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SIMULATED QUANTUM ANISOTROPIC ANNEALING APPLIED TO ARTIFICIAL
NEURAL NETWORK WEIGHT SELECTION

THESIS
Justin Fletcher
First Lieutenant, USAF

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THESIS

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Master of Science in Computer Science

Justin Fletcher, B.S. CEC

First Lieutenant, USAF

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Justin Fletcher, B.S. CEC

First Lieutenant, USAF

Approved:

<hr/> Dr. Michael J. Mendenhall Thesis Advisor	<hr/> Date
<hr/> Dr. Gilbert L. Peterson Committee Member	<hr/> Date
<hr/> Capt. Charlton D. Lewis Committee Member	<hr/> Date

Preface

Justin Fletcher

Table of Contents

	Page
Preface	iii
List of Figures	vi
List of Tables	vii
List of Symbols	viii
List of Abbreviations	ix
Abstract	x
I. Introduction	1-1
II. Background	2-1
2.1 Artificial Neural Networks	2-1
2.1.1 Biological Inspiration	2-1
2.1.2 Historical Overview	2-2
2.1.3 Network Topology	2-10
2.1.4 Activation Functions	2-10
2.1.5 Learning Strategies	2-11
2.2 Related Works in Simulated Annealing	2-11
2.2.1 Reheating	2-12
2.3 Related Works in Quantum Mechanics	2-12
2.3.1 Quantum Tunneling	2-12
2.3.2 Quantum Annealing	2-12
2.4 Notation and Terminology Conventions	2-13

	Page
III. Methodology	3-1
3.1 Simulated Quantum Annealing	3-1
3.2 Traversing the Error Manifold	3-1
3.2.1 Unidimensional Weight Perturbation	3-1
3.2.2 Omni-dimensional Weight Perturbation	3-1
3.2.3 Constrained Step-Size Omni-dimensional Weight Per- turbation	3-1
3.2.4 Quantum Weight Perturbation	3-1
3.2.5 Stochastic-Anisotropic Quantum Weight Perturbation	3-1
3.2.6 Quantum Annealing	3-2
IV. Results	4-1
V. Conclusion	5-1
Appendix A. First appendix title	A-1
A.1 In an appendix	A-1
Bibliography	BIB-1
Vita	VITA-1

List of Figures

Figure

Page

List of Tables

Table

Page

List of Symbols

Symbol

Page

List of Abbreviations

Abbreviation	Page
ANN Artificial Neural Network	ix
ANN	

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Abstract

Stub.

SIMULATED QUANTUM ANISOTROPIC ANNEALING APPLIED TO ARTIFICIAL NEURAL NETWORK WEIGHT SELECTION

I. Introduction

Stub.

II. Background

This chapter serves as a comprehensive review of the physical and computational concepts material to the topic of this thesis. A broad overview of artificial neural networks and the application and history thereof is presented. Next, simulated annealing is described, along with a summary of some related works and a description of the physical inspiration for the algorithm. The chapter concludes with a very brief overview of the quantum mechanics, with emphasis placed on those concepts which will be employed throughout this thesis document. Finally, the notation and terminology conventions adopted in this document are established.

2.1 Artificial Neural Networks

It has long been recognized that the capacity of biological information processing systems to flexibly and quickly process large quantities of data greatly exceeds that of sequential computing machinery. This information processing capability arises from the complex, nonlinear, parallel nature of biological information processor. The family of models designed to replicate this powerful information processing architecture are collectively called artificial neural networks. In the most general sense, artificial neural networks are parallel distributed information processors (11) comprising many simple processing elements. Networks store information about experienced stimuli and can make that information available. In such a network, interneuron connection strengths are used to encode information, and are modified via a learning strategy. Artificial neural networks are characterized by three features: a network topology or architecture, an activation function, and a learning strategy. Each will be discussed in the following sections. I will also review the history of artificial neural networks, and the biological inspiration for the computational model.

