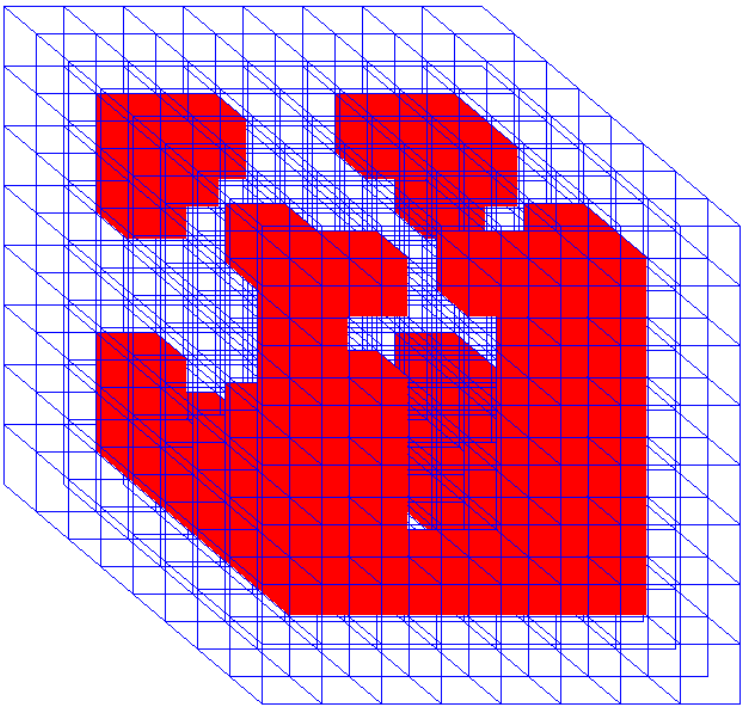

FIGURE 2. the whole fields in binary values

4. Evolution and equation—-re-substitution methods

The Schrodinger equation for atom is considered

$$-iF_t = k\nabla^2 F - QF/r$$

We needs the stable solution of it

$$F_t = iEF$$

A real solution is obtained

$$R = k\nabla^2 R - QR/r$$

By solving the operator

$$R = k\nabla^2 R + G$$

An equation is obtained

$$R = C(e^{-k/r}) * (R/r)$$

Now it's easy to constructs algorithm for this equation: obviously, it's a recursive algorithm. But there is one more skill necessary to operates on:
1) Choosing a point randomly on a 16x16x16 cube (with the charge in the center of it) , which point's value is taken as a Dirac function supported by the point. Then the equation is simpler than ever to be calculated. In fact the right part is a distribution, according to which statistic a point is chosen randomly by the method of Russian Roullete.
2) The chosen point is re-substituted to the step 1.

