GENERALIZED INTELLIGENT BEHAVIOR AND EVENT RECOGNITION METHOD FOR NUCLEAR ENGINEERING APPLICATIONS

An Undergraduate Research Scholars Thesis

by

ZACHARY HARDY

Submitted to the Undergraduate Research Scholars program at
Texas A&M University
in partial fulfillment of the requirements for the designation as an

UNDERGRADUATE RESEARCH SCHOLAR

Approved by Research Advisor: Dr. Pavel Tsvetkov

May 2017

Major: Nuclear Engineering

TABLE OF CONTENTS

ABSTRACT

Generalized Intelligent Behavior and Event Recognition Method for Nuclear Engineering Applications

Zachary Hardy
Department of Nuclear Engineering
Texas A&M University

Research Advisor: Dr. Pavel Tsvetkov
Department of Nuclear Engineering
Texas A&M University

In many fields of engineering it is desirable, and often required, to identify certain characteristics of processes, properties, and systems. This effort focuses on the development and demonstration of an intelligent behavior and event recognition method. Using a black-box approach, the method was generalized and applied to several different applications as proof of concept. Quantum mechanics, nuclear supply chain management, and nuclear composition characterization problems were considered. The method utilized data synthesis and genetic algorithms, an artificial intelligence method, to achieve the desired results. This will allow the user to have a single optimization tool which can be applied to a diverse problem set.

ACKNOWLEDGEMENTS

I would like to thank my research advisor, Dr. Pavel Tsvetkov, for the opportunities he has given me and his continued support and guidance throughout this process.

NOMENCLATURE

GA	Genetic Algorithms
QM	Quantum Mechanics

CHAPTER I

INTRODUCTION

There are many tools available when solving an optimization problem. However, in many cases, these tools have a small scope of application types. Further, the computational cost must be considered based on the level of accuracy needed in the solution. It is desirable to have a tool which can handle most types of problems in a computationally efficient manner, while still yielding a relatively high degree of accuracy. This paper will outline the development of a generalized method using genetic algorithms (GA) to solve a diverse problem set.

Theory:

Heuristic Methods:

Arriving at exact solutions to optimization problems can often be computationally very expensive requiring large amounts of both memory and time. Heuristic methods are much more time efficient, but come at a cost in accuracy and quality assurance. Heuristic methods often model natural processes such as natural selection [6].

Genetic Algorithms:

A GA is a stochastic optimization tool used for high-dimensional, multimodal, nonlinear, discontinuous, or nondifferentiable problems. They require little knowledge of a system. There are two requirements for a problem to be posed by a GA. Solutions must be composed of multiple components, known as a genetic formulation and there must be some objective function which can give information on the accuracy of a solution. GAs do not require the gradient of the mathematical model to be continuous or smooth, which vastly expands the scope of applicability of the algorithm. The following section will outline the implementation of a GA.

Evolution:

Per Charles Darwin's principle of natural selection, the strongest, or most fit, individuals within a population will survive the adversity presented in an ecosystem and reproduce passing their genetics onto their offspring in the subsequent generation. In a GA, a series of solutions in the solution domain (population) is generated with random values for each parameter (chromosome). These solutions are then ranked based on their fitness to some criteria set in the objective function. The more fit solutions are selected to create offspring in which they pass on their genetic material. By mixing strong genetic material, the algorithm is able to increase its level of accuracy. This process is repeated until some criteria is met or a specified number of generations is reached. Each step will be discussed in more detail in the following sections.

Initialization:

The initialization step of a GA arbitrarily generates a set of solutions in the solution space using Monte Carlo methods. This set forms the initial population which progresses through the fitness evaluation, ranking and selection, and into the mating process.

Selection:

The selection process involves the fitness evaluation of each solution with the objective function and subsequent ranking by fitness. Selection can be accomplished using any number of methods. Two popular methods are fixed and tournament selection. In fixed selection, a fixed percentage of the top solution are kept and the rest discarded. In tournament selection, two solutions are paired together randomly. The top solution is kept and the bottom discarded. Using this method, a larger genetic pool is maintained.

