

Group 2 Project Proposal

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Abstract: Group 2 proposes to study the convergence properties of simulated annealing, genetic algorithms, and ant-colony approaches towards finding optimal solutions for various travelling salesman problems. Code will be tested to find convergence rate, wall-clock time, and for solution space exploration. For future studies, we will consider looking at parallel and/or GPU solutions to accelerate algorithms.

1. Introduction

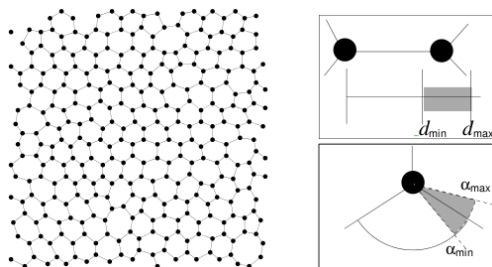


Figure 1: An example of an amorphous solid under simulation. A maximum vertex number of 3 is defined, along with minimum and maximum angles and bond lengths; taken from: Ref. 3

2. Simulated Annealing

Simulated annealing is a stochastic approach towards minimizing an energy function.

3. Genetic Algorithms

Unlike simulated annealing, genetic algorithms rely on a population approach to

4. Ant-Colony Approaches

Ant Colony Optimization [2] draws inspiration from the behavior of ants as they develop a path from their nest to a food source. As ants travel, they deposit pheromones. These pheromones can be detected by other ants and the ants are more likely to follow a path with higher pheromone concentration. In addition to the ants depositing pheromones, these

pheromones will evaporate over time. This means that shorter paths will allow larger pheromone concentrations to buildup as ants will be depositing pheromones quicker than they evaporate. Eventually, the system will converge on a minimum solution. A global minimum is pursued by starting out with a large number of ants and by tuning the weight at which pheromones influence decisions.

5. Go with the Winner Approaches

Simulated annealing probabilistically converges to the optimal solution at the rate of $O(\frac{1}{n})$ where n is the number of independent runs. Using heuristic schemes such as the “Go with the Winner” [1], hereby referred to as GWW, one can improve this convergence rate to $O(\log \frac{1}{n})$ and have recently found their way into molecular modeling applications [3]. In general terms, the GWW algorithm mirrors that of simulated annealing; however, each independent run is periodically reassessed to determine if one is converging upon a losing solution. Runs with no chance for success are immediately discarded while runs with the best chance of finding an optimal solution are replicated; thus, GWW generates an ensemble of independent runs filled with “winners”.

6. Analysis

To test the performance of these optimization schemes, we will minimize the energy of depositing particles on a surface. Given that the deposition pattern of particles is not unique, all of the optimization schemes will need to generate an ensemble of models representing local minima on the potential energy surface. To quantify the phase space coverage of these optimization schemes, we will generate multiple deposition models and study how the results cluster. Additionally, we will study the convergence rate and wall-clock time for each algorithm.

References

- [1] Aldous D. and Vazirani U. Go with the winners algorithms. *Proceedings of the 35th IEEE Symposium on Foundations of Computer Science*, pages 492–501, 1994.
- [2] Marco Dorigo, Vittorio Maniezzo, and Alberto Coloni. The ant system: Optimization by a colony of cooperating agents. *IEEE TRANSACTIONS ON SYSTEMS, MAN, AND CYBERNETICS-PART B*, 26(1):29–41, 1996.
- [3] Marcus Peinado and Thomas Lengauer. ‘go with the winners’ generators with applications to molecular modeling. *RANDOM*, pages 135–149, 1997.