Travelling Salesman Problem:
Convergence Properties of Optimization Algorithms

Group 2

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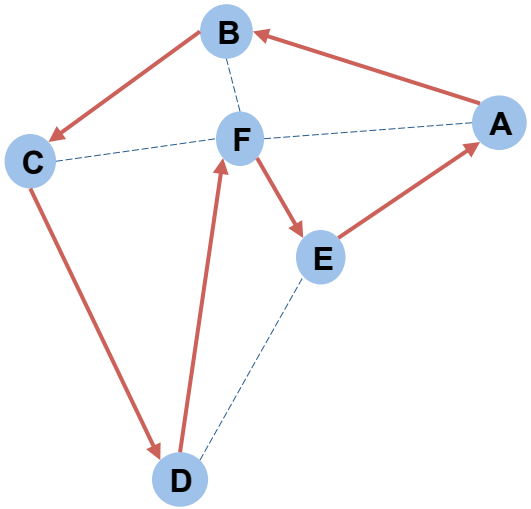
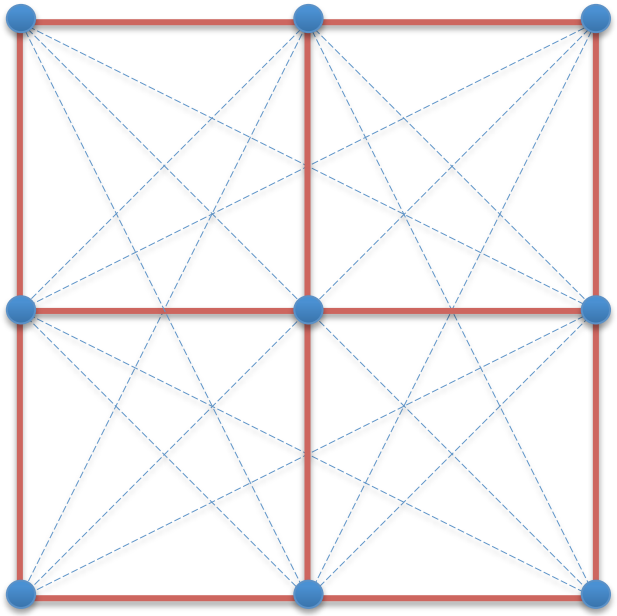
Introduction



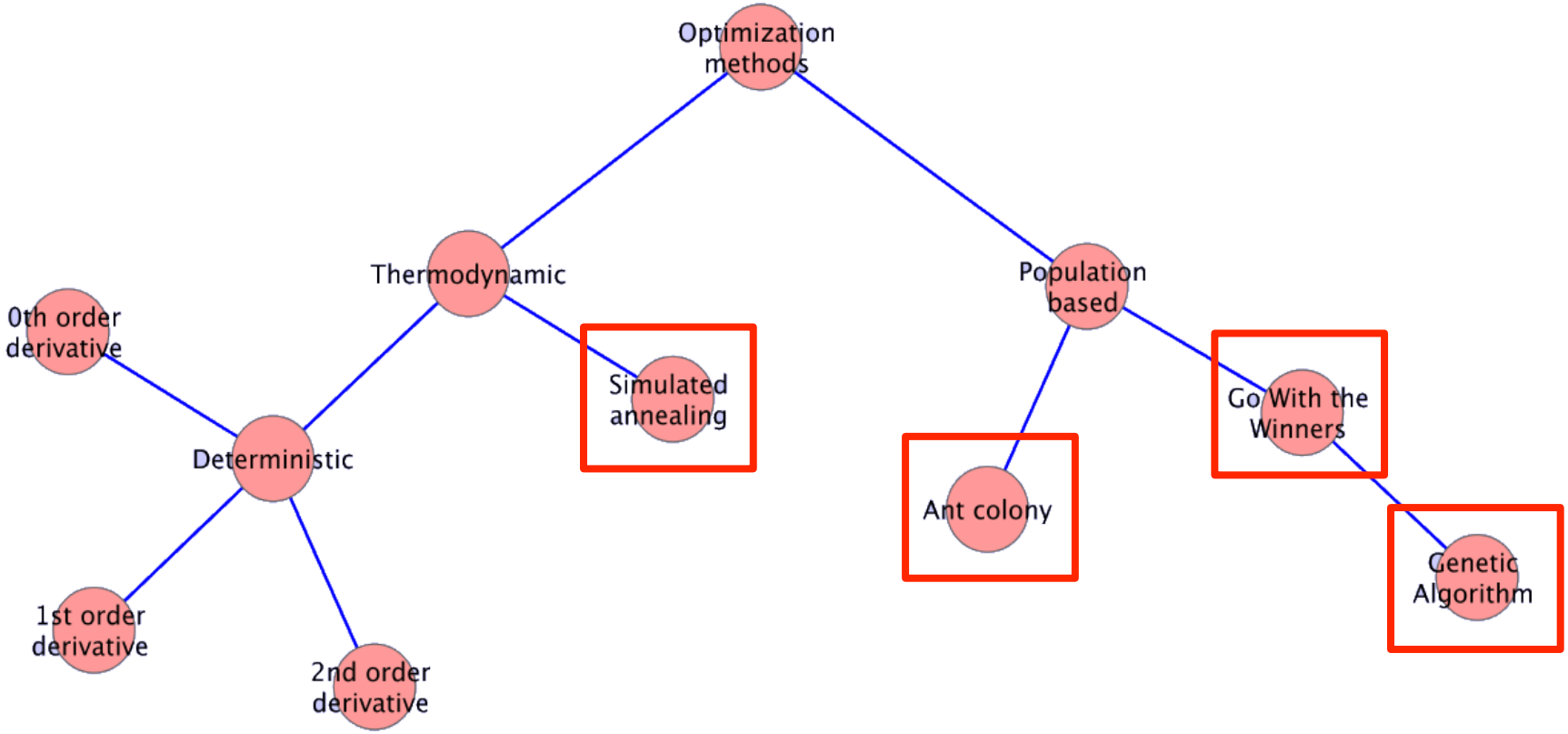


Travelling Salesman Problem

Surface Reconstruction

1. Marcus Peinado and Thomas Lengauer. `go with the winners' generators with applications to molecular modeling. RANDOM, pages 135{149, 1997.

Hierarchy of Optimization Methods



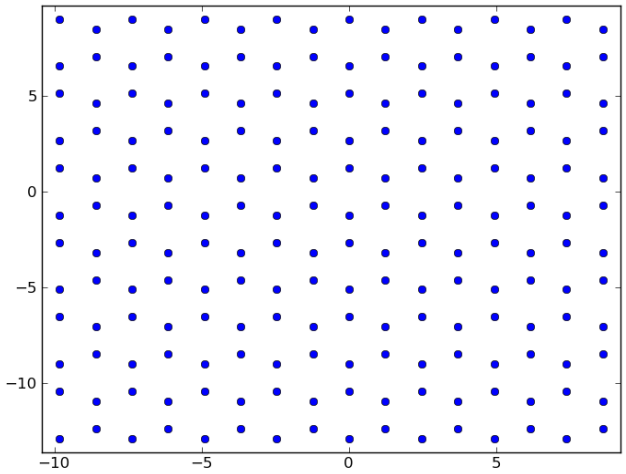
Hamiltonian Description

$$H(r_0 \ldots r_n, V_0 \ldots V_n) = k_b \sum_{i,j}^{n,n} (r_i - r_j)^2 + k_v \sum_{k}^{n} \| V_k - V_0 \|$$

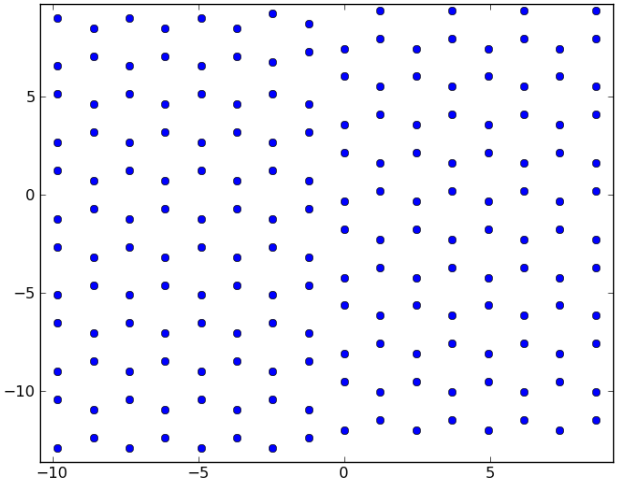
Penalizes vertices with connections unequal to required connection

Where,
r_i is the position of $particle_i$
V_k is the number of vertices $particle_i$ is connected to
V_0 is the actual number of vertices $particle_i$ should be connected to
$k_b = 1$, bond constant
$k_v = 1024$, vertex constant