Crossover and Mutation:

Crossover and mutation make up the mating phase. In this phase two solutions pass their parameter values on to offspring solutions to improve accuracy. A population of the same size as the initial population is bred to replace the initial population. Crossover can be achieved in any number of ways. Two important crossover methods are per parameter and pivot crossover. Per parameter crossover is typically applied to problems with continuous domains. In this method, a random number generator coupled with assigned probabilities for each parent determines which chromosomes are passed on to the child solution. Weights are assigned to favor the more fit solutions. Pivot crossover is typical in discretized problems with a finite number of potential solutions which can be represented by binary strings. In this method, a pivot point is randomly selected and all chromosomes past it are swapped. This generates two child solutions.

Mutation plays a key role in ensuring that the GA does not converge early on a local optimum. By adding in new, random parameter values throughout the breeding process, the spread in the solution domain being searched can be widely expanded. Mutation is typically carried out probabilistically per parameter. Either a new chromosome value is generated randomly, or a bit is swapped in the binary string, creating a new solution.

In some cases, it may be necessary to have adaptive crossover and mutation rates. This can help further help the algorithm avoid early convergence on a local optimum. By having these adaptive rates, as the solution begins to converge, mutation probabilities can be increased to allow the solution to spread out over the solution space. With this, care must be taken to ensure that the best solutions are not lost. Safeguards must be built into algorithms using this method to combat the algorithm losing the true solution.

Convergence:

A GA iterates the previously described processes a number of times, generating a number of generations. With each generation, the solution parameters are mixed together, making the overall fitness of the population greater. As it nears a global optimum, the spread of the population should converge towards that optimum point. The GA is terminated when an optimization criteria – desired fitness level – is met or a certain number of generations is completed.

Parameter Tuning:

One of the challenges that face genetic algorithms is finding the correct algorithm parameters (population size, crossover method, crossover rate, mutation rate, etc.) to use for different applications of GA. Tuning these parameters to fit each application can become a tedious task because there is no definite method to determine ideal parameters. Tuning can be done iteratively or non-iteratively by random sampling and checking parameters.

Objectives:

This project aims to develop a nondestructive method to characterize nuclide composition by using artificial intelligence methods such as genetic algorithms.

Strategy:

The development of a basic, functional genetic algorithm outlined in the Harrison text will be the first step to solve a quantum mechanics (QM) problem [3]. Following this, the three cases will be mathematical formulated and then each problem parametrized. The computational method will then be integrated into the algorithm and finally, evaluated for viability and performance on several simplified examples.

CHAPTER II

QUANTUM MECHANICS OPTIMIZATION

This chapter will give a brief overview of the QM background relevant to this application, a problem description, the implementation of a GA to the problem, and the results achieved. The GA and problem were derived from the Harrison text and the results will be compared to those of those presented [1].

Background & Problem Description:

The fundamental concept of QM is that a system can be fully described by a wave-function. A wave-function can be a single function, or a linear combination of many, as shown in Eq. 1, where a_i represents a coefficient and ψ_i represents a basis state wave-function.

$$\psi = \sum_{i=1}^{k} a_i \psi_i \qquad \text{(Eq. 1)}$$

Wave-functions which are composed of a linear combination of several, are systems in a state of superposition, in which the system is said to be in all those states simultaneously. The square of each coefficient represents the probability of measuring the system in the corresponding state. Because of this, the coefficients must be between -1 and 1 and the sum of their squares must equal 1.