2.1.1 Biological Inspiration. This is all one big stub.

Fig[an image of a neuron, mapped to a schematic of a neuron, mapped to a processing element]

Integration of magnitude-encoded, rather than frequency-encoded, signals. Threshold functions relationship to the biological shape, size... Papers needed.

Biological neural networks are many orders of magnitude slower than those based in ... It is not the size of the network or the number of interconnections alone which confer upon the human brain its remarkable efficiency (Faggin, 1991). Though size and connectivity are necessary, it is the structure, or topology of the network of interconnections that en

Activation time-line: The concentration of neurotransmitters in the extra-synaptic fluid increases, raising the instantaneous membrane potentiality, possibly breaching the threshold potential causing a fire-and-reset, where there is some physical limit on the rate at which the reset step can occur, thus causing the diminishing response seen in Figure 2 of Neurocomputing, whence the fire causes either excitatory or depressive neurotransmitters to be released at the synaptic clefts formed at the end of the axon, thus propagating the activation through the net.

What is changed in synaptic modification is the efficiency with which a particular post-synaptic site is able to convert neurotransmitters in the surrounding intercellular environment, which is to say in the synaptic cleft, into a change in charge inside the cell.

Activation function: A neuron's activation function is just a phenomenon emerges from the combination of its potential threshold and rest rate, both of which are physiological properties which can change after cell formation. (Instructing Perisomatic Inhibition by Direct Lineage Reprogramming of Neocortical Projection Neurons, 2015)

2.1.2 Historical Overview. The study of artificial neural networks began with a 1943 paper (19) by McCulloch and Pitts. In this paper, McCulloch and Pitts united, for the first time, neurophysiology and formal logic in a model of neural activity. This landmark paper marked the beginning of not only the computational theory of neural networks but also the computational theory of mind, and eventually led to the notion of finite automata (24). In this paper McCulloch and Pitts introduced a very simple model of a neuron, which acted as a threshold-based propositional logic unit. Significantly, McCulloch and Pitts showed that a network of these neuron models, interconnected, could

represent a proposition of arbitrarily-high complexity. Said differently, a network of these neurons can represent any logical proposition. These models, often called McCulloch-Pitts Neurons, allow only discrete input values which are summed and compared to a threshold value during a fixed time quantum, and do not possess any learning mechanism. These neurons are able to incorporate inhibitory action, but the action is absolute and inhibits the activation of the neuron without regard to any other considerations. These models are of theoretical significance, but cannot be applied to practical problems.

[Graphic Stub: Simple McCulloch-Pitts neuron.]

Though McCulloch and Pitts made mention of learning in their 1943 paper, thirteen years would pass before this concept was formalized into a mathematical and computational model. In 1956 Rochester, Holland, Haibt, and Duda (25) presented the first attempt at using a physiologically-inspired learning rule to update the synaptic weights of a neural network. This model was based on the correlation learning rule postulated in 1949 by Hebb¹. In his book *The Organization of Behavior*, Hebb suggested that synaptic plasticity, that is the capacity of synaptic strengths to change, is driven by metabolic and structural changes in the both neurons near the synaptic cleft (12) such that if two cells often fired simultaneously the efficiency with which they cause one another to fire will increase. This efficiency is now called a synaptic weight. Rochester et. al. showed that the addition of variable synaptic weights alone was not sufficient to produce a network capable of learning. It was also necessary that these weights be capable of assuming inhibitory values.

[Graphic Stub: simple perceptron terminology, figure.]

