

# Optimization by Simulated Annealing

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# Combinatorial Optimization

- Central to science, engineering, CS
- Optimizing objective (cost) functions of complicated systems
- Determination of global extremum of objective functions
- Deterministic methods unrealistic as number of parameters becomes very large
  - Traveling Salesman Problem
  - Computer Design

# Introduction to the Traveling Salesman Problem

- **Problem 1:** Minimize cost function (E) of a salesman traveling between N number of cities and back
  - Cost to travel between cities proportional to distance between cities

Simplest form :

$$E = L \equiv \sum_{i=1}^N \sqrt{(x_i - x_{i+1})^2 + (y_i - y_{i+1})^2}$$



Give me your money!

# Intro. Traveling Salesman Problem

continued...

- Number of possible path configurations =  $N!$
- Exact solutions to minimization of  $E$  computationally determined for magnitudes of  $N < \sim 10^2$  (as of 1983)
- Non-deterministic polynomial time complete (NP-C) problem
  - Computing effort for exact soln. increases exponentially with  $N$
- Heuristic methods for near-optimal solutions
  - “Divide and Conquer” and “Iterative Improvements”
    - Monte Carlo (MC) & Simulated Annealing (SA)

# Metropolis Monte Carlo Algorithm

- 1) Start with known configuration, objective function (ie, energy), some Temperature value
- 2) Random change configuration (ie, add small random displacement)
- 3) Calculate new energy value ( $E_2$ )
- 4) Compare to energy at previous position ( $E_1$ ):
  - If  $E_2 < E_1$ , keep new position
  - If  $E_2 > E_1$ , keep new position if the Boltzmann factor for transition is greater or equal to a random number between 0 and 1

$$\text{Rand}(0, 1) \leq \exp[-(E_2 - E_1)/kT]$$

- 5) Repeat steps 2) – 4) K number of times

# Simulated Annealing (SA)

- Concept of SA from annealing process
  - Slowly cooling melt to form perfect crystals
- SA provides a temperature schedule for the Metropolis method
  - Start at effectively high temperature and gradually decrease the temperature by increments until  $T$  slightly above 0 ( $<1$ )
  - At every temperature, Metropolis algorithm is run (nested-loop)
- Benefits
  - Ability to escape local minima at non-zero temperatures
  - “Divide and Conquer” -> Gross features of final state appear at high temp. while fine details appear at low temp.

# SA Application: The Traveling Salesman

- Kirkpatrick et al solved problem where  $N=400$ 
  - Re-arrangement involved random selection of string of cities and reversal of order (Lin-Kernighan method)

- Side of square boundary has length of  $N^{1/2}$

- Cities grouped into nine clusters

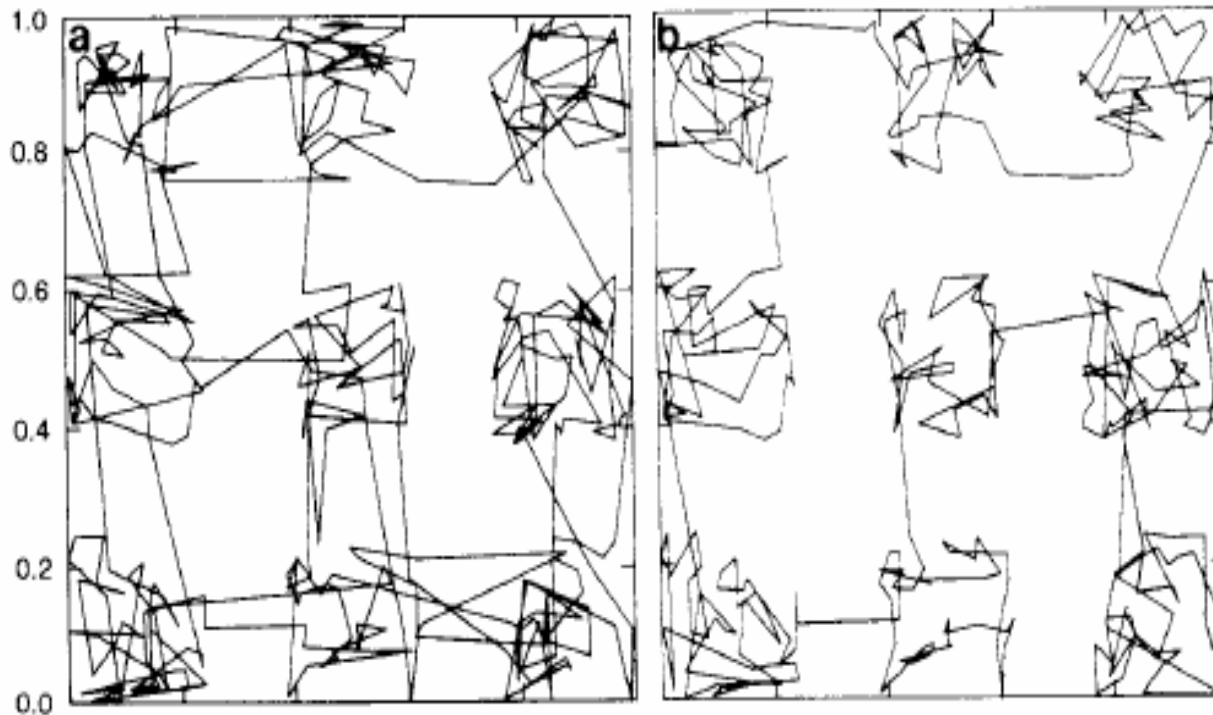
- Solved problem in “Manhattan” metric space so thus,