Due to the nature of QM, exact values for physical characteristics cannot be acquired, only expected values. Physical characteristics, such as energy, momentum, or position are extracted from the wave-function by applying operators. The energy operator applied to the wave function is shown in Eq. 2,

$$(\mathcal{H} + V(z))\,\psi = E\psi \qquad \text{(Eq. 2)}$$

Where $\mathcal{H}$ is the Hamiltonian operator, V(z) is the potential function, and E is a constant representing the expected energy of the system. Eq. 3 shows the definition of the Hamiltonian operator.

$$\mathcal{H} = -\frac{\hbar}{2m}\frac{\partial^2}{\partial z^2} \qquad \text{(Eq. 3)}$$

This method seeks to find the ground state wave-function and associated energy of an electron in a parabolic potential. By definition, ground state is the minimum energy a system can have. In approaching this eigenvalue problem, there is one more unknown than the number of basis states in the wave-function – each wave-function's coefficient and the energy eigenvalue. This method will avoid the computationally expensive and mathematically more intricate processes seen in using matrix methods or quantum perturbation theory to solve this problem and use a GA to obtain accurate results in a short amount of time.

Mathematical Formulation & Implementation:

To achieve the desired results of this minimization problem, a basis wave-function, shown in Eq. 4, was chosen and the coefficients, a_i, were taken as the parameters to be the genetic representation of the problem. Four basis states were used in the GA.

$$\psi_i = a_i\sqrt{\frac{2}{L}}\sin\left(\frac{i\pi z}{L}\right) \qquad \text{(Eq. 4)}$$

The fitness of each function was checked by applying the Hamiltonian operator, shown in Eq. 3, to the wave-function. The Hamiltonian operator was applied by multiplying the complex conjugate of the wave function, $\psi*$ to Eq. 2. After this, the expected energy, E was isolated and the opposite side of the equation was integrated over all space, shown in Eq. 5.

$$< E > = \frac{\int \psi^* \mathcal{H} \psi \, dz}{\int \psi^* \psi \, dz} \qquad \text{(Eq. 5)}$$

Random sampling was used to generate an initial population which was then checked and ranked by the fitness function. Numerical methods were used for the fitness evaluation because it contained both derivatives and integrals. To do this, the shooting method was used. In the shooting method, the algebraic expansion of the second derivative, given in Eq. 6, was used to carry out a numerical integration.

$$\frac{d^2\psi}{dz^2} = \frac{\psi(z+dz)-2\psi(z)+\psi(z-dz)}{(dz)^2} \quad \text{(Eq. 6)}$$

In this method, the wave-function was initialized at 0 with a defined step length. Each integral was performed separately over all space. The quotient of the integrals was found yielding the expected energy [1].

Once the pilot population was generated, and each solution was evaluated for fitness, ranked, and paired. The algorithm used a basic probabilistic crossover and mutation process in which there is the largest probability of the child getting the more fit parent's gene, followed by the lesser fit, with a small mutation probability incorporated.

Results & Discussion:

This algorithm was written in MATLAB modeled after the one presented in the Harrison text written in C++. The algorithm parameters used to yield the results presented below are listed in Table 1. These closely mimicked those from the text, except for the crossover and mutation probabilities. The fitter parent probability was increased by ten percent and the less fit probability decreased by twenty percent with a ten percent mutation probability added.

Upon comparison to the results of the GA presented in the text, the developed GA achieved better results using weighted crossover probabilities and mutation probabilities. The results are shown in Table 2.

Table 1: Algorithm parameters.

Parameter	**Value**
# of Basis States	4
Solutions per Generation	100
# of Generations	3
Fitter Parent Crossover Probability	60%
Less Fit Parent Crossover Probability	30%
Mutation Probability	10%

Table 2: Comparison of GA performance [1].

Generation	**$E_{Harrison}$ (meV)**	**E (meV)**	**% Difference**
1	9.366462	8.420066	-10.10%
2	7.512481	7.449304	-6.32%
3	7.512481	6.983623	-7.04%

From comparison, it was evident that the GA which used a bias and mutation performed better than that of the text, yielding a lower expected energy in each generation. Upon convergence, the GA converged at roughly 6.9576 meV after ten generations, just below the 6.983623 meV achieved after just three generations, shown in Figure 1. This was indicative of the level of accuracy that can be achieved with a small amount of computation time. The bulk of the runtime spent was spent in making small refinements to the solution to increase accuracy.