The next major contribution to the field would come in 1958 with Rosenblatt's introduction of the perceptron (26). The perceptron was the first (2) well formed, computationally oriented neural network. Crucially, and unlike most preceding neural models, the model Rosenblatt presented in his 1958 paper was associative. That is, the model learned to associate stimuli with a response. This learning is accomplished by modifying the synaptic weights of the model such that the difference between an input pattern and

¹It should be mentioned that, while Hebb was the first to postulate the correlation learning rule as it relates to neurons and synaptic connection strength, the abstract rule was foreshadowed as early as 1890 by William James (14) in Chapter XVI of *Psychology (Briefer Course)*.

the desired output pattern is minimized. The responsibility for the error, or difference between the correct and computed output patterns, is divided among the weights in proportion to their magnitude. Thus, large synaptic weights will be reduced more than small synaptic weights for a large, positive error. This weight update strategy is represented mathematically as:

$$w_i(t+1) = w_i(t) + \alpha(d_j - y_j)x_{j,i} \quad (2.1)$$

where $w_i(t)$ the synaptic weight for feature i at discrete time t , α is the tunable learning rate parameter, d_j is the desired output, y_j is the computed output, and $x_{j,i}$ is the input pattern. This method constitutes a form of reinforcement learning.

Rosenblatt's perceptron was found to be successful at predicting the correct response class for stimuli only if the responses were correlated. It was not until Block's 1962 publication that the reason for this observed performance was elucidated. In this paper, Block presented two key findings: first, that simple perceptrons require linearly separable classes to achieve perfect classification and second, the perceptron convergence theorem (4). Linear separability is the ability of the response classifications to be separated by a hyperplane in the n -dimensional space of the input stimuli to which they correspond. The requirement of linear separability arises directly from the way in which the output of a perceptron response unit is calculated. The output of a perceptron response unit is given by:

$$y_j = \begin{cases} -1 & \sum_{i=1}^n w_{i,j}x_i \leq \Theta \\ +1 & \sum_{i=1}^n w_{i,j}x_i > \Theta \end{cases} \quad (2.2)$$

where y_j is the response value of response unit j , $w_{i,j}$ is the synaptic weight of the connection between activation unit i and response unit j , x_i is the activation value of activation unit i , and Θ is the threshold value of the perceptron. Block's crucial observation was that the form of the summation in the response determining equation is isomorphic to a hyperplane in an n -dimensional space. Thus, in order for the perceptron to achieve perfect classification a hyperplane must be able to separate them in the n -dimensional input space. The corollary of this observation is the perceptron convergence theorem. The theorem proves that for some learning rules, if a perfect classification is possible it will be

found by the perceptron. Specifically, the class of learning rules which were found effective were those which did not change synaptic weights when a correct classification occurs. While the condition does ensure convergence, it often causes very slow convergence, as the synaptic weights change much more slowly when only a small number of samples remain misclassified. Considerably faster guaranteed convergence can be achieved using a error gradient descent learning rule (30), as described by Widrow and Hoff.

In 1969 Minsky and Papert published *Perceptrons*, a book on mathematics and theory of computation. In this book Minsky and Papert mathematically and geometrically analyzed the limitations inherent in the perceptron model of computation. The authors reasoned that the each response unit of Rosenblatt's perceptrons was actually computing logical predicates about the inputs it received, based on the observation that response units can either be active or inactive. This analytical framework allowed the authors to construct unprecedented geometric and logical arguments about the computational capabilities of a perceptron. They found that there were several classes of problems which were unsolvable by linear perceptrons (21). In the final chapter of the *Perceptrons* Minsky and Papert extended their judgments regarding the ineffectiveness of single-layered perceptrons to all variants of perceptrons, including the multi-layered variety. This conjecture would turn out to be one of the most significant of the entire book, as it likely resulted in a reduction of funding for neural network research (2) which lasted for several years. Unfortunately, this judgment was false.

While it is true that the pace of development in the field of neural networks slowed considerably after the publication of *Perceptrons*, there was still progress made during the 1970s. In 1972, both Anderson (1) and Kohonen (16) published models of what would come to be known as linear associative neural networks, which are a generalization of Rosenblatt's perceptron. As with the perceptron, neurons in a linear associative neural network compute their output by summing the product of each input signal the synaptic weight associated with that input. Unlike the perceptron, the output of these networks is proportional to this sum, rather than a binary value computed by applying a threshold function to the sum. Though still unable to achieve perfect classification on many classes

of problems, these networks were able to successfully associate input patterns with output patterns.