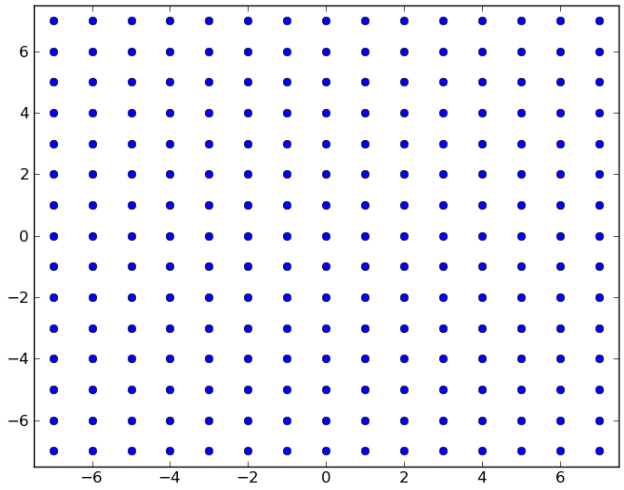
Test Systems



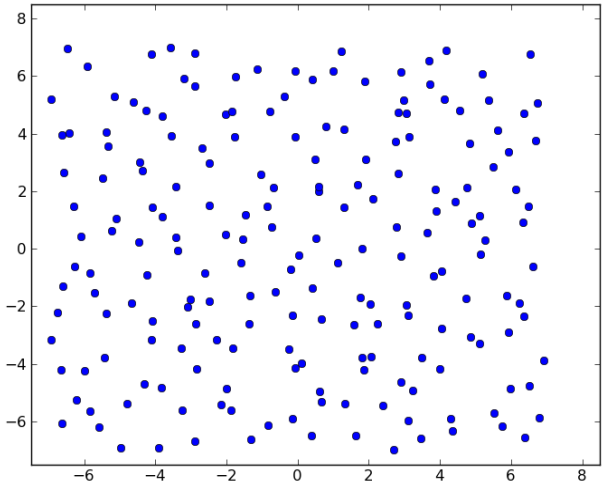
Honeycomb Lattice



Sheared Honeycomb Lattice



Square Lattice



Square Lattice – Random Positions

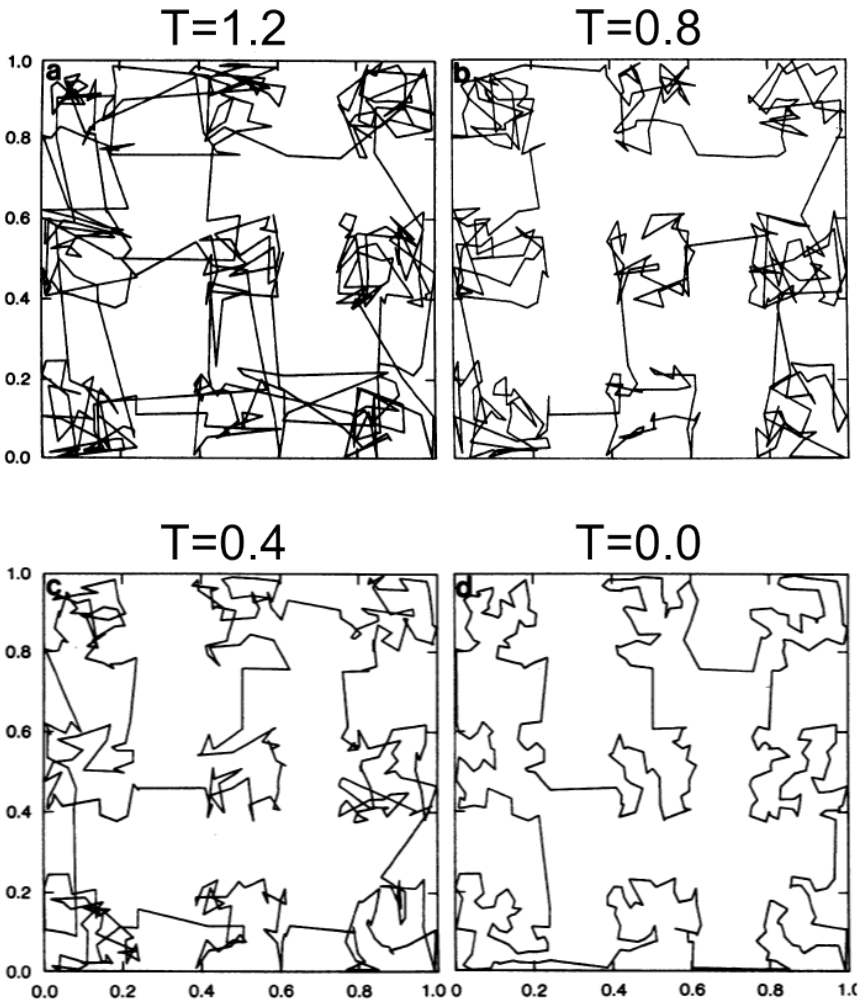
Code Implementation

- **Java – *Heavylifting***
  - Cross-Platform
  - Abstraction
  - TDD - JUnit
  - Threads
- Python – *Analysis*
- Tcl (VMD) – *Analysis*
- Awk – Input File
-

```
//Test copy constructor
surf.disconnectAll();
Surface clone = new Surface(surf);
clone.connect(0,1);
assertEquals(2,clone.missingVertex(0));
assertEquals(3,surf.missingVertex(0));
assertEquals(true,clone.connected(0,1));
assertEquals(false,surf.connected(0,1));
```

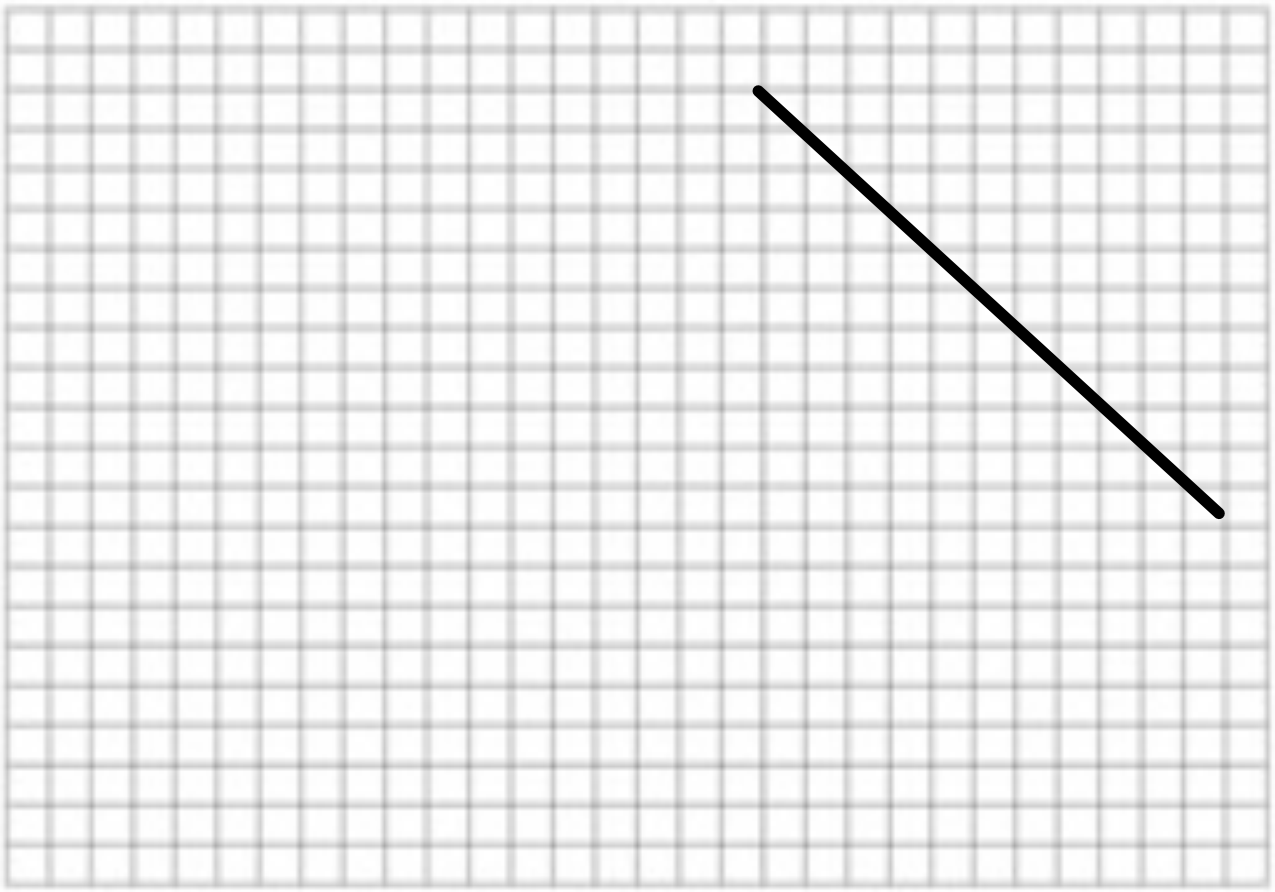
Simulated Annealing: Controlled Cooling

$$e^{-E/k_B T}$$



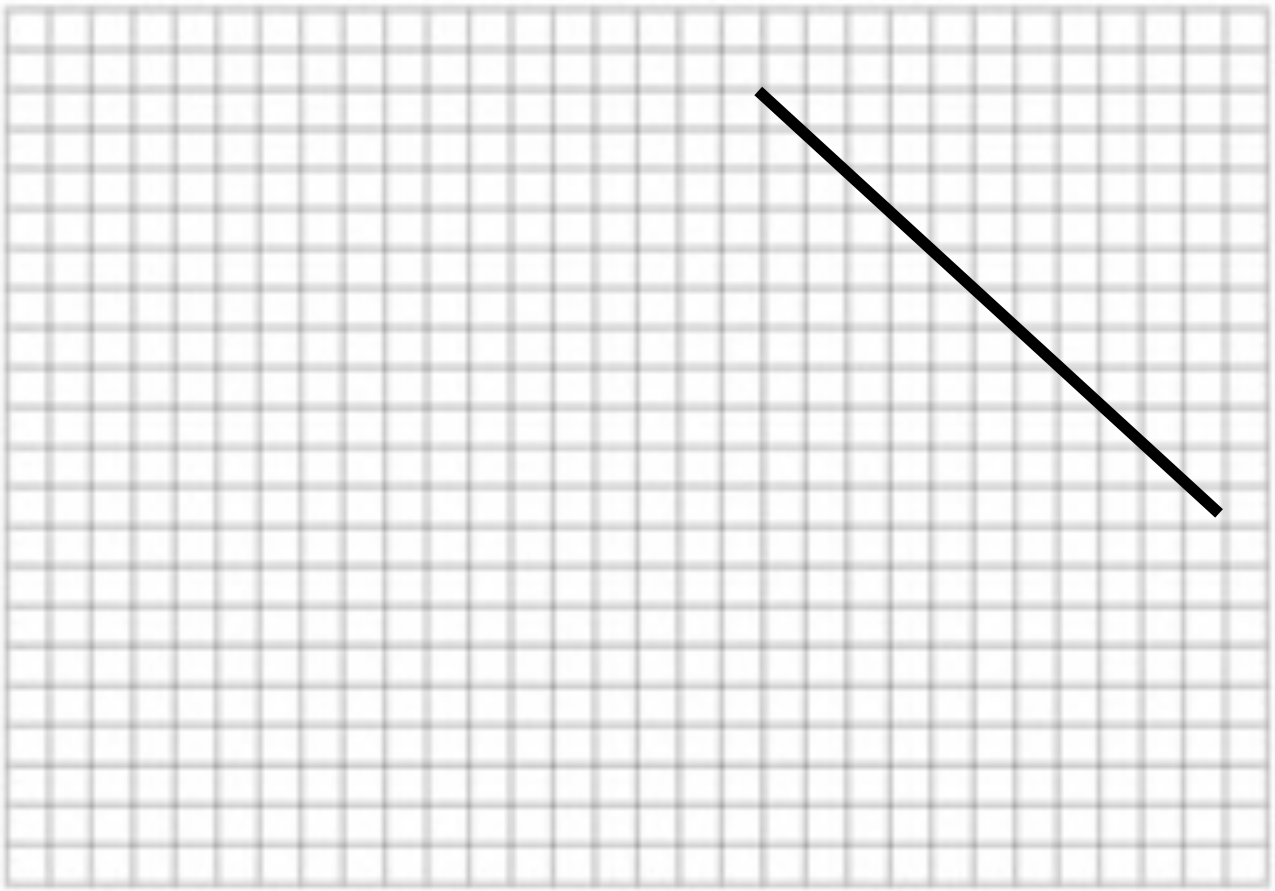
1. "Optimization by Simulated Annealing" S. Kirkpatrick, C. D. Gelatt, Jr., and M. P. Vecchi, Science 13 May 1983: 220 (4598), 671-680.