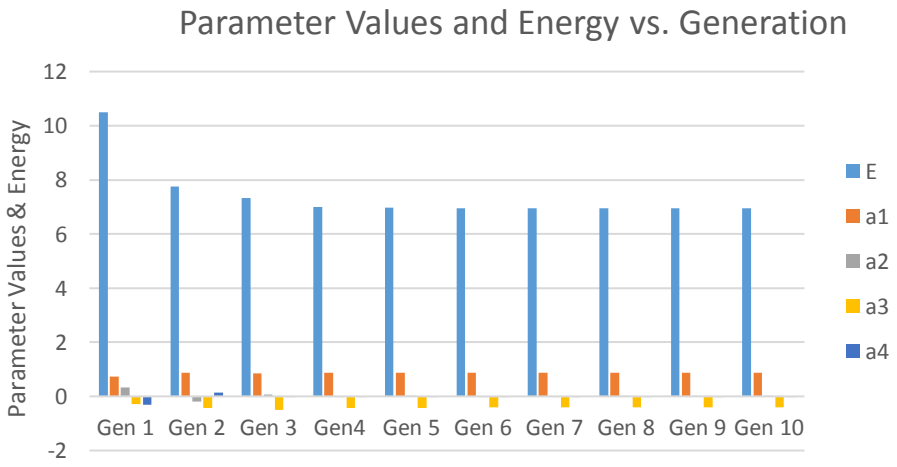

Figure 1: Plot of optimization parameters and associated fitness levels for 10 generations.

By using GAs, the wave-function of an electron in a parabolic potential well. This was done by using the Hamiltonian operator as the objective function to minimize. Generally, to solve this type of problem, quantum perturbation theory or matrix methods, which feature much more complex mathematics than the GAs are needed. Using a GA, these methods were avoided and a reasonable answer was found in a relatively short amount of time. If this problem was for a two or three-dimensional case, the number of unknowns increases by a factor of n for each dimension. Computational savings can be more apparent for these types of problems. The GA developed to solve this one-dimensional QM problem achieved an accurate result in a short amount of time and avoided vastly more complex methods at reaching a similar result.

CHAPTER III

NUCLEAR SUPPLY CHAIN OPTIMIZATION

This chapter will address the development of a method for optimization of a supply chain for a nuclear reactor. It will discuss necessary background information, the problem statement, and the data collection method. The mathematical formulation and implementation will be presented next followed by the results and discussion on the method. The results obtained are simply a proof of concept. Further development would be used by a company with sufficient industry data.

Background & Problem Description:

For any engineering product, without a supply chain, the product cannot be successful. Without a good supply chain, the materials to create a product cannot reach an assembly site and the finished product cannot be distributed to be used by consumers. This is especially true for a nuclear power plant because of the already high operation costs. Without an economic supply chain, the construction and operation of a nuclear power plant could become unfeasible.

The goal of this application is to aid in the decision-making process for a global supply chain. Because of limitations on the available supplier and transporter data, the focus will be to produce region specific data which could give some indication of the best transportation method and to show that the algorithm will converge using a simple road shipping model.

Data Collection Method:

The data collected for this application was found from two sources, World Energy Outlook 2012 [8] and the CIA World Factbook [9]. The World Energy Outlook 2012 gave

information such as the number of nuclear power plants in 2012 versus the expected number in 2035 in which the percent expected growth can be determined. This gave a good estimate of how for or against nuclear power a country may be and was a good representation the amount of resources that will be tied up in construction the near future. This data is presented in Table 3. The CIA World Factbook provided infrastructure and geographic data which could aid in determining the best transportation mode and supplier in different regions of the world.

Table 3: Nuclear infrastructure data [8].