$$E = L \equiv \sum_{i=1}^N ( |x_i - x_{i+1}| + |y_i - y_{i+1}| )$$

- Solved problem several times and averaged optimal step lengths ( $\alpha$ )

# SA Results: Traveling Salesman

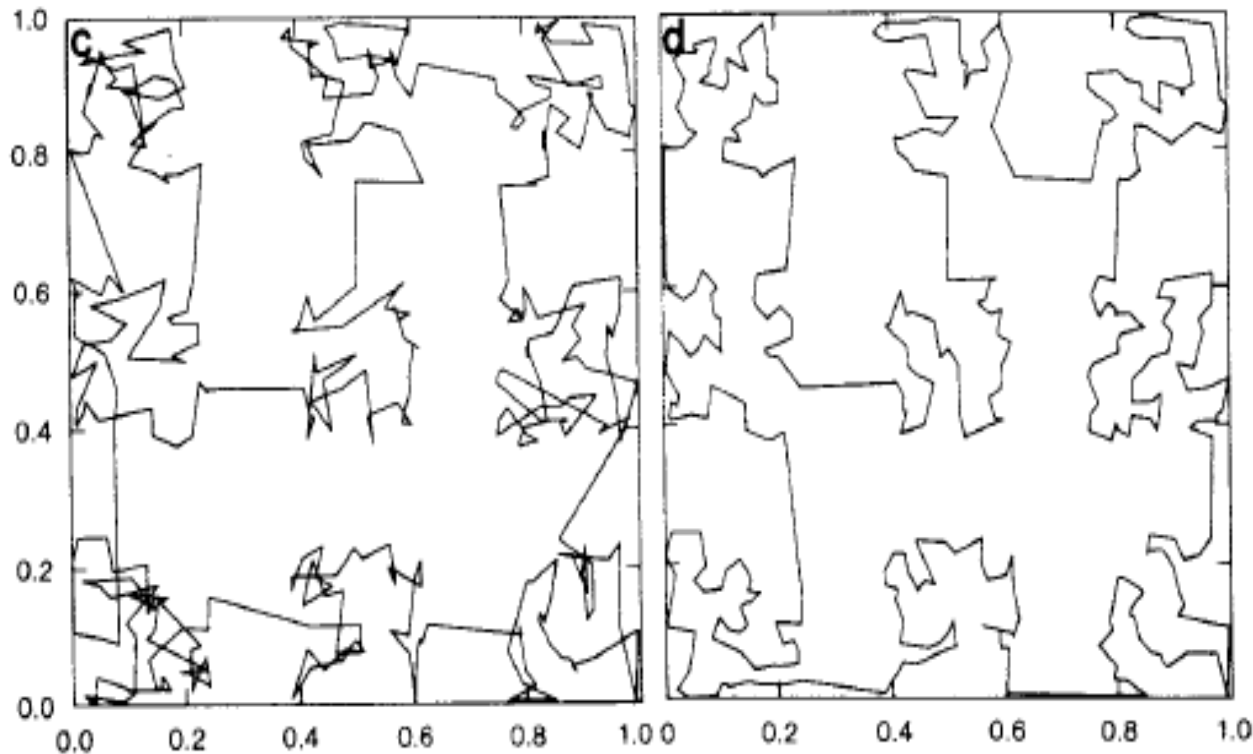
- a) Results at  $T = 1.2$  ( $\alpha = 2.0567$ )
- b) Results at  $T = 0.8$  ( $\alpha = 1.515$ )