Simulated Annealing Moves



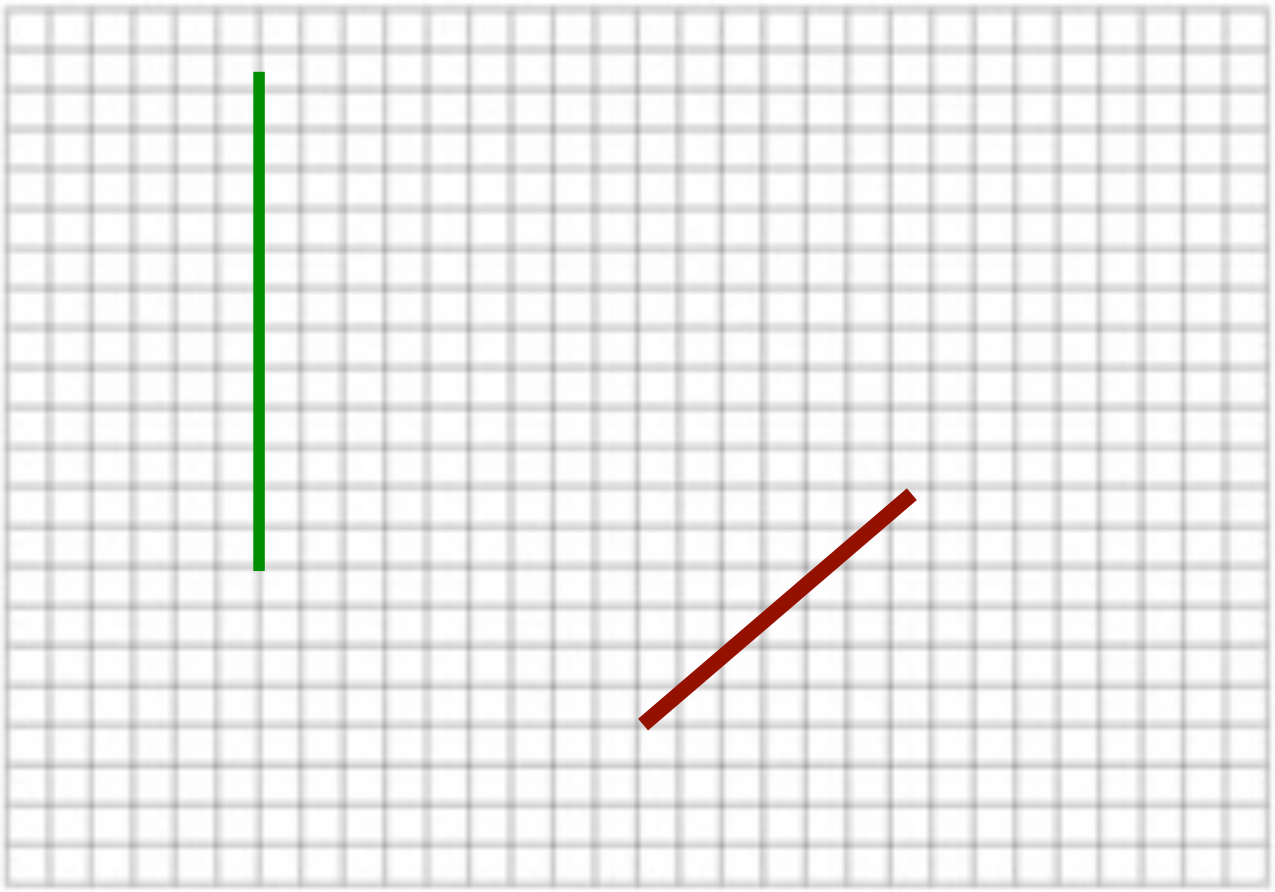
http://mathbits.com/mathbits/studentresources/graphpaper/graphpaper.htm

Simulated Annealing Moves



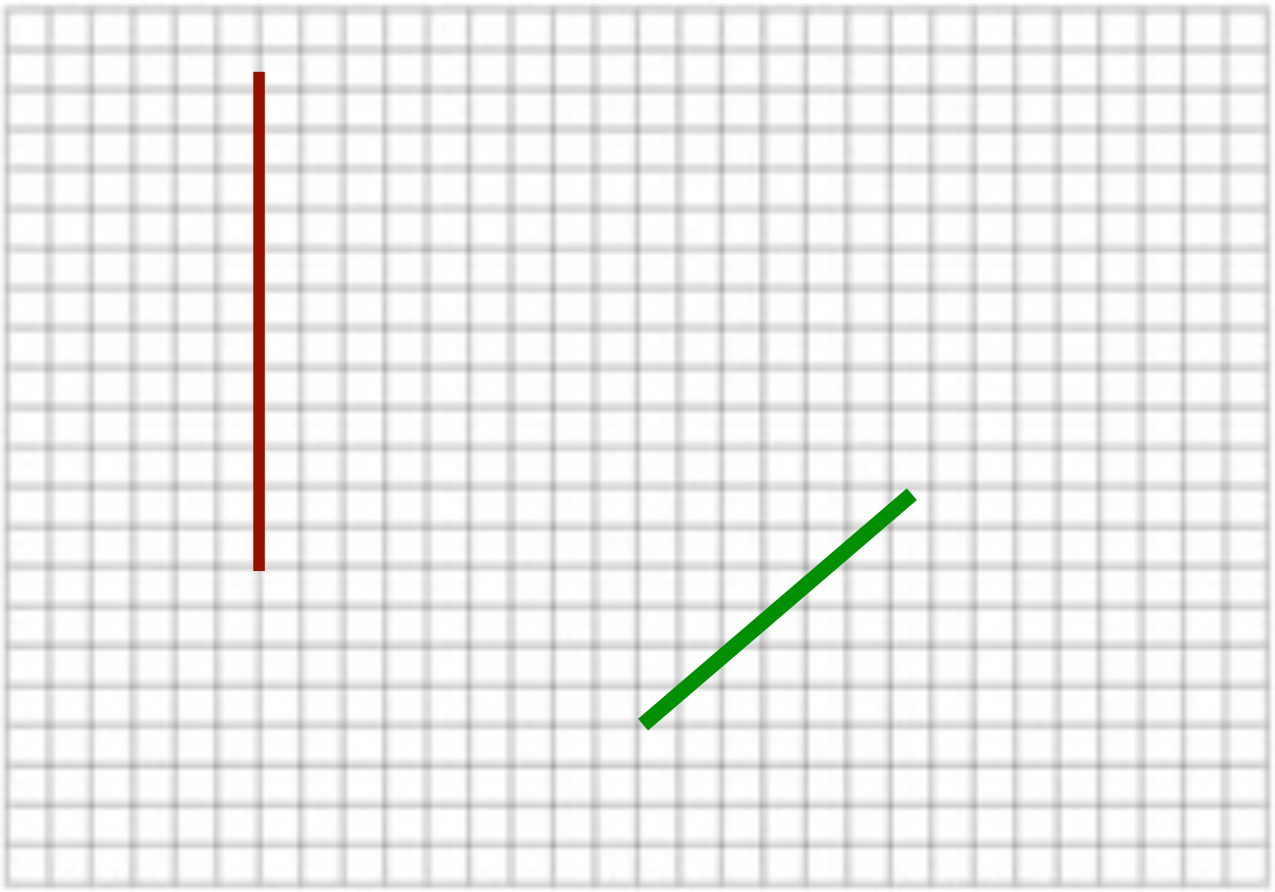
http://mathbits.com/mathbits/studentresources/graphpaper/graphpaper.htm