Region	**Number of NPP (2011)**	**Number of NPP (2035)**	**% Growth**
India	4	30	650.00%
Russia	22	39	77.27%
European Union	130	118	-9.23%
China	16	130	712.50%
U.S.A.	100	124	24.00%
Pakistan	4	8	100.00%
Brazil	2	6	200.00%
Argentina	3	5	66.67%
Canada	19	21	10.53%

Another dataset of interest was that of transportation infrastructure, both water and land. Quantifying the number of seaports in a country gave a good indication of the feasibility of using an international supplier. The number of river ports gave information on whether barging would be a feasible primary transportation mode or not. In looking at waterways, roadways, and railways, it was important to look at the length per area so that different country's infrastructures could be compared on a normalized scale. For instance, the United States of America is a larger country by area than the European Union and has more total roadway length. However, when

comparing roadway density in the two regions, the European Union's roads are about twice as dense as those in the United States. Below in Table 4 and Table 5 is the data for water and land transportation. Although this data was not directly applied to the model in the next section, it allows any users to incorporate it into their models to give a good first approximation on what transportation modes will be better in specific regions.

Table 4: Water transportation infrastructure data [9].

Region	**Number of Seaports**	**Number of River/Lakeports**	**Waterway Desnity (km/km^2)**
India	8	0	4.411E-03
Russia	5	1	5.966E-03
European Union	25	0	1.234E-02
China	7	1	1.146E-02
United States of America	11	1	4.170E-03
Pakistan	2	0	0.000E+00
Brazil	7	1	5.871E-03
Argentina	5	3	3.956E-04
Canada	3	5	6.370E-05

Table 5: Land transportation infrastructure data [9].

Region	Railroad Density (km/km^2)	Roadway Density (km/km^2)	Paved Airport Density (km^-2)
India	2.085E-02	1.429E+00	7.696E-05
Russia	5.097E-03	7.506E-02	3.474E-05
European Union	5.331E-02	2.447E+00	4.352E-04
China	1.993E-02	4.279E-01	4.824E-05
United States of America	2.985E-02	6.698E-01	5.140E-04
Pakistan	1.492E-02	3.315E-01	1.357E-04
Brazil	3.351E-03	1.857E-01	8.197E-05
Argentina	1.328E-02	8.322E-02	5.791E-05
Canada	7.805E-03	1.044E-01	5.238E-05

Mathematical Formulation & Implementation:

A large corporation may have large datasets containing information on the specifications of many shipping companies. The objective function should be able to obtain the optimum set of specifications for the minimum cost, and then choose the most fit entity listed in the dataset. Because this type of data is not readily available and often only comes from negotiations, the data used in this research was based off of industry mean costs [11].

In the development of this function, the list of parameters that could be applied is large. For choosing a road transportation method, parameters such as truck type, nearest location of transporter, the maximum load of the roads to be used, the heights of the bridges the truck will pass under, the width of the lanes, different types of costs associated with road transportation, and many more. To remain general, the specifications for interstate roads were used and are given in Table 6.

Table 6: Interstate specifications and regulations. [10]

Specification	Value
Maximum Weight	80,000 lbs
Minimum Bridge Height	16 ft
Lane Width	12 ft

A transportation cost model from the National Transportation Library was chosen to be the objective function [11]. In this model, many different types of shipping vehicles are listed with specifications such as gross vehicle weight (GVW), payload, average percentage of unloaded miles travelled, and various costs associated with the shipment. Below, in Eq. 7, the basic objective function for optimizing road shipping is given. In this function, f is the percent of the total distance travelled unloaded, d is the distance travelled, P_m is the price per total miles travelled, P_{lm} is the price per loaded mile travelled, W is the weight of the payload, and P_{tm} is the price per ton-mile. Constraints on this model are listed in Table 7. For this problem, the constraints used were those of the interstate regulations.

$$C = (1 + f)dw_m P_m + d(w_{lm} P_{lm} + W w_{tm} P_{tm}) \quad \text{(Eq. 7)}$$

Table 7: Objective function constraints [11].