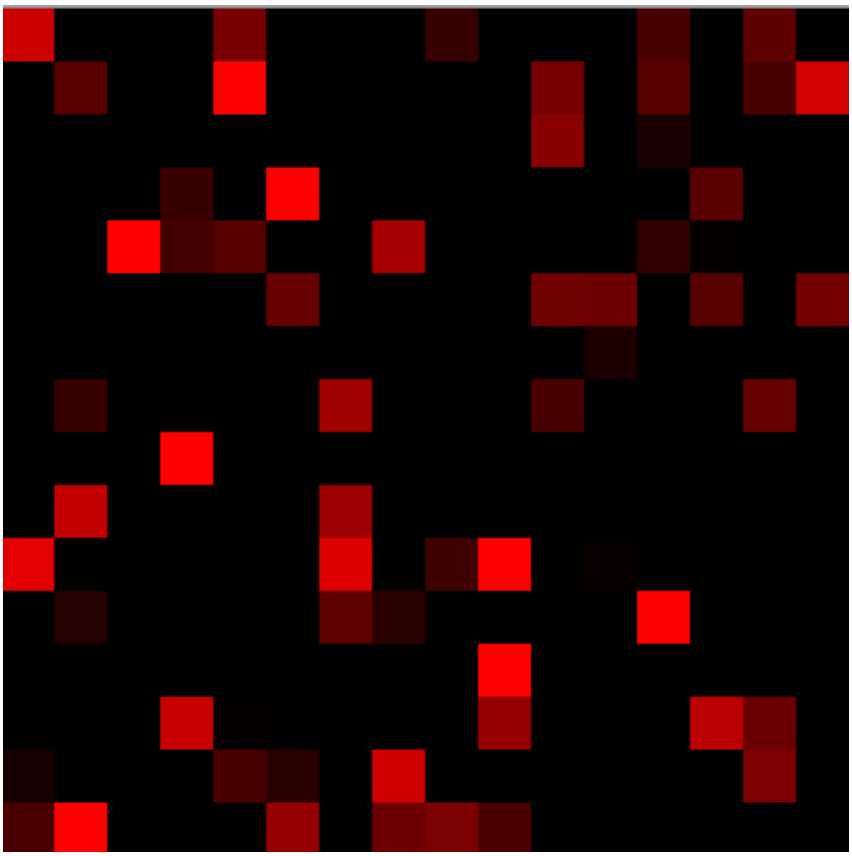

FIGURE 3. a slice of the fields

3) Every chosen point is added on to the scores S for each point.
The result is

$$R + C' = S$$

The program is similar to the one above and is omitted here. The figure of the solution of the field is like the following figures 3,4.

From the figures we can get a strong impression that it's very much like a d track of electrons outside of nuclei, because it has so many horns in each plane (5 or so) and the picture in the slice is completely a branch of tracks in x-y plane with a little tilt.

5. Conclusion

By the demonstration above the hybrid between evolution and Monte Carlo methods is powerful. The algorithm above is simple, but it's effective because the two computations in personal computer have run 10000000 loops in 8-12 seconds each to output satisfactory results.

It's hopeful to look to this method for solving complex molecules or nucleons

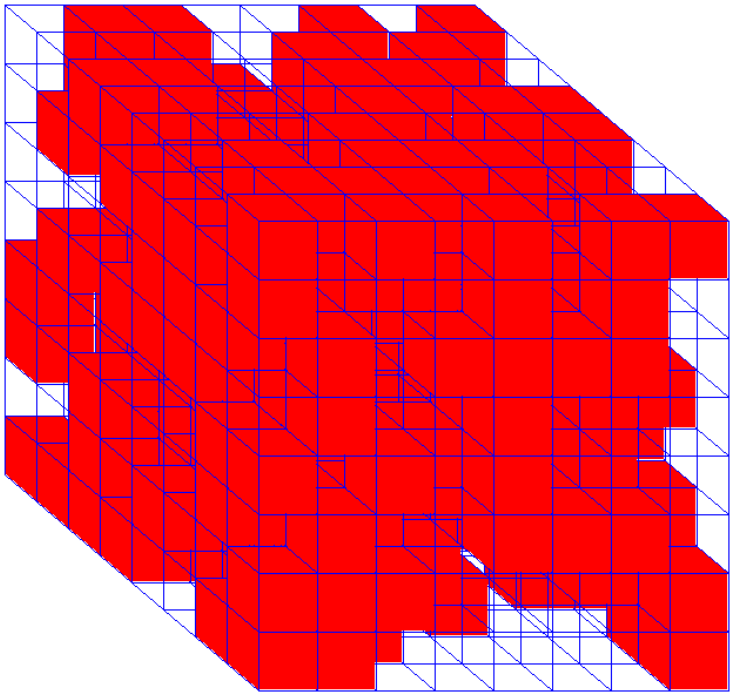

FIGURE 4. the whole field in binary value

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[1] Berg, Bernd A. (2004). Markov Chain Monte Carlo Simulations and Their Statistical Analysis (With Web-Based Fortran Code). Hackensack, NJ: World Scientific. ISBN 9812389350.

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