Simulated Annealing Moves



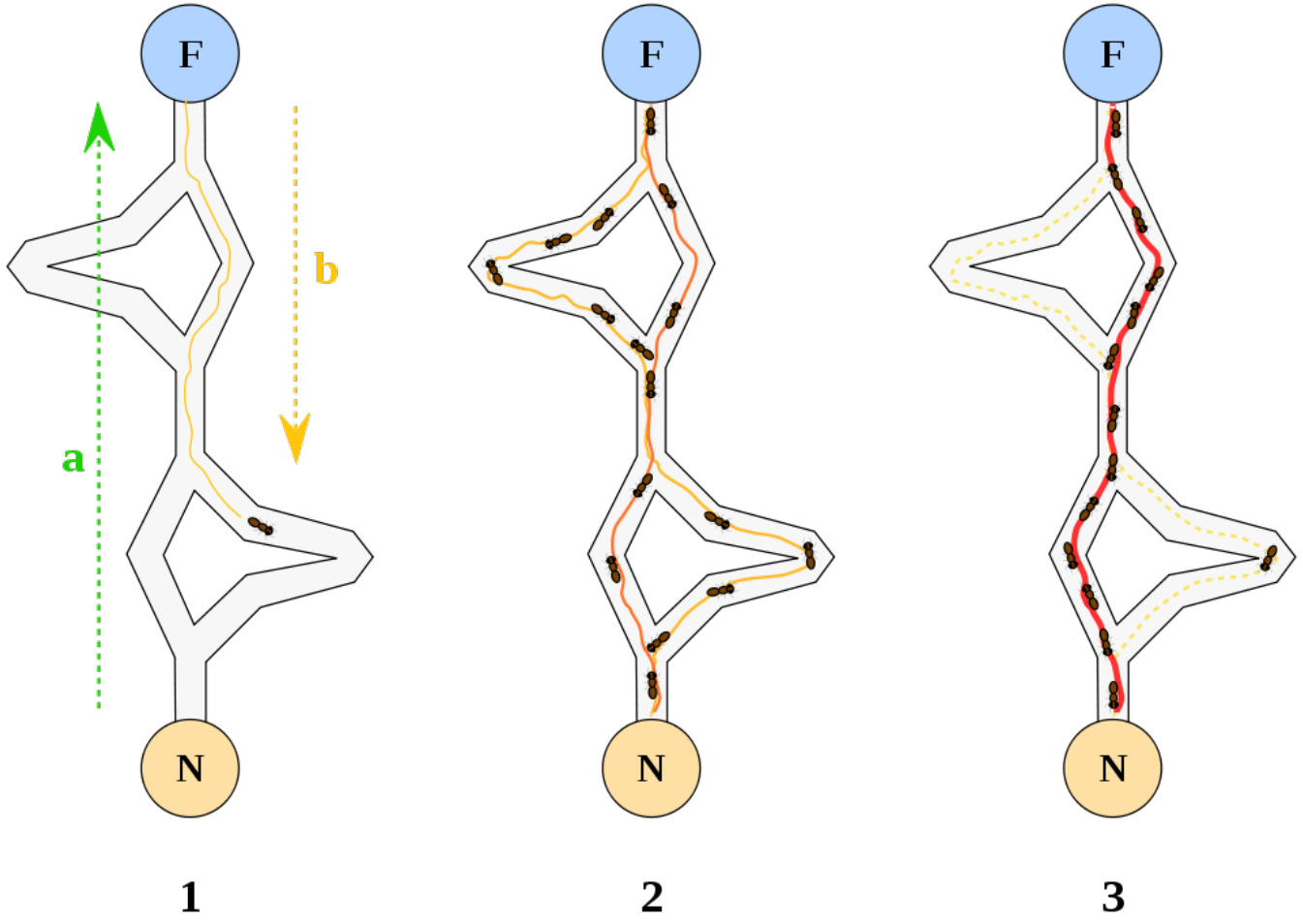
http://mathbits.com/mathbits/studentresources/graphpaper/graphpaper.htm

Simulated Annealing Moves



http://mathbits.com/mathbits/studentresources/graphpaper/graphpaper.htm

Ant Colony



1.http://en.wikipedia.org/wiki/File:Aco_branches.svg

Ant Colony - Implementation

- Pheromone Matrix
- Each Ant Constructs a Solution
- Update Pheromone Matrix
-

Ant Colony – Implementation (contd..)

- Update pheromones based on energy

$$P_{ij} = (1 - r)P_{ij} + \sum_{k} \frac{Q}{L_k}$$

Ant Colony – Implementation (contd..)

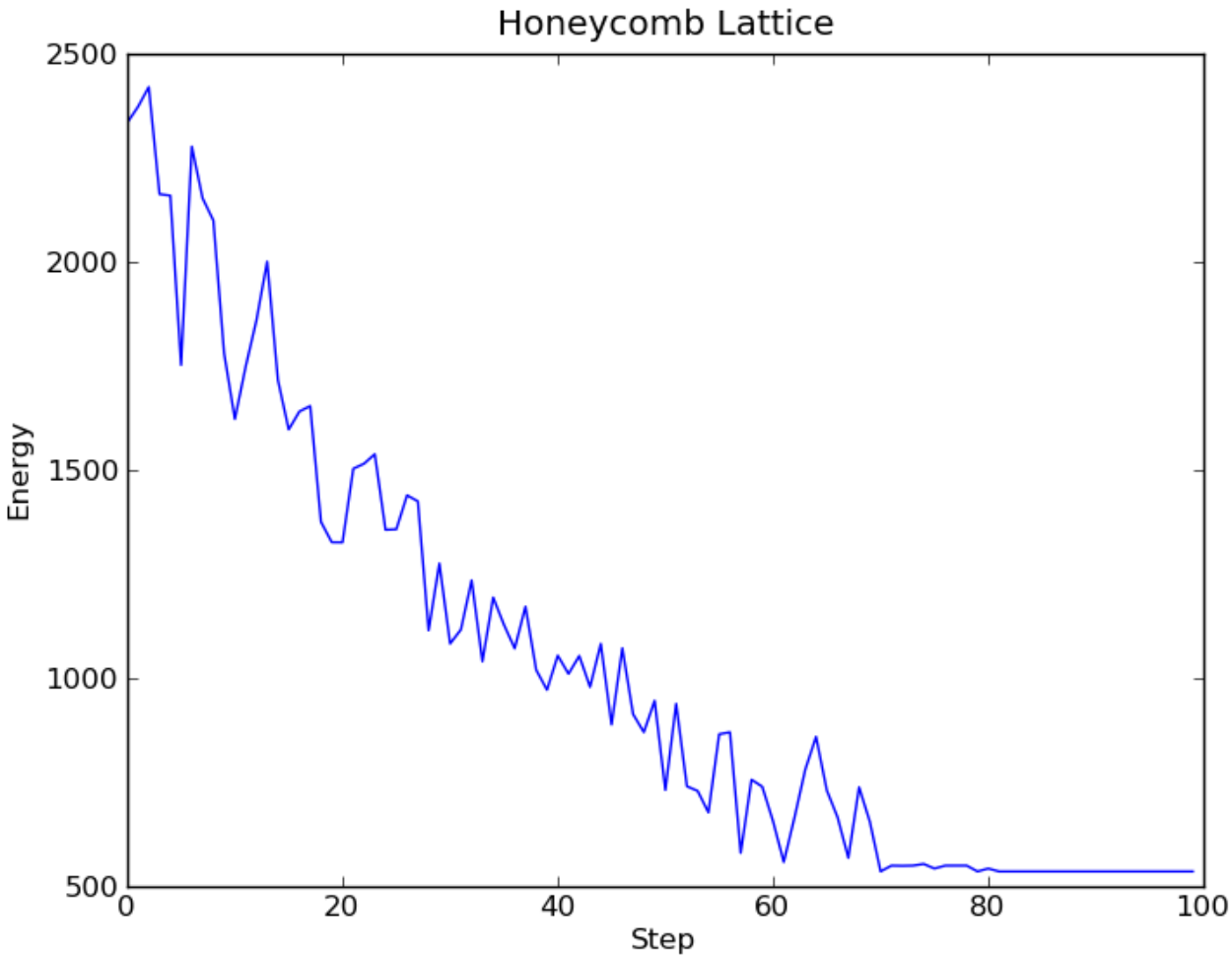
- Update pheromones based on energy:

$$P_{ij} = (1 - r)P_{ij} + \sum_{k} \frac{Q}{L_k}$$

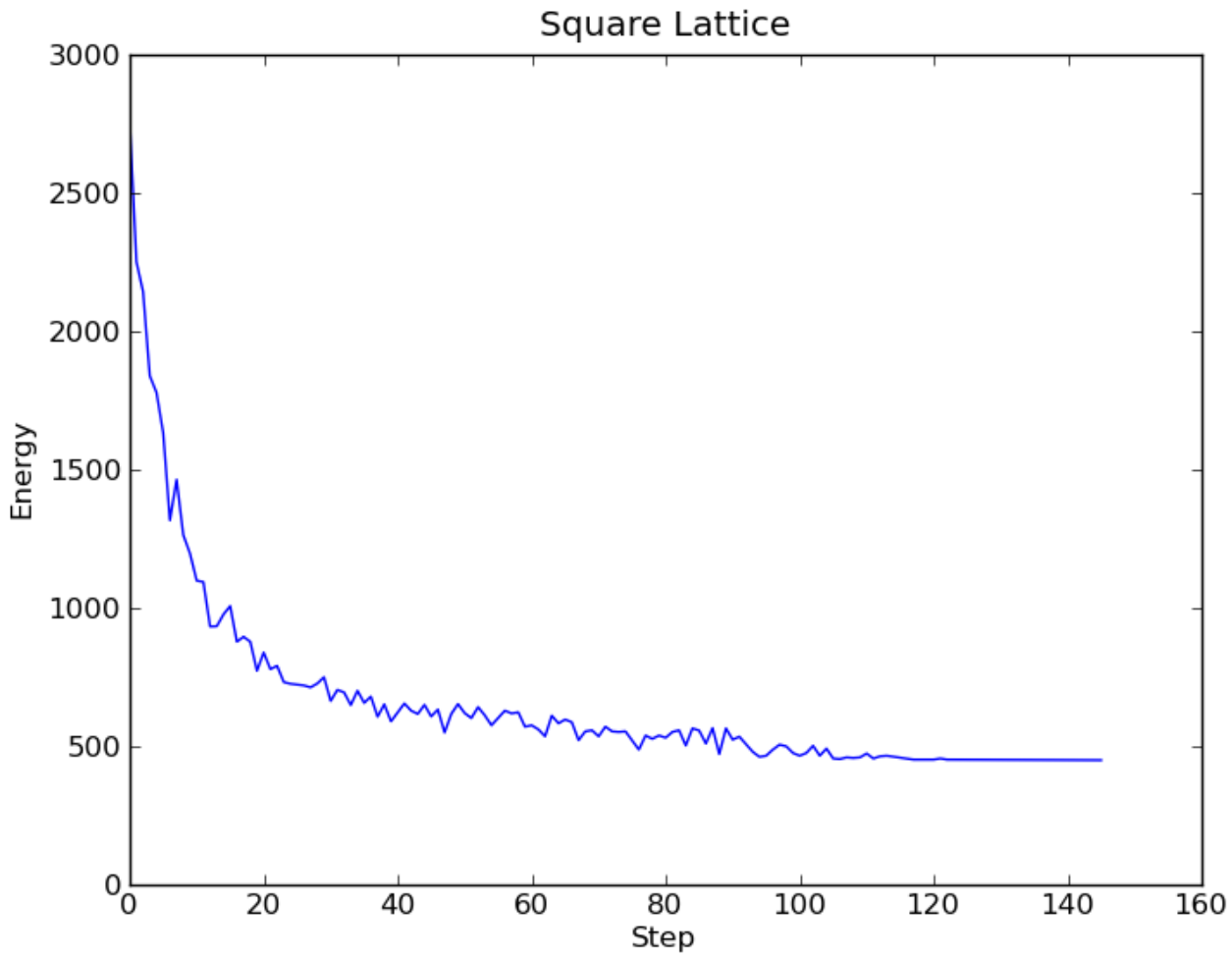
- Accept moves during walk with probability:

$$A_{ij} = \frac{1}{Z} \frac{(P_{ij})^{\beta}}{(d_{ij})^{\alpha}}$$

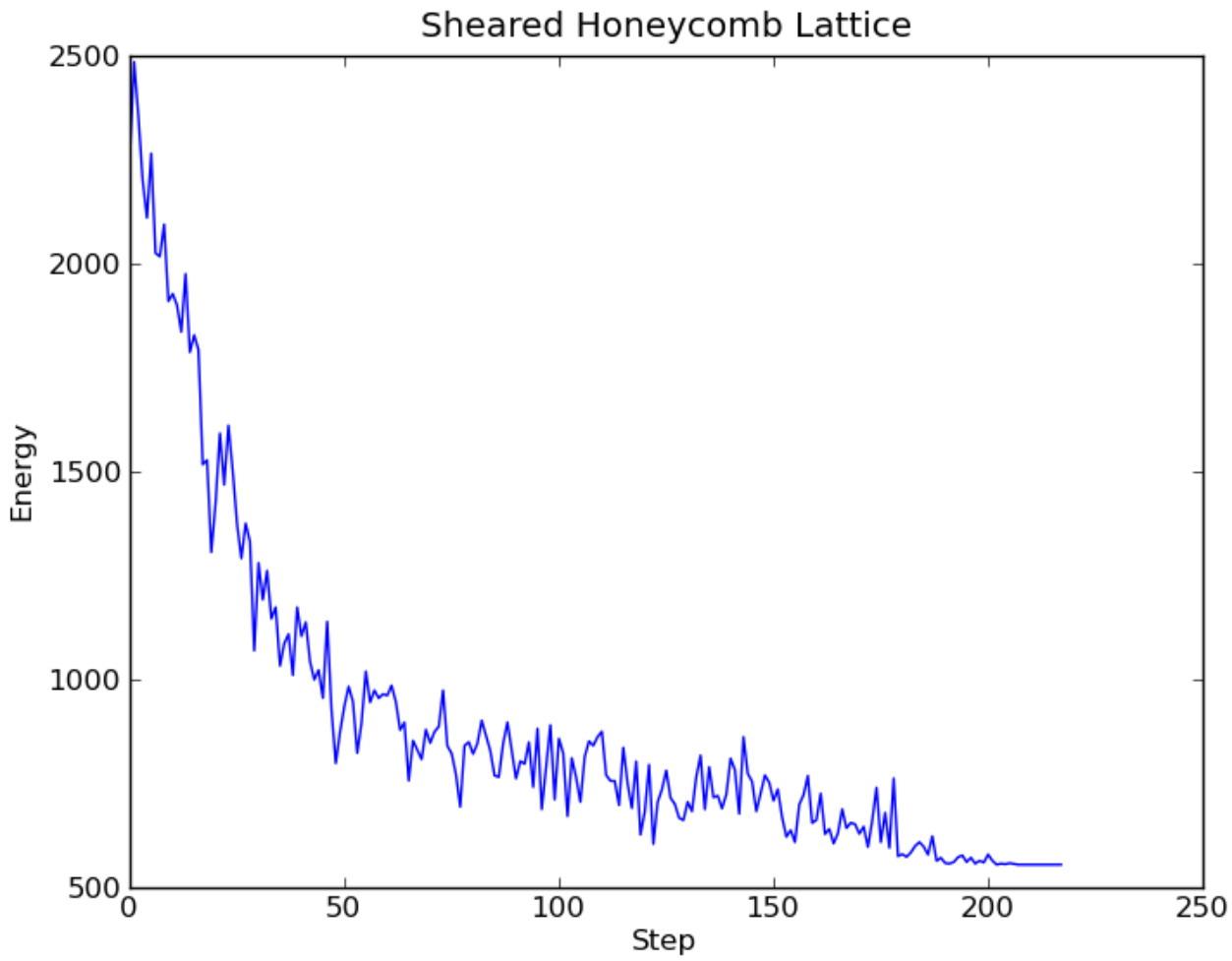
Ant Colony – Discussion



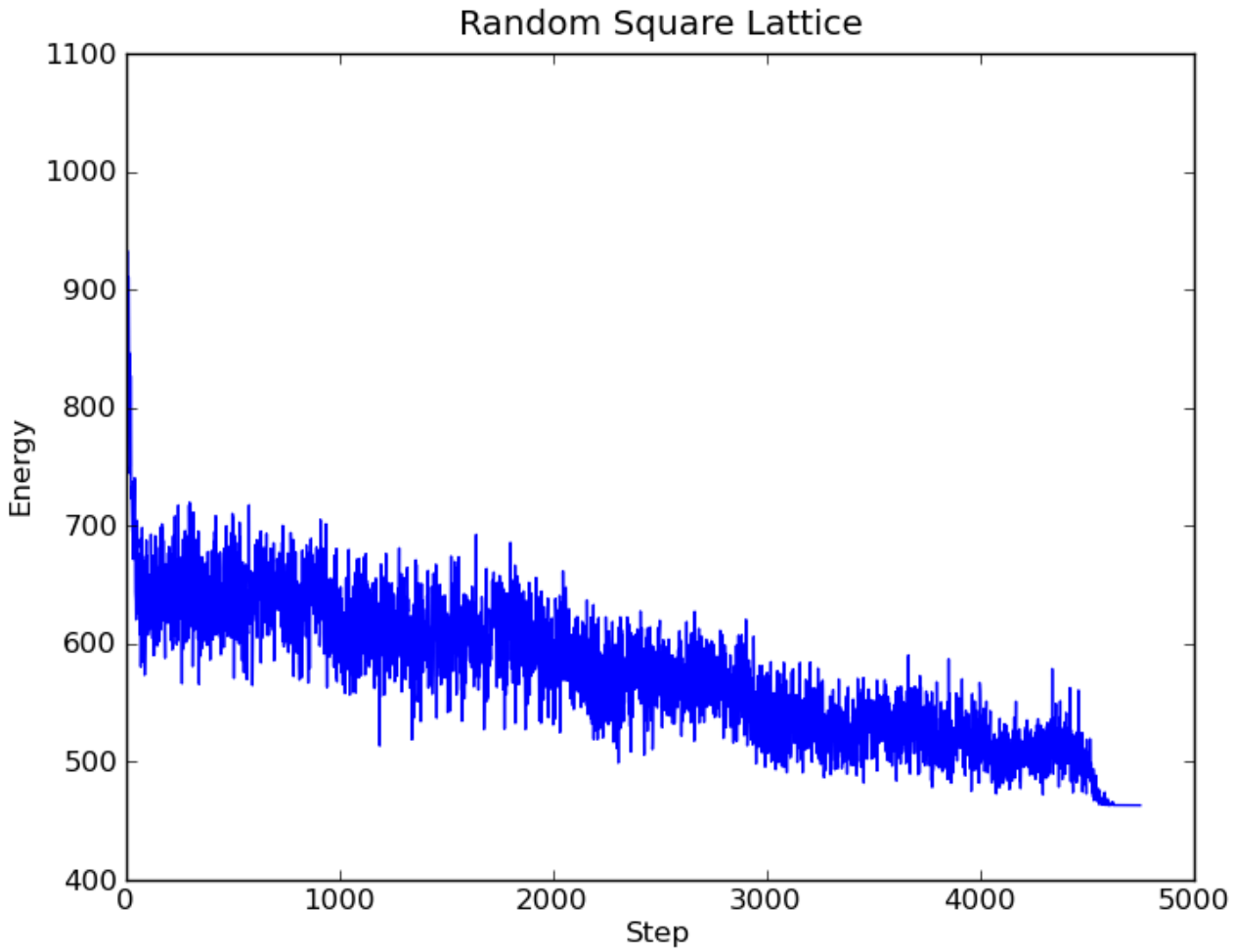
Ant Colony – Discussion



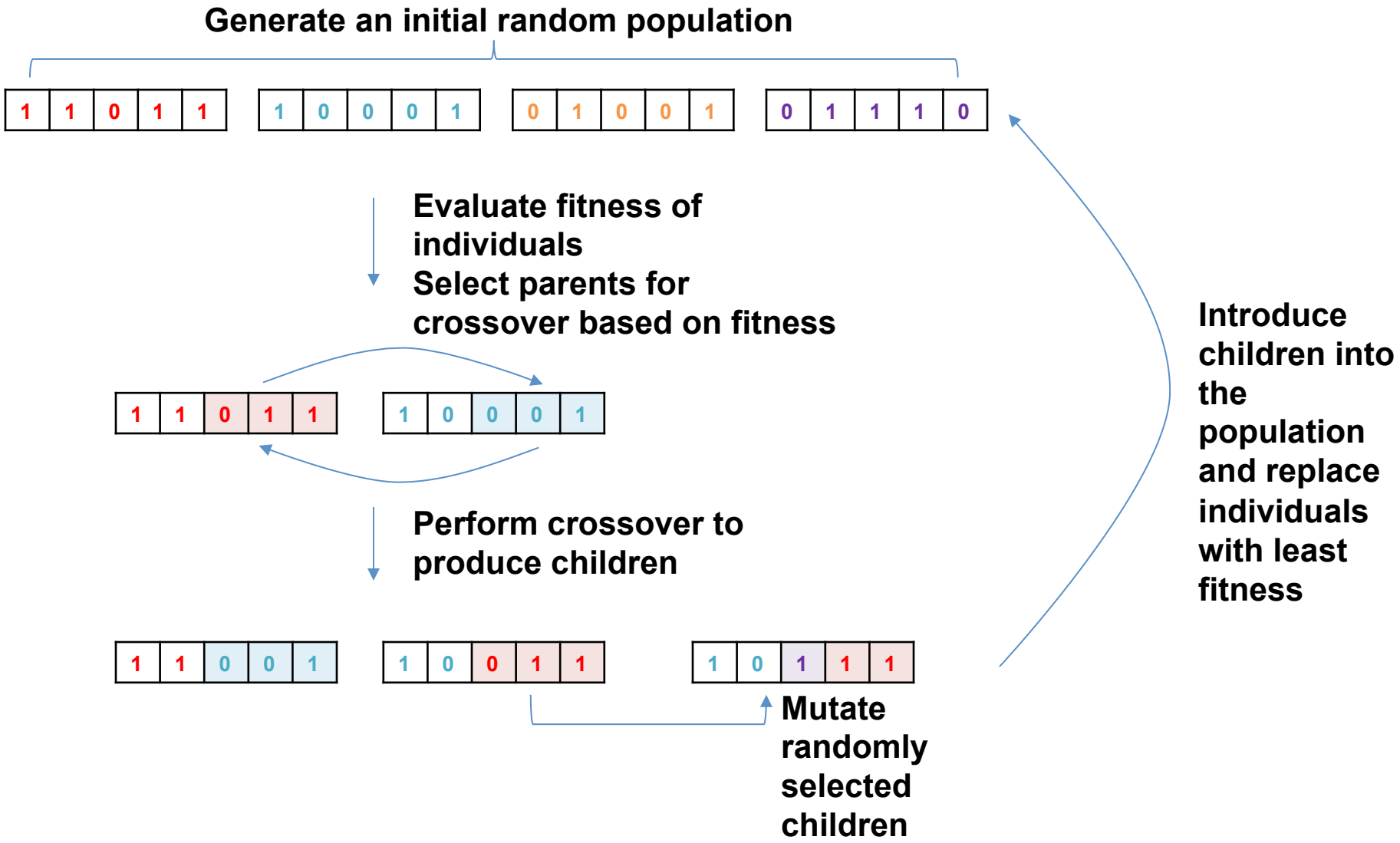
Ant Colony – Discussion



Ant Colony – Discussion



Genetic Algorithms: Survival of the Fittest

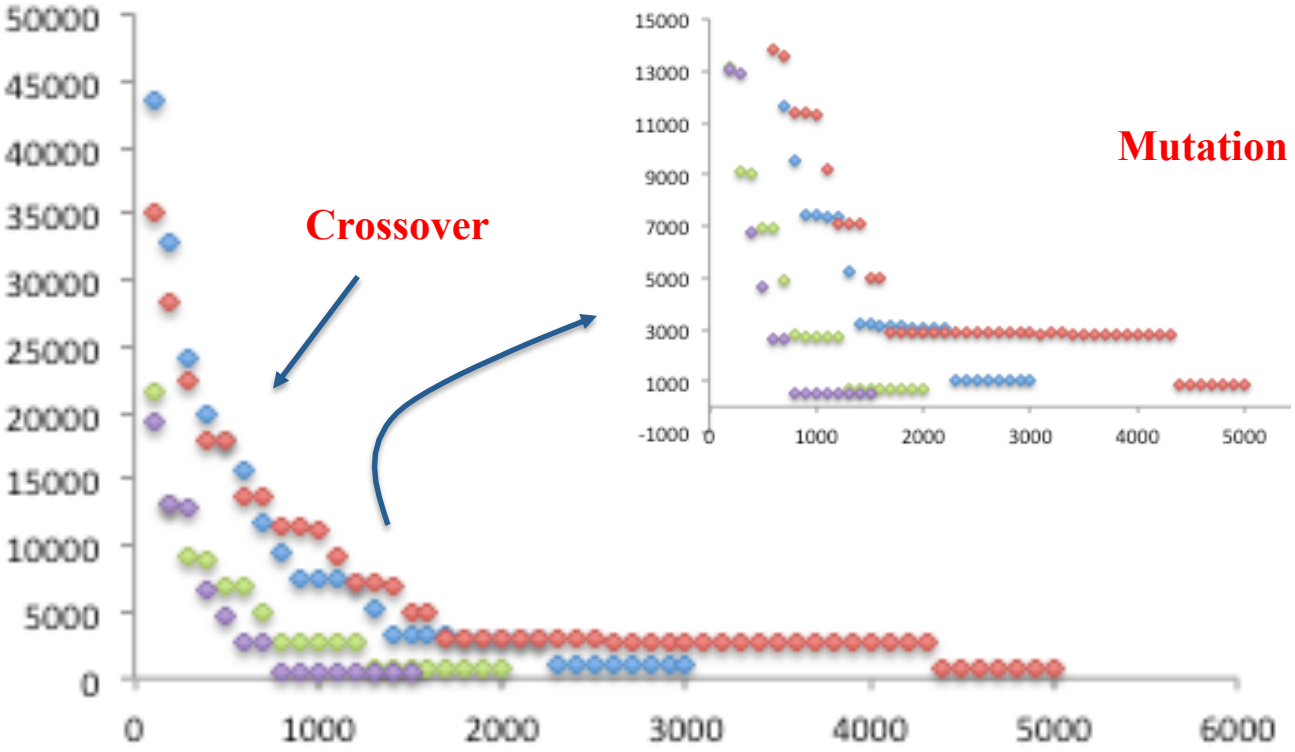


1. "A genetic algorithm tutorial", Darrell Whitley , Statistics and Computing, Volume 4, Number 2, 65-85, DOI: 10.1007/BF00175354

Genetic Algorithm: Generation Rules

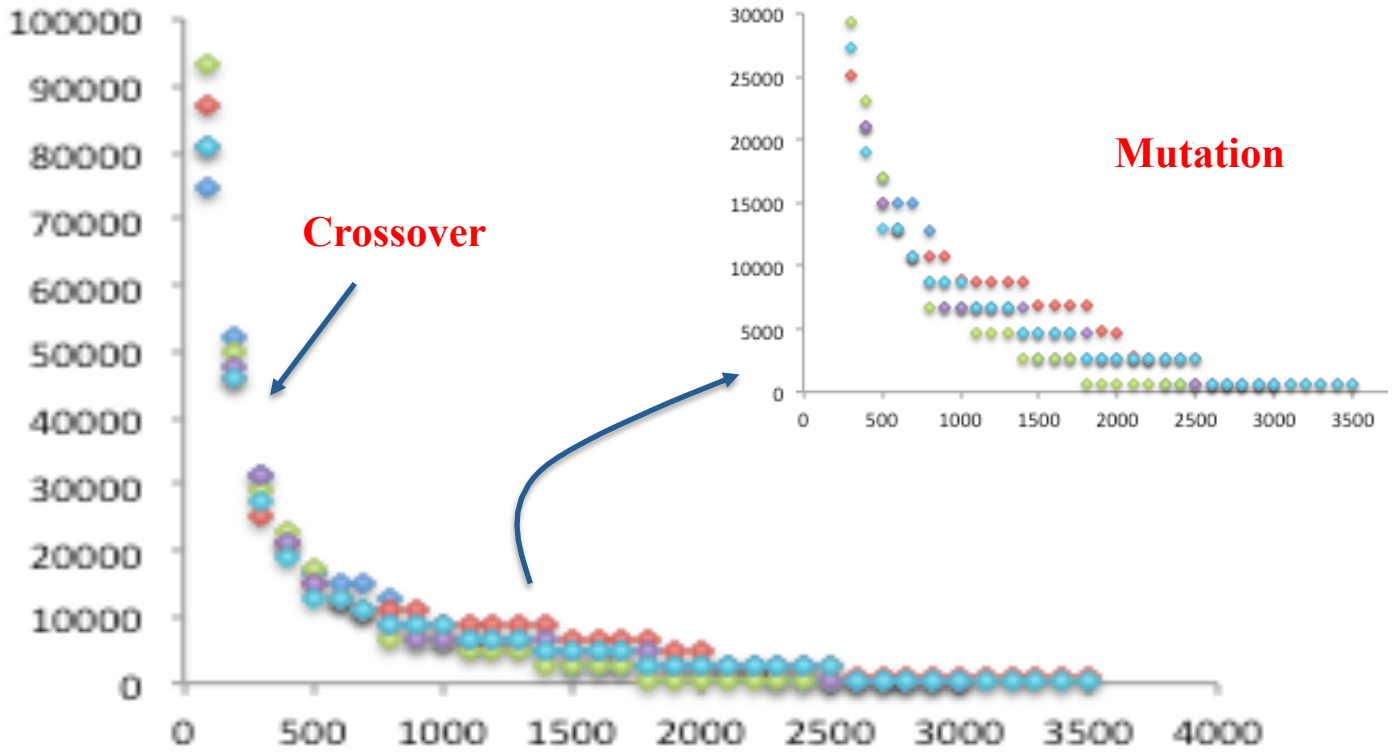
- **Selection - Fitness proportionate/roulette-wheel selection:**
  - Area of the wheel assigned to each parent in proportion to fitness
- **Crossover - Matrix Crossover Variant:**
  - Select a column M at random and interchange column data between parents
  - After interchange, $V_k > V_0$ for any particle, disconnect from farthest neighbor
- **Mutation - 2-Opt Operator Variant:**
  - Connect all particles between two randomly chosen points i_1 and i_2 with a randomly chosen neighbor
  - After interchange, $V_k > V_0$ for any particle, disconnect from farthest neighbor