Constraint	Condition
Height	$H_{platform} + H_{object} < \min(H_{bridge})$
Width	$w_{object} \leq \min(w_{lane})$
Length	$l_{object} \leq l_{trailer}$
Weight	$W_{object} \leq$ payload

To test the algorithm's performance, a simple case was considered in which one full 5 axel 48' flatbed trailer transported materials from a Westinghouse Electric Company manufacturing plant in New Hampshire to the V.C. Summer Nuclear Generating Station in South Carolina. To determine the distance between these two locations, Google Maps was used. The route which used mostly interstates was found to be 980 miles. Using the data listed below in Table 8 and Eq. 7, the shipment cost was found to be $4068.10.

Table 8: Flatbed trailer (5 Axle 48') averaged data [11].

Specification	Value
GVW	78,000 lbs
Payload	50,400 lbs
Price per Mile	$1.08
% Unloaded	25%
Price per Loaded Mile	$1.40
Price per Ton-Mile	$0.0556

To limit the search space to non-trivial choices, a condition was implemented in the initialization step such that the weights assigned were between 0.5 and 1.5. This was done because it is unlikely that pricing varies past that extend. Further, a condition was introduced to guarantee that the mean of the weights was one.

Results & Discussion:

Because this problem was generalized, the numerical result was trivial. The most important consideration investigated was the downward trend in cost and convergence to a single point or small region. The main purpose of this demonstration was to show that the algorithm would in fact converge to some optimum value for mathematical cost models. Using the algorithm parameters listed in Table 9, the plot in Figure 1 was produced.

Table 9: Algorithm parameters for supply chain analysis.

Parameter	Value
Number of Individual Costs	3
Potential Solutions per Generation	100
Number of Generations	50
Fitter Parent Crossover Probability	60%
Less Fit Parent Crossover Probability	30%
Mutation Probability	10%

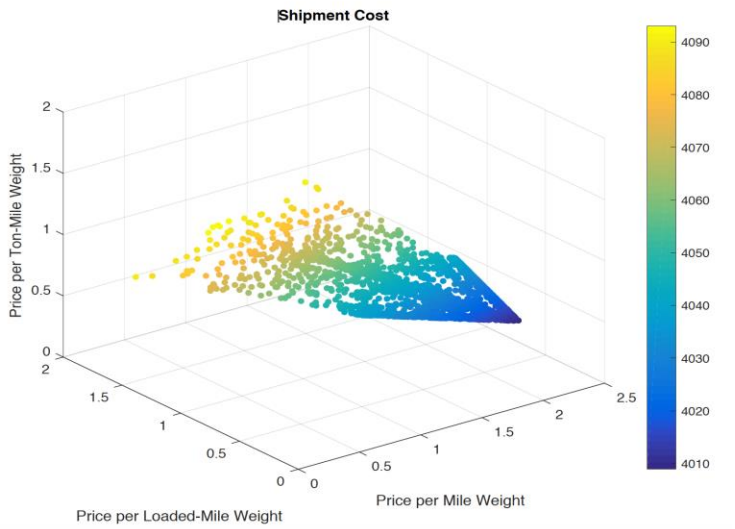

Figure 2: Plot of the three model parameters versus associated shipment cost.

At the completion of the algorithm a cost of $4008.66 was reached. Figure 2 clearly shows that the algorithm performed as expected and converged towards a single optimum. From this point, the user could find the cheapest supplier by identifying the closest fit to the optimum prices produced by the algorithm. This algorithm could be expanded quite significantly to account for costs incurred by risks using the data presented in the beginning of this chapter and to aid in the determination of the cheapest transportation mode.

Although no meaningful numerical results were gathered from the specific model tested, this could be of great use to an organization with data on suppliers and transporters. To gather meaningful information, an organization can use their own cost models for various transportation methods and risk models which can incorporate the region-specific data above. With this, an organization could gather preliminary insights onto which mode of transportation and which companies within those modes would most likely be the best choice.