The decade also saw the advent of self-organized maps, which are a type of competitive learning neural network. Self-organization in neural networks was first demonstrated by van der Malsburg in a paper (28) published in 1973. This paper analyzed the response of simulated cortical cells to a simulated visual stimulus. The paper is interesting both for the complexity of the neural model developed, and because it contained the first direct comparison between computer simulation and physiological data (2).

Throughout the decade progress was also made in the understanding of the physiology of biological neural networks. Of particular interest are those papers describing the lateral retinal system of *Limulus polyphemus*, the horseshoe crab. Chosen for the ease with which experiments may be conducted on its compound lateral eye, *Limulus* features prominently in the neurophysiological research. Several works were published on the *Limulus*, perhaps the most significant of which came near the end of the decade with the 1978 publication of a paper describing the dynamics of the retina of a *Limulus* when exposed to moving stimuli. In this paper, the *Limulus* eye was analyzed as a linear system, and the results of this analysis were compared to the actual response of the system to input pattern. The agreement between the linear² model and the biological output signals was found to be in excellent agreement (5). This finding was interesting for the purposes of perceptron simulation, but was ultimately found not to hold for larger collections of neurons.

Several events conspired to create a reinvigoration of neural network research in the early 1980s. Theoretical advances in the physiology of biological neural networks. processor manufacturing technology had advanced sufficiently to allow for much larger-scale simulations. simulation capability...

In 1982, John Hopfield published *Neural networks and physical systems with emergent collective computational abilities*. This momentous work is regarded by many to be the beginning of the renaissance of neural network research (2), and contains many novel insights.

²Linear, in this context of this system, means that the output of the system when presented with the sum of a set of inputs is equivalent to the sum of the outputs of the system when presented with each input individually.

Hopfield begins the paper differently than past researchers. Rather than proposing a learning rule or network topology and then evaluating the results of this proposition, Hopfield begins by considering an alternative purpose for a neural network. Hopfield suggests that the network be thought of as a means to develop locally stable points, or attractors, in a state space. The state space comprises the set of states which are the activation value of each neuron. Thus, learning should be the process of modifying the synaptic weights such that they cause the system to flow into local attractors which represent the desired output. In such a model, a noisy or incomplete input would result in an activation pattern which resides on a gradient in the state space. The neural network would then change the activation pattern in such a way as to move the system down the gradient into the attractor state. Hopfield suggests that this process is a general physical description of the concept of content-addressable memory.

[Graphic Stub: notional activation state space with letters and noisy letters as points.]

Hopfield then proposes a network architecture to achieve this behavior (13). The chosen model is one which has binary neural output values and recurrent connections. Neural networks of this type are now called Hopfield networks. Like Rosenblatt's original perceptron model, the neurons used in Hopfield's work had a non-linear, threshold activation function. The network topology was recurrent, with the restriction that no neuron could provide input to itself. Hopfield adopted a variation of Hebb's learning rule to update the synaptic weights.

In Hopfield's network model, the connection strength between two neurons i and j is denoted as T_{ij} , and the activation status of a neuron i is denoted as V_i . T is therefore the connection matrix of the neural network, with each element representing an individual connection strength and zeros along the diagonal. It is from this organization of the connection strengths that one of the most important insights of this work originates. Hopfield recognized that, in the special case of the model in which $T_{ij} = T_{ji}$, a quantity E could be defined such that

$$E = -\frac{1}{2} \sum_{i \neq j} \sum T_{ij} V_i V_j. \quad (2.3)$$

The change in this quantity as a result of a change in one of the activation values, V_i in the following equation, is then represented as

$$\Delta E = -\Delta V_i \sum_{j \neq i} T_{ij} V_j. \quad (2.4)$$

From this equation, it is clear that any change in V_i ³ will reduce the value of E . This decrease in E must necessarily continue until some local minimum of the value of E is reached. Here, Hopfield observed that this case is isomorphic with an Ising model,” referencing the statistical mechanical model of magnetic spins. In this isomorphism, the quantity E maps to the energy of a physical system described by an Ising model. It is difficult to overstate the importance of this observation. It both provided a novel mechanism by which physical theory could be applied to neural networks, and legitimized the study of neural networks as a physical system, encouraging many physicist to join in the development of the theory.

