Genetic Algorithms and Solutions of an Interesting Differential Equation
Real World Applications Track

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ABSTRACT
The Schrodinger equation is a second order differential equation that describes and governs many real world systems of interest. Analytical techniques are sufficient to solve this equation for some simple systems, and numerical techniques can provide adequate approximate solutions for somewhat more complex problems. However, attempts to use numerical techniques for yet more complex systems, some of great interest, have proven to be beyond the capabilities of conventional computing resources. Computational intelligence techniques have been applied in some approaches to addressing this problem. This paper reports an approach to using genetic algorithms with "mixed" analytical wave functions, to solve the Schrodinger equation.

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1. INTRODUCTION
Schrodinger's equation is a second order partial differential equation that sits at the heart of quantum mechanics [9]. Its solutions describe and govern many systems of interest in physics, chemistry, finance and biology. Closed form analytical solutions of this equation are known for some simple systems. More complicated systems require more complicated versions of the equation. For systems without known closed form analytical solutions other approaches are used. These approaches are based on simplifying assumptions regarding the equation itself and/or the use of numerical methods for solving the equation. Extensive work on both of these approaches has been done, and substantial and useful results have been obtained [8]. Yet even these innovations have not been sufficient to obtain usable solutions to

Schrodinger's equation for many systems of great interest. Would it be possible to formulate it, protein folding might be such a system [1].

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Accordingly, it seems useful to enquire into other approaches that might contribute to making the solution of this equation more computationally feasible. Computational intelligence techniques might be considered, separately or in combination. An incremental approach to such a development effort seems prudent, and might start by applying a single CI technique to multiple versions of the problem (multiple systems), beginning with very simple systems and working up to more complicated systems.

Genetic algorithms and genetic programming have already been applied to the solution of differential equations. Koza [6] demonstrated the use of genetic programming to solve differential equations. In celestial mechanics Bello-Mora *et al.* [2] used genetic algorithms to explore the solution space for weak stability boundary transfer orbits. Howard and Roberts [5] presented a method for the challenge of solving the steady state convection-diffusion equations directly as an alternative to the imperfect and ad-hoc methods of today: weighted residual methods (Petrov-Galerkin finite elements, upwind finite differences, etc.) by means of genetic programming; Howard and Kolibal [4] later advanced an alternative approach that combined stochastic interpolation and genetic programming, and which offered more generality and the potential for the solution of 2D and 3D convection-diffusion equations and Navier-Stokes equations with arbitrary boundary conditions. With both methods they discovered a type of "GA deceptive problem" [3] concerning high Peclet numbers.

This paper reports an approach to using genetic algorithms with "mixed" analytical wave functions, for Schrodinger's equation.

2. APPROACH ALTERNATIVES
We may distinguish three paths to solution of the equation of interest:

1. Attempts to directly solve the (un-simplified) equation, with closed form (but possibly approximate) analytic solutions;

2. Attempts to solve versions of the equation that have been subjected to simplifying assumptions; and

3. Attempts to apply numerical techniques to either the un-simplified equation, or to versions of the equation that have been subjected to simplifying assumptions.

Any of theses approaches might possibly be rendered more computationally feasible by the application of CI techniques.

It would be tempting to try to estimate the computational efficiency of any of these approaches by applying them to small-

scale systems followed by scaling the results up to large scale systems. However, the convergence of techniques such as genetic algorithms is difficult to predict, so estimates of scale-up are unreliable or need to be investigated.

Similarly, we might try to compare the computational demands of a CI approach with those of a traditional numerical approach for simple systems, determining which was the more computationally efficient. However, given the difficulty of forecasting the convergence of both CI techniques and traditional numerical techniques when applied to very complicated problems, this approach seems futile. At best, mathematical numerical analysis will only yield error estimates which indicate orders of convergence that are bound by unknown constants. It seems that we must try out the CI techniques in order to determine their effectiveness.

3. A GENETIC ALGORITHM SOLUTION OF THE SCHRODINGER EQUATION

3.1 Formulation and Representation

Solutions consist of complex-valued functions of position called ψ, the wave function, and E, a corresponding real-valued eigenvalue. It is tempting to try to use the GA to directly estimate numerical values of ψ and E. E is a single value, and ψ could be approximated by its value at a grid of points [7]. We note that this representation would allow the wave function to take dramatically different values at adjacent points, with the potential for dramatically different values of the (approximated) second derivative of ψ at some of those points. However, the Schrodinger equation itself constrains the value of the second derivative. For lower energy solutions, we expect low values of the second derivative. We seek to use this constraint to reduce computational demands by avoiding computations that allow excessive values for the second derivative of the wave function.

How then can we represent the potential solutions for the GA? The ψ functions could be represented by analytical functions, such as sine and, cosines, and/or exponentials, and/or Laguerre polynomials, etc., or as sums of analytic functions. The use of analytic functions to represent ψ has the great advantages of (1) in limiting the magnitude of the second derivative (smoothly varying functions) and (2) in reducing the computational load that is requires to compute the fitness.

3.2 Solution Approach

This representation would allow the wave function to take dramatically different values at adjacent points, which is physically excluded for many interesting problems. Solutions of the Schrodinger equation are defined in terms of sets of basis functions (sets of basis vectors). "Good" sets of basis functions facilitate solution, while less appropriate sets hinder solution. Where exact analytic solutions are known, the appropriate sets of basis vectors are also well known [9].

What constitutes appropriate sets for problems without known analytic solutions? In particular, for molecules and for atoms more complicated than hydrogen (which has a known analytic solution), what then are the appropriate sets? The Linear Combination of Atomic Orbitals (LCAO) approach is widely used. Wave functions for single electrons centered on individual nuclei constitute the basis set. These wave functions might be, for example, the analytically derived solutions for hydrogen-like atoms (called Slater-type orbitals). Alternatively, the selection of these basis functions may be based more on computational efficiency rather than on a physical motivation. Gaussian orbitals are a widely used example of such basis functions [8].

The following solution approach is proposed. Create prospective approximate basis sets from combinations of finite subsets of analytically derived solutions from various problems, and computationally motivated basis sets also. For example, truncate the (infinite) set of solution functions from a variety of problems (e.g., hydrogen atom, infinite potential well, varieties of finite potential well, etc.) to finite subsets, and merge those subsets. Add a (finite) subset of Gaussian functions to this merged set. In attempting solutions to the Schrodinger equation the GA will use the resulting set, here termed "mixed set".

First efforts to use these sets must be on problems with known solutions as this enables validation of the approach by a comparison with the known analytical solutions. This also facilitates numerical experiments with regard to the minimum sizes and compositions of the mixed sets. Experiments on problems without known analytical solutions follow. These would start with more complicated (than hydrogen-line) atoms and with simple molecules.

4. REFERENCES

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