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Abstract

Here an abstract will show up in some months to follow.

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Thesis domain (Socrates-Erasmus subject area codes)

11.3 Informatyka

Subject classification

D. Software
D.127. Blabalgorithms
D.127.6. Numerical blabalysis

Tytuł pracy w języku polskim

Tytuł po polsku

Contents

Introduction

Here describe what quantum computing is and its brief history -Feynamnn lecture -shores algorithm

Chapter 1

Current state of Quantum Computing

Quantum computing has seen a rapid growth in recent years. Major players in the tech industry, governments and universities invest their time, money and effort.

1.1. Gate model

Some text about the gate model computers

1.1.1. Error correction

Some for subsection of error correction - Google quantum supremacy? - biggest chip so far

1.2. Problems of practical QC - NISQ

Some text about NISQ

1.3. Quantum Annealing

Quantum annealing has some interesting properties. It is analog in nature and because the computation happens in a ground state it is unaffected by decoherence [**?**].

Chapter 2

What actually is Quantum Annealing

Quantum annealing is a computational process, an optimization metaheuristic proposed theoretically in 1988 in [1], as an analogy to simulated annealing, formulated five years earlier [5]. It was first simulated classically, to finally become realised in an analog hardware by D-Wave Inc. First working quantum annealer was presented in 2007 and contained 16 qubits [4]. To fully understand the term and to develop a bottom-up intuition of the process it is best to track the gradual development of the concept.

2.1. Thermal Annealing

Traditionally annealing refers to thermal annealing, a metallurgical process known to humanity for centuries. Annealing reduces hardness and increases ductility of a (most often) metal peace, making it more workable. The peace is heated until glowing (for steel) and kept in high temperature. The temperature increases the rate at which atoms diffuse in the metal, eradicating dislocations of the crystalline structure, hence moving towards equilibrium state - lower internal stresses. Lower number of dislocations results in higher ductility. The process of stress-relief is spontaneous, so it also progresses at room temperature, although at a very slow pace. It is the heat that increases the energy of thermal fluctuations, making transitions more probable. This concept is the basis on which, by analogy, optimisational algorithms were build. Annealing may also be applied to glass, with similar purposes and process. As glass has no crystalline structure, the mechanics differ [2].

A process with opposite effects is quenching, where hot material is cooled rapidly. This results in sub-optimal configuration of the material. Remaining stresses make the material harder but more brittle [3].

2.2. Simulated Annealing

As an optimizational algorithm, simulated annealing emerged in the early '80 in a paper by Kirkpatrick, Gelatt, and Vecchi [5]. As of 2021, it was cited almost 50 000 times, indicating how influential the idea is. The work of Kirkpatrick et al. is based on much older concept, the Metropolis algorithm by Metropolis et al. [6]. The authors devised a computational method for studying aggregate properties of the large number of particles, a subject of the statistical mechanics. As the number of particles is typically big (an order of $10^23/cm^3$) only the most probable behaviour of the system is observed in the experiments. To calculate parameters of this observable state, a Gibbs ensemble is used. It is an average of a parameter taken over all possible configurations, each defined by particle positions and weighted by a corresponding

Boltzmann probability factor:

$$p \propto e^{-E/kT}$$

where k is the Boltzmann constant, T is temperature, E the potential energy of the configuration, defined as:

$$E = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} V(d_{ij})$$

where V is the potential between particles, d is the distance between them.

The averaging involves integration over a high-dimensional configuration space. As the number of particles is high, so is the dimensionality of the integral. Metropolis et al. proposed a computational method for tackling the problem of integration, based on Monte Carlo method. They studied a group of interacting particles (56 or 224) packed in a two-dimensional, closed space, at a given temperature. Standard Monte Carlo method involves random, uniform sampling of points and assigning them a weight which represents the probability of finding a particular configuration. Any randomly selected state will most probably be far from "optimum", hence with high energy and finally with low weight (probability) assigned. Standard Monte-Carlo method which involves sampling from a uniform distribution would require a huge number of configurations to be calculated, most of which with a very low contribution. Instead the authors choose configurations with probability $e^{-E/kT}$ and weight them evenly.

The algorithm starts from a random particle configuration of the particles, next following steps are executed in a loop :

1. Move a chosen particle to new positions:

   $$X \to X + \alpha\gamma_1$$

   $$Y \to Y + \alpha\gamma_2$$

   where X, Y are the coordinates of the particle, α is the maximum allowed step, γ_1 and γ_2 are random numbers between -1 and 1.

2. Calculate the change in energy ΔE. If $\Delta E < 0$ the move is always allowed, so we always accept "better" solution. If $\Delta E > 0$ the move is allowed with probability $e^{-E/kT}$. To realise the probability, γ_3 between 0 and 1 is randomly selected. If $\gamma_3 < e^{-E/kT}$ the move is accepted, else rejected.

3. Whether the configuration has changed or not, each step is taken into account for counting the ensembles.

The described algorithm allows for studying the properties of a set of particles at a given temperature. There is a connection with optimisation as we have discussed states of lower energy, the optimal ones. Still there is a little chance of finding them randomly. So how to transform a computational method of statistical mechanics into a optimisation algorithm? Kirkpatrick et al. realised that by lowering the temperature of the algorithm, one would simulate cooling process. At the end of the process, the Boltzmann distribution collapses into the lowest energy states. Unfortunately, low temperature is not a sufficient condition for finding the optimal state. We can refer to previous section 2.1

2.3. Quantum Annealing

Chapter 3

The problem

Chapter 4

Practical relization of The problem

Chapter 5

Conclusions and remarks

Chapter 6

Scratchbook

Ocean tool-kit is the software suite currently used by DWave to solve computational problems. It consists of various sub-modules, each aimed at different stage of the process. The tool-kit is freely available on Github [**?**].

Bibliography

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