Hopfield constructed a model of the system described in the paper, and presented it with random input patterns⁴. He found that the network can indeed recall a small number of patterns, on the order of approximately 15 percent of the network dimensionality, before the recall error becomes significant.

In 1985, Ackley, Hinton, and Sejnowski, extended the neural network model proposed by Hopfield⁵. Hopfield networks are deterministic with respect to energy; by definition any change in a Hopfield network always reduces the energy of the system or leaves it the same. This is a useful property if it is acceptable to find one of many local minima, or attractors. However, if a single, global minima in the state space is sought this model is likely to converge prematurely to a local attractor state. In order to surmount this limitation Ackley, Hinton, Sejnowski modified the Hopfield neural model to activate stochastically. The probability of state transition, p is given by

$$p = \frac{1}{1 + e^{-\Delta E/T}} \quad (2.5)$$

³An identical conclusion would be reached if V_j was changed instead of V_i . It is merely a matter of convention.

⁴Hopfield calls these input patterns entities or *Gestalts*.

⁵Though a Hopfield network was used for the work done by Ackley, Hinton, and Sejnowski it is not necessary to use network with recurrent connections.

where ΔE is the change in energy of the system resulting from a transition to a new state and T is the artificial temperature of the system. Thus the relative probability, P_α/P_β of moving to either of two arbitrary global states, α and β , goes as

$$\frac{P_\alpha}{P_\beta} = e^{-(E_\alpha - E_\beta)/T} \quad (2.6)$$

which is a form isomorphic to the Boltzmann distribution. Thus, a neural network with transition probabilities described by equation 2.5 is called a Boltzmann machine. The effect of probabilistic state transitions of this form is that state transitions from low energy states to higher energy states are possible, thereby allowing the system to escape local minima.

Inspection of equations 2.5 and 2.6 reveals that the probability of transition is determined by both ΔE and T . A large value of ΔE , which corresponds to a large increase in total energy, will decrease the probability of transition. Conversely, a large value of T will increase the probability of transition for any arbitrary value of ΔE . The systems artificial temperature therefore acts as a tuning mechanism for the exploration of the state space. A high temperature value will result greater exploration of the space state, but will result in less gradient descent and therefore may cause the system to depart the attractor basin of the global minimum. A low artificial temperature parameter may cause premature convergence. Ackley, Hinton, and Sejnowski solved this tuning problem by recognizing a deep connection to another concept born of statistical mechanics: simulated annealing. Simulated annealing decreases the artificial temperature of a system slowly over the course of a simulation, and as a result increases the likelihood that the final state of the system will be the ground state, which is to say the global minimum. This algorithm is discussed in detail in section 2.2.

With a procedure for finding the global minimum of a space state in place, the authors proceeded to construct state spaces for which the global minimum was of interest. One way to construct such a state space is to include hidden units in the neural network. Hidden unit are neural units which are neither input nor output units. These hidden units allow the network to solve interesting problems that are out of reach of simple associative neural networks(2). However, like all neurons in any neural network, the connection weights of

these neurons must be modified in order for the network to learn. It is not immediately clear how hidden unit synaptic weights can be modified to account for the performance of the network. This deficiency is often called the credit assignment problem(3). The application of simulated annealing in Boltzmann machines avoids the problem of assigning credit to hidden units, thereby enabling their inclusion in the model. This is historically significant because it was the first successfully-implemented multi-layered neural network (11).

