



CSE Case Studies Seminar

S. Kirkpatrick et al.: Optimization by Simulated Annealing

Beat Hubmann

Optimization by Simulated Annealing

S. Kirkpatrick, C. D. Gelatt, Jr., M. P. Vecchi

In this article we briefly review the central constructs in combinatorial optimization and in statistical mechanics and then develop the similarities between the two fields. We show how the Metropolis algorithm for approximate numerical simulation of the behavior of a many-body system at a finite temperature provides a natural tool for bringing the techniques of statistical mechanics to bear on

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Since the NP-complete class of problems contains many situations of practical interest, heuristic methods have been developed with computational require-

Summary. There is a deep and useful connection between statistical mechanics

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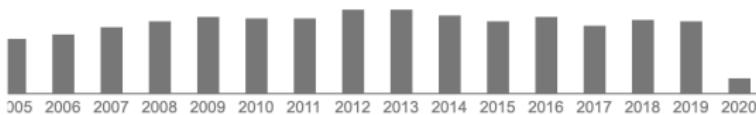
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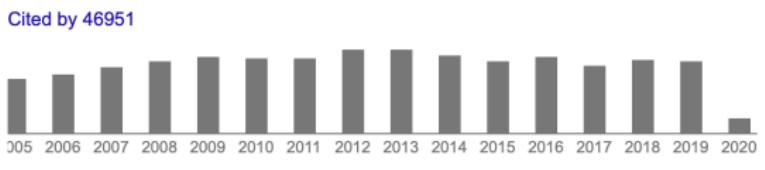
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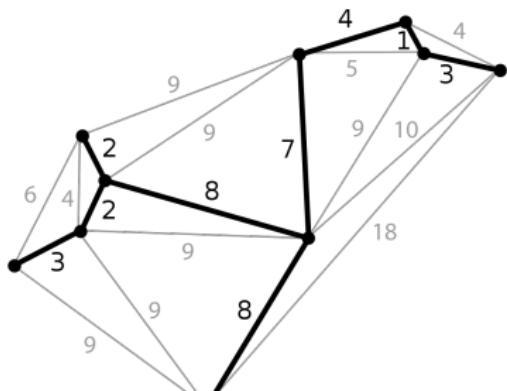
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[2]

Combinatorial optimization

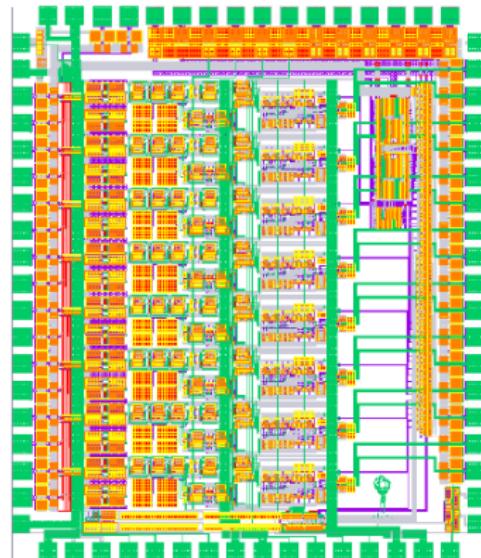


[3]

- finding optimum of function of '**very many**' independent discrete variables
- in many cases, exhaustive search **not tractable**
- often **NP-hard**

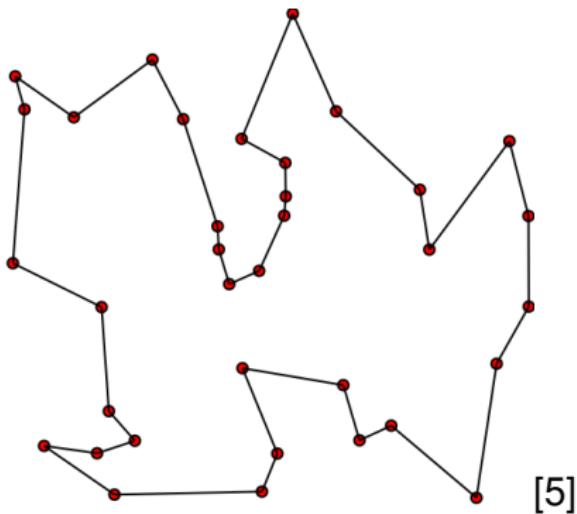
Example case 1: Chip design

- circuit placement
- wiring routes
- in general **NP-hard**



[4]

Example case 2: Travelling Salesperson Problem



- shortest possible route visiting each city and returning to origin
- generalized: vehicle routing problem (VRP)
- NP-hard

TSP: Exact algorithms

- brute-force: $\mathcal{O}(n!)$
- dynamic programming: $\mathcal{O}(n^2 2^n)$ (Held-Karp)

