# Literature Review

Describe the chapter and the sections it has.

## 1 Annealing Metaheuristics

In this section we will discuss a class of metaheuristics that are inspired by the physical process of *annealing*. At the beginning, we will explain what it is. Then we will talk about multiple annealing metaheuristics that are relevant to this work.

### Annealing

Annealing is a heat treatment process of matter like glass or metal (Collins, 1921; Wu and Fan, 2020). It involves heating up the material and then carefully cooling it down at a controlled rate. By following that process, it is possible to achieve a stable crystal structure.

If, however, this rate is exceeded, the resulting crystal will have defects as only locally optimal structures were allowed to form (Kirkpatrick, Gelatt and Vecchi, 1983). The lack of equilibrium will make such crystal metastable.

### Simulated Annealing

Simulated annealing (SA) is a metaheuristic that uses the concept of temperature to approximate global optimum of a combinatorial optimization problem. The temperature (*T*) is a variable that controls the likelihood of making locally non-optimal uphill moves. Just as in physical annealing, we start the optimization with a high temperature and decrease it at a controlled rate. If that rate is low enough (reference), we are guaranteed to find a global optimum. However, it is possible to find good approximations of the optima significantly faster at higher cooling rates.

The temperature concept allows the algorithm to explore and exploit during the optimization process. The SA starts with a high temperature to allow the algorithm to “explore”. At that point the algorithm acts like random walk, choosing random moves with high probability, which prevents us from being stuck at local optima.

At the end of the SA, when the temperature is low, the algorithm prioritizes advantageous moves, and that is when exploitation happens. The algorithm acts like greedy algorithm and tries to find the optima. As we shift from higher to lower temperatures, we gradually shift from exploring the search space to find the optimum.

Let *c* be current node, *n* be next node and *evaluation(x)* be the function that evaluates the energy of the node *x*. Then the quality of the move, or the energy transition, (*ΔE*) can be defined by the following formula, when minimizing:

*ΔE = evaluation(c) - evaluation(n)*

*ΔE* and *T* are the variables that will affect the probability of choosing node *n*, where *ΔE* defines the energy drop that the proposed node will introduce and *T* controlling how *ΔE* influences the probability of choosing this node:

The *acceptance probability function* is the function that maps current node, proposed node, and Temperature to a probability. There are many functions that suit this purpose, we will use sigmoid.

If that probability is higher than a uniformly generated random number, then node *c* is rejected in favour of node *n*. In the original paper, always resulted in choosing the proposed node, but that is not necessary for SA to work.

The pseudocode of SA is given by:

c ← initial node

**While** T > threshold:

n ← generate next node(c)

**if** P(c, n, T) >= random(0, 1)

c ← n

**end if**

T = cooling(T)

**End while**

### Quantum Annealing

Quantum annealing (QA) is a metaheuristic that uses quantum-mechanical fluctuations to find a global minimum of a function (Ohzeki and Nishimori, 2010). In QA we start with a strong quantum field and gradually decrease its strength (quantum fluctuation) to find a ground state that is optimal. This is analogous to SA, where we decreased the temperature (thermal fluctuation) to achieve the same result.

QA begins in a coherent superposition of all possible states, but as we decrease the strength of quantum field, we approach a single solution state. This is shown on figure 1.

FIGURE 1

QA does not have neighbouring nodes that are located 1 permutation away like SA but has neighbouring nodes in a certain range that we can transition into. This range is also defined by the strength of the quantum field, slowly ceasing in the process of annealing.

If there is a short wall between current state, which happens to be a local minimum, and the global minimum, SA algorithm will need to make a series of disadvantageous moves to reach a better solution or in other words *“climb”* the wall. This is avoided by QA as It can tunnel through short walls. This effect is called *quantum tunnelling*. Comparison of thermal hopping and quantum tunnelling can be seen on Figure 2.

FIGURE 2

"The ability to rapidly sample from many states and hence characterise the shape of the energy landscape is a key benefit of this technology" (Higham and Bedford, 2021). Quantum Annealer has been developed and commercialised by D-wave and is currently used to solve real-world problems.

### Digital Annealing

## 2 Quadratic Binary Unconstrained Optimization

* 1. links

<https://www.tandfonline.com/doi/abs/10.1080/01621459.2013.872993>

https://faculty.washington.edu/aragon/pubs/annealing-pt1.pdf

* 1. links

<https://arxiv.org/pdf/1202.5868.pdf>

<https://arxiv.org/pdf/1006.1696.pdf>

<https://www.nature.com/articles/nature10012>

# References

Collins, E. F. (1921) ‘ELECTRICALLY HEATED GLASS ANNEALING LEHR1’, *Journal of the American Ceramic Society*, 4(5), pp. 335–349. doi: 10.1111/J.1151-2916.1921.TB18664.X.

Higham, C. F. and Bedford, A. (2021) ‘Quantum Deep Learning: Sampling Neural Nets with a Quantum Annealer’. Available at: https://arxiv.org/abs/2107.08710v1 (Accessed: 11 November 2021).

Kirkpatrick, S., Gelatt, ; C D and Vecchi, ; M P (1983) ‘Optimization by Simulated Annealing’, *New Series*, 220(4598), pp. 671–680.

Ohzeki, M. and Nishimori, H. (2010) ‘Quantum annealing: An introduction and new developments’.

Wu, H. and Fan, G. (2020) ‘An overview of tailoring strain delocalization for strength-ductility synergy’, *Progress in Materials Science*, 113, p. 100675. doi: 10.1016/J.PMATSCI.2020.100675.