The next major development in neural networks came in 1986 with the introduction of the back-propagation algorithm. Though the formalisms required involved in this algorithm had been developed earlier (6) (29), and the method was simultaneously discovered independently by two other groups (23) (18), it was Rumelhart, Hinton, and Williams that applied the algorithm to machine learning (27). Back-propagation can be thought of as a generalization of the gradient descent⁶ algorithm presented Widrow and Hoff (30), which includes the errors associated with connection strength of hidden units, or internal representation units. A detailed discussion and derivation of the back-propagation algorithm is included in Section 2.1.5.1. Though back-propagation in multilayered perceptrons cannot be guaranteed to find an exactly correct solution, the algorithm is demonstrably capable of solving difficult and interesting problems, thus disproving the speculation of Minsky and Papert in *Perceptrons*.

With the advent of Boltzmann machines and back-propagation, it became possible to analyze the properties and capabilities of multilayered neural networks. In 1989 Cybenko showed that a multilayer feedforward neural network with nonlinear activation function is in principle capable of approximating any continuous function (8). This finding is striking because it implies that, given the correct learning rule and a sufficiently large network, a multilayer neural network can learn a pattern of arbitrary complexity.

2.1.3 *Network Topology.* Stub.

2.1.4 *Activation Functions.* Stub.

⁶The gradient descended here is the gradient of the error surface in the space of states of synaptic weights, not the gradient of the activation state surface, as with a Hopfield network.

2.1.5 Learning Strategies. Stub.

2.1.5.1 Back Propagation Training. Stub.

2.1.5.2 Simulated Annealing. Stub.

2.2 Related Works in Simulated Annealing

Simulated annealing is a stochastic optimization algorithm which can be used to find the global minimum of a cost function mapped from the configurations of a combinatorial optimization problem. The concept of simulated annealing was introduced in by Kirkpatrick et al. in (15) as an application of the methods of statistical mechanics to the problem of discrete combinatorial optimization. Specifically, simulated annealing is an extension of the Metropolis-Hastings (20) algorithm which can be used to estimate the ground energy state of a many-body systems at thermal equilibrium. Kirkpatrick et al. applied the Metropolis-Hastings algorithm sequentially, with decreasing temperature values in order to approximate a solid slowly cooling to low temperatures. Later work by Goffe (10), Corana et al. (7), and Lecchini-Visintini et. al. (17) extended simulated annealing to the continuous domain. The basic simulated annealing algorithm is presented in [Algorithm Stub: SA].

[Algorithm Stub: SA]

Stub: discuss the statistical mechanical formalism for SA.

In the parlance of simulated annealing (15) a system at its maximum temperature is said to be *melted*. In the melted state, most perturbations of the system configuration are accepted by the algorithm. Analogously, a system that has a temperature of zero, which indicates that the algorithm cannot move to any higher-error state, is said to be *frozen*. Note that a frozen system may still be perturbed into a lower-energy state.

When considering only the influence of classical thermal fluctuations in particle energy levels, the probability of a particle traversing a barrier of height ΔV at a temperature T is on the order of:

$$\mathcal{P}_t = e^{-\frac{\Delta V}{T}} \quad (2.7)$$

2.2.1 Reheating. Stub.

2.3 Related Works in Quantum Mechanics

Quantum mechanics is the branch of physics concerned with the physical laws of nature at very small scales. Many aspects of physical reality are observable only at these scales. Several techniques described in this document are either inspired by, or are simple models of quantum mechanical processes. These concepts are very briefly reviewed in this section.

2.3.1 Quantum Tunneling. One of the quantum phenomena for which there is no classical analog is potential barrier penetration, also known as quantum tunneling. This phenomenon arises from the probabilistic and wavelike behavior of particles in quantum physics. Tunneling plays a significant role in the behavior of bound and scattering quantum mechanical systems.

A particle with energy E incident upon a potential energy barrier of height $\Delta V > E$ has a non-zero probability of being found in, or past, the barrier. Classically, this behavior is forbidden. The probability of tunneling, \mathcal{P}_t , through a step barrier of height ΔV is described by:

$$\mathcal{P}_t = e^{-\frac{w\sqrt{\Delta V}}{\Gamma}} \quad (2.8)$$

where Γ is the tunneling field strength (22). Figure [Graphic Stub: Quantum tunneling] depicts a one-dimensional example of quantum tunneling.