CHAPTER IV

CONCLUSION

The developed method was tested on two vastly different examples. On the supply chain problem, a simple non-physical polynomial model was optimized with respect to cost. In the QM problem, a much more complicated model involving a high-level of physics was optimized with respect to wave-function basis state coefficients. This was possible because of the inherent variability of a GA to handle nearly any objective function. Using Eq. 5, shown below, the

$$< E > = \frac{\int \psi^* \mathcal{H} \psi \, dz}{\int \psi^* \psi \, dz}$$

energy and associated quantum mechanical wave-function of an electron in a parabolic potential was determined. In doing this, complex, tedious matrix methods were avoided and the only knowledge of the physics required was a basic definition. Using Eq. 7, shown below, the

$$C = (1 + f) d w_m P_m + d(w_{lm} P_{lm} + W w_{tm} P_{tm})$$

optimal relationship between cost parameters was found. This demonstrated that a GA could be applied to a supply chain problem given mean industry data, risk models, infrastructure data, and individual company data to determine the most beneficial mode of transportation and best companies to choose. Its success on each application indicates that the algorithm is model independent and that many more applications are within its scope. In improvement of the algorithm's performance, work should be done to implement better selection, crossover, and mutation methods and sensitivity studies should be done for each problem to find the optimum algorithm parameter set for each problem.

Future Work:

This section will discuss the next application of this method.

Nuclear Composition Characterization:

Current nuclear composition characterization methods use destructive methods, such as mass spectrometry. A nondestructive method to characterize nuclear composition is desirable since it would be done remotely using input datasets from detectors without any disruption of the system or destruction of material. Using a response-function approach linked with simulation data will aid in the reconstruction of the nuclear composition [4]. This can be done with limited knowledge of the system by using artificial intelligence methods such as genetic algorithms. This method could be applied to several different areas such as nuclear security, nuclear forensics, and burnup analysis among others.

Using the algorithm discussed in this paper a similar approach will be taken for the characterization problem. First a mathematical model must be developed. The model should include neutron energy spectra, cross section data for possible nuclides in the mixture, response functions, and given input detector data with a set of all nuclide concentrations as the unknown genetic formulation of the problem. The concentrations will be characterized by detecting and recognizing energy signatures unique to specific nuclear reactions. Once this is complete, the objective function will be tested by comparison to a known sample and efforts will be undertaken to quantify uncertainties. The algorithm parameters will then be tuned to optimize the algorithm's performance.

REFERENCES

[1] Harrison, P. (2001). Computational Methods in Physics, Chemistry, and Biology. Chichester: Wiley.

[2] Kumar, A., & Tsvetkov V., P. (n.d.). Parametric Analysis and Optimization using Multivariate Regression Analysis and Genetic Algorithms. Department of Nuclear Engineering, Texas A&M University.

[3] Cook, T. (2016, August). Cyber Security R&D. Nuclear Energy R&D Workshop for Universities.

[4] Gillis, W. C., Rose, P., & Erickson, A. (2016). Interpreting Detector Response via Photon Spectral Unfolding. Journal of Nuclear Instruments and Materials Analysis.

[5] Find Global Minima for Highly Nonlinear Problems. (n.d.). Retrieved from https://www.mathworks.com/discovery/genetic-algorithm.html

[6] Kumar, A. (2016, August). An Iterative Optimization Method Using Genetic Algorithms and Gaussian Process Based Regression in Nuclear Reactor Design Applications. Texas A&M University.

[7] Eiben, A. E., and S. K. Smit. Evolutionary Algorithm Parameters and Methods to Tune Them. N.p.: Springer, 2012. Web. 8 Jan. 2017.

[8] International Energy Agency. (n.d.). World Energy Outlook, 2012 (World Energy Outlook) (pp. 190–191).

[9] Central Intelligence Agency. (n.d.). The World Factbook [Database].

[10] A Policy on Geometric Design of Highways and Streets. (2014, April 11). Washington DC: American Association of State and Highway Transportation.

[11] Cambridge Systematics, Inc. (n.d.). Appendix F: Estimating Transport Costs. National Transportation Library.

[12] Freeman, D. W., Edwards, D. R., & Bolon, A. E. (1998). Genetic algorithms Ð A new technique for solving the neutron spectrum unfolding problem. *Elsevier*.