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- dynamic programming: $\mathcal{O}(n^2 2^n)$ (Held-Karp)
- \Rightarrow need heuristic methods:
- constructive heuristics
- divide-and-conquer
- iterative improvement
- randomized improvement

TSP: Exact algorithms

- \Rightarrow need heuristic methods:
- randomized improvement
- \hookrightarrow simulated annealing

Simulated annealing: Idea

- inspired by condensed matter physics
- find ground state configuration in low temperature limit

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- probability of state x : $P(x) \propto \exp(\frac{-E(x)}{k_B T})$
- sample configuration space with MCMC: **Metropolis**

Simulated annealing: Idea

- inspired by condensed matter physics
- find ground state configuration in low temperature limit
- probability of state x : $P(x) \propto \exp(\frac{-E(x)}{k_B T})$
- sample configuration space with MCMC: Metropolis
- annealing schedule: $\lim_{t \rightarrow t_{\text{end}}} T = 0$

Molecular dynamics vs. TSP (1/4): System configuration description

phase space

$$\mathbf{r} = \{\vec{r}_i\}_{i \in N}$$

tour as ordered list
of vertices

$$T = [1, 2, \dots, N]$$

Molecular dynamics vs. TSP (2/4):

Random moves

randomly change
one/several
coordinates $\mathbf{r} \rightarrow \mathbf{r}'$

randomly swap two
vertices $T =$
 $[..., 3, 7, 8, ...] \rightarrow$
 $T' = [..., 8, 7, 3, ...]$

Molecular dynamics vs. TSP (3/4): Quantitative objective function

$E \equiv$ Hamiltonian
 $\mathcal{H}(\mathbf{r})$

$E \equiv$ Length of tour
 $L(\mathbf{T})$

Molecular dynamics vs. TSP (4/4):

Acceptance probability and annealing

Changed configuration acceptance probability

$$P_{\text{acc}} = \min(1, \exp(-\frac{\Delta E}{k_B T}))$$

Molecular dynamics vs. TSP (4/4):

Acceptance probability and annealing

Changed configuration acceptance probability

$$P_{\text{acc}} = \min(1, \exp(\frac{-\Delta E}{k_B T}))$$

Annealing schedule $\lim_{t \rightarrow t_{\text{end}}} T = 0$

Simulated annealing for 400-city TSP

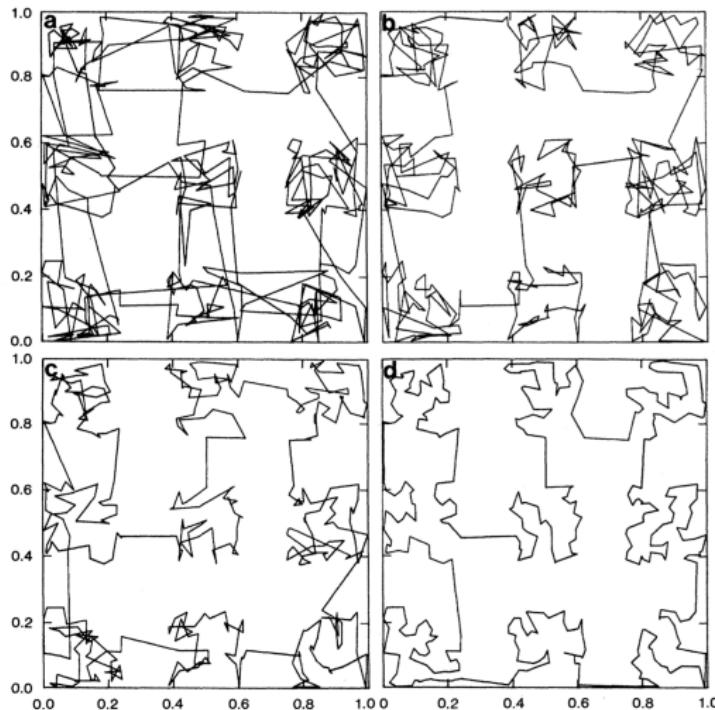


Fig. 9. Results at four temperatures for a clustered 400-city traveling salesman problem. The points are uniformly distributed in nine regions. (a) $T = 1.2$, $\alpha = 2.0567$; (b) $T = 0.8$, $\alpha = 1.515$; (c) $T = 0.4$, $\alpha = 1.055$; (d) $T = 0.0$, $\alpha = 0.7839$.

Animated simulated annealing for 125-city TSP

[6]

Simulated annealing: The gist

- 'a balance between exploration and exploitation'
- based on statistical mechanics
- improves iteratively, but has probabilistic component to avoid getting stuck in local minima

Simulated annealing: Advantages

- 'decent enough' approximate optimum in fixed amount of time
- well suited for discrete search spaces
- agnostic to system type, objective function
- relatively simple and independent of problem complexity to implement

Simulated annealing: Challenges

- deciding set of moves and objective function requires insight into problem and may not be obvious
- annealing schedule usually to be determined empirically

My conclusion

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