[Graphic Stub: Quantum tunneling]

2.3.2 Quantum Annealing. Quantum annealing is the use of quantum, rather than thermal fluctuations to traverse the free energy landscape of a system. This is accomplished by introducing an additional Hamiltonian term that does not commute with the classical Hamiltonian. The term is introduced to account for the presence of a tunneling field which controls the frequency with which quantum fluctuations occur in the system. In effect, this term controls the relative importance of quantum effects on the behavior of the modeled system. This term, much like thermal energy in simulated annealing, is

gradually reduced over the course of the simulation (9). The time dependent Schrödinger equation ⁷ for such a system has the form (22):

$$[\lambda(t)H' + H_0]\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (2.9)$$

where $\lambda(t)$ is the time-variance function of the tunneling field, H' is the Hamiltonian term describing the tunneling field, and H_0 is the classical Hamiltonian.

The fluctuations induced by the tunneling field are tunneling events, which transition the system from one configuration to a different, lower-energy configuration directly, without assuming any of the higher energy configurations between the two. Said differently, the quantum tunneling field enables the penetration of energy barriers. The addition of these quantum fluctuations also ensures that each possible state of the system can be reached (9).

2.4 *Notation and Terminology Conventions*

There is a great deal of academic writing describing quantum annealing in the language of physics, but very little writing describing the concept from an algorithmic perspective. For this reason a new, more specific term is introduced in this document. Simulated quantum annealing (SQA) is the quantum mechanical counterpart of simulated thermal annealing.

The term neuron will be used in this document to describe the information processing elements of a neural network. This convention is selected both for conciseness and for the useful adjectival form, neural, which will be of great explanatory utility in the coming chapters.

⁷Note that the presence of the Schrödinger equation in section does not imply that quantum annealing requires the annealed system must be an approximation to a wavefunction. It merely serves as an exposition of the properties of physical system which is modeled.

III. Methodology

3.1 Simulated Quantum Annealing

It is instructive to contrast equations 2.1 and 2.2. Both describe the same value, but the importance of the width and height of the traversed barrier in the two equations is considerably different. For systems in which quantum tunneling is possible, the probability of penetrating a barrier of height ΔV is increased by a factor of approximately $e^{\Delta V}$, for large values of ΔV . This relationship is depicted graphically in Fig. 2 which shows the probability of barrier traversal for a system which allows quantum fluctuations, divided by the same probability for a system which only considers thermal fluctuations. Therefore, physical models which considers quantum effects are much more likely predict penetration of tall, thin energy barriers than those which only include classical thermal effects.

[In both the simulated thermal and quantum annealing algorithms the Metropolis acceptance criterion is utilized, which is given by

$$\mathcal{P}_t = e^{-\frac{w\sqrt{\Delta V}}{\Gamma}} \quad (3.1)$$

[goto page 78 in SA eq 5.1]

[Graphic Stub: QSA/SA advantage curve.]

[Graphic Stub: arbitrary 2-parameter error space performance graph]

3.2 Traversing the Error Manifold

3.2.1 Unidimensional Weight Perturbation.

3.2.2 Omni-dimensional Weight Perturbation.

3.2.3 Constrained Step-Size Omni-dimensional Weight Perturbation.

3.2.4 Quantum Weight Perturbation.

3.2.5 Stochastic-Anisotropic Quantum Weight Perturbation.

3.2.6 *Quantum Annealing.*

IV. Results

V. Conclusion

Appendix A. First appendix title

A.1 In an appendix

This is appendix section A.1.

Note: I highly recommend you create each chapter in a separate file including the `\chapter` command and `\include` the file. Then you can use `\includeonly` to process selected chapters and you avoid having to latex/preview/print your entire document every time.

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Vita

Insert your brief biographical sketch here. Your permanent address is generated automatically.

Permanent address: 452 Orchard Drive
Oakwood, Ohio 45419