Genetic Algorithm: Energy v/s Iterations



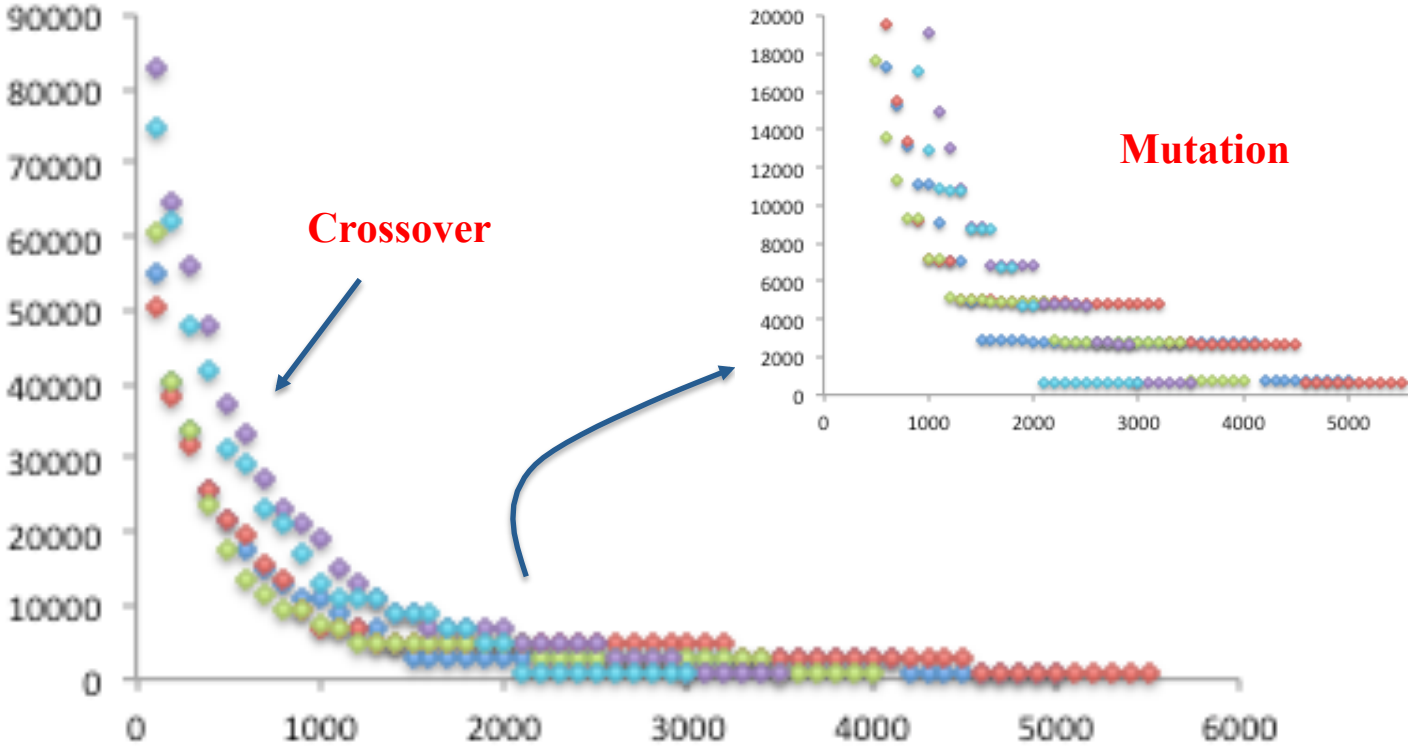
Hexagonal Lattice

Genetic Algorithm: Energy v/s Iterations



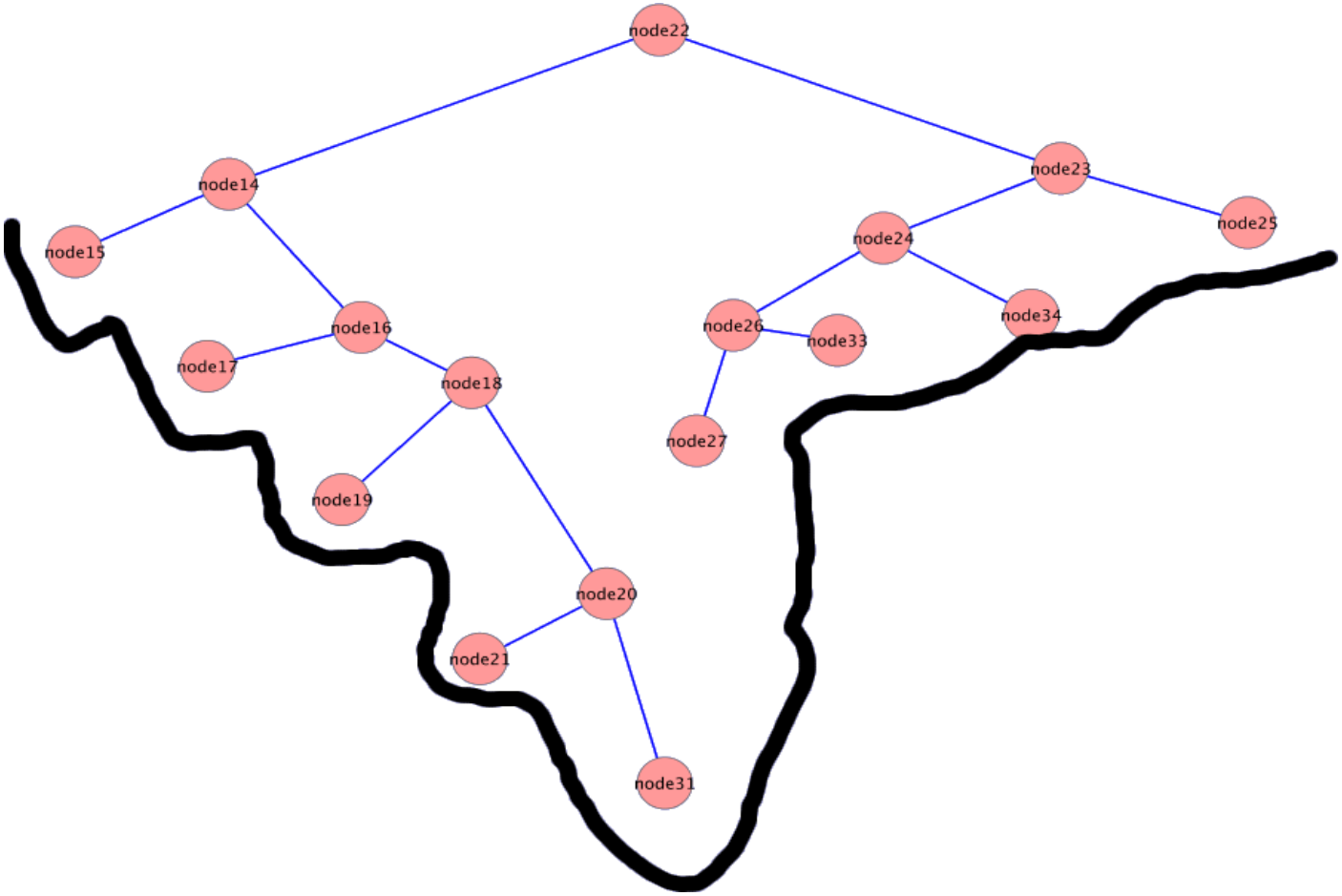
Sheared Hexagonal Lattice

Genetic Algorithm: Energy v/s Iterations



Square Lattice – Random Positions

Go With The Winners



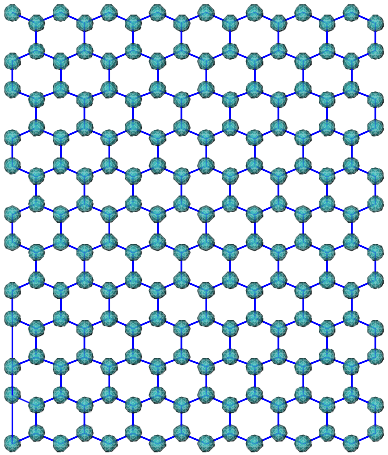
Go With The Winners

GWTW – Simulated Annealing with survival of fittest

- Moves are predetermined
  - Create/destroy bonds
  - Swap bonds to explore phase space faster
- Survival of the fittest
  - Select single winner of system
  - Kill off lower half of population
  - Repopulate single winner clone

Honeycomb Lattice: Comparison

Best Solutions

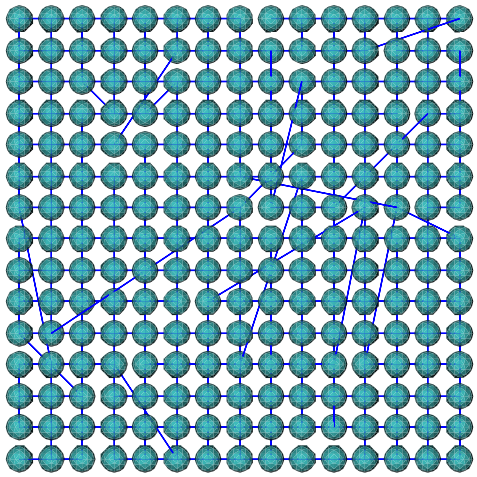


All Algorithms

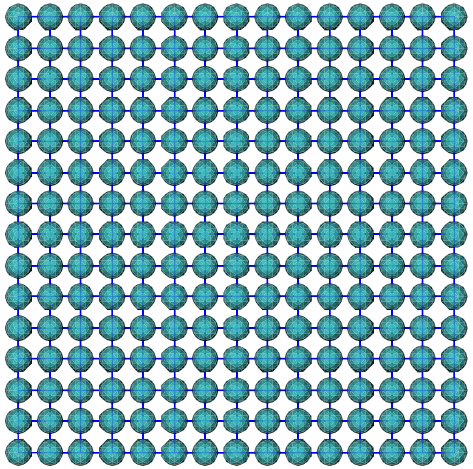
	Simulated Annealing	Ant Colony Optimization	Genetic Algorithm	Go With the Winner
Avg Energy	535.967999	535.967999	703.6449	535.967999
Best Energy	535.967999	535.967999	535.967999	535.967999
Avg Run Time (s)	797	9	113	1422
Avg Iterations	800000	94	2800	400000

Square Lattice: Comparison

Best Solutions



Simulated Annealing

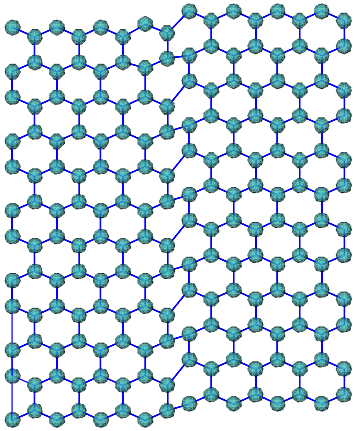


Other Algorithms

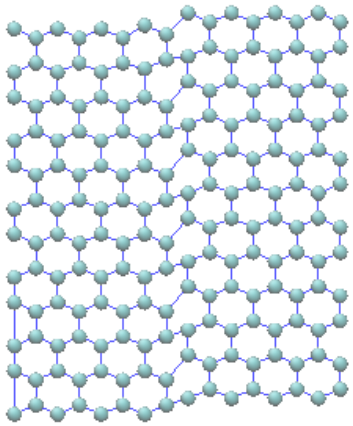
	Simulated Annealing	Ant Colony Optimization	Genetic Algorithm	Go With the Winner
Avg Energy	1277	450	450	1518
Best Energy	1277	450	450	450
Avg Run Time (s)	1093	24	113	1713
Avg Iterations	800000	128	2800	400000

Sheared Hexagonal Lattice: Comparison

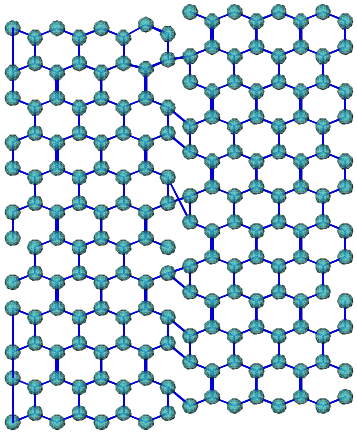
Best Solutions



Ant Colony Optimization



Genetic Algorithm

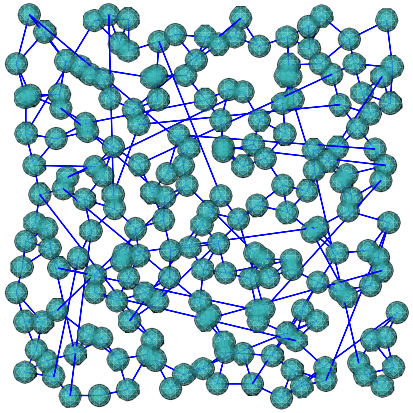


Go With the Winner

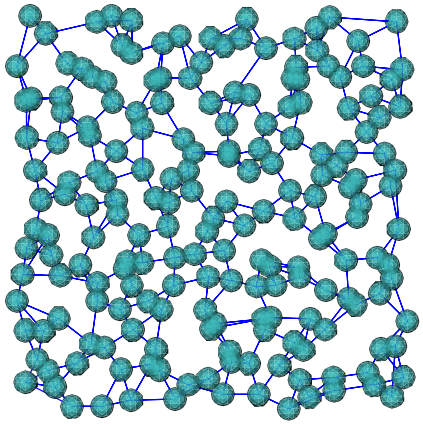
	Ant Colony Optimization	Genetic Algorithm	Go With the Winner
Avg Energy	554.928	606.89764	962.64
Best Energy	554.928	554.928	962.64
Avg Run Time (s)	4	155	940
Avg Iterations	243	3100	400000

Square Lattice-Random Positions: Comparison

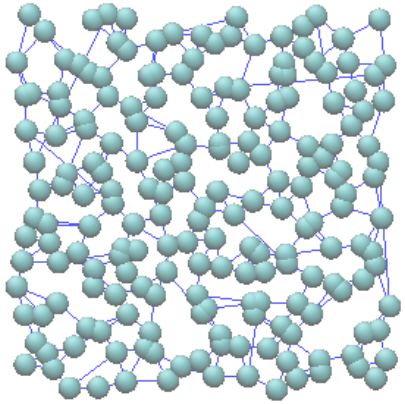
Best Solutions



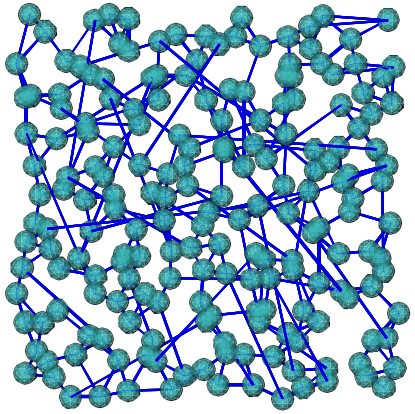
Simulated Annealing



Ant Colony Optimization



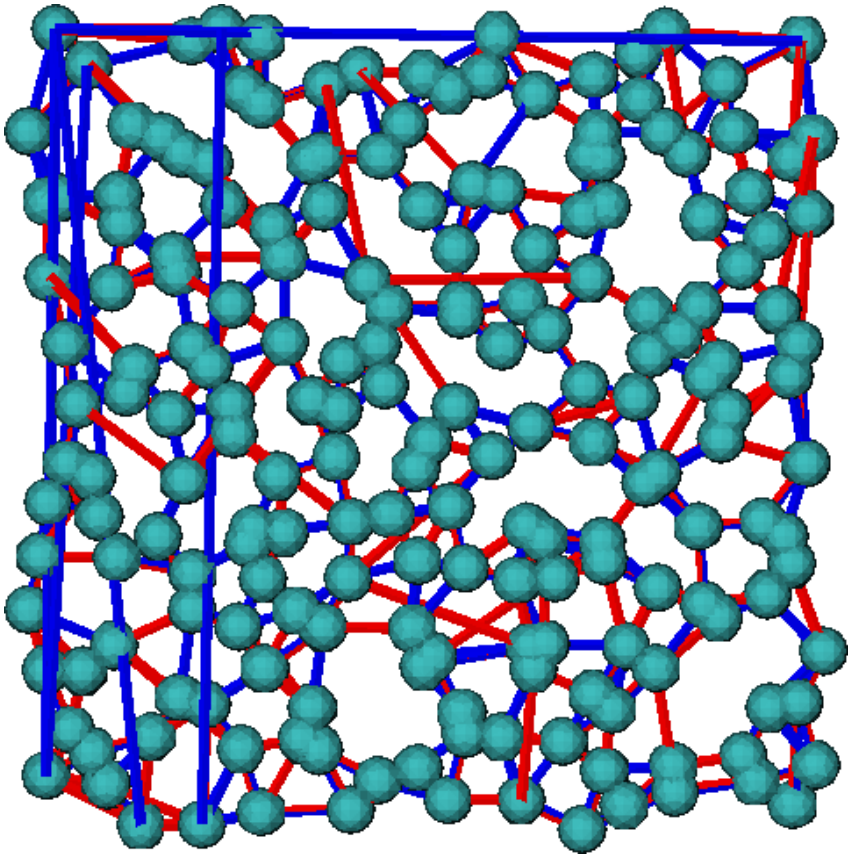
Genetic Algorithm



Go With the Winner

	Simulated Annealing	Ant Colony Optimization	Genetic Algorithm	Go With the Winner
Avg Energy	2999.99	463.1	672.762708	2708.94068
Best Energy	2999.99	463.1	612.181165	2571.18136
Avg Run Time (s)	821	715	187	1435
Avg Iterations	800000	5101	4200	400000

Comparison Between Solutions

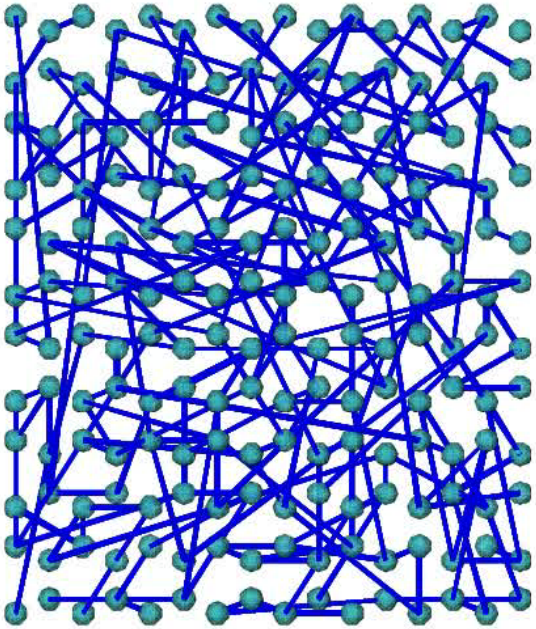


Square Lattice - Random Positions
ACO
GA

Connections
634 similar
270 unique

138 : 132 Left v/s Right

Sample Optimization: ACO for Honeycomb



Conclusion

- ACO outperforms other algorithms in all test cases
- GA generates multiple solutions – search space exploration
- SA is not very efficient for this problem
- GWTWs accelerates convergence of SA methods; also yields lower energy solutions
- Choice of move is essential for efficient computation
- Must highly tune code to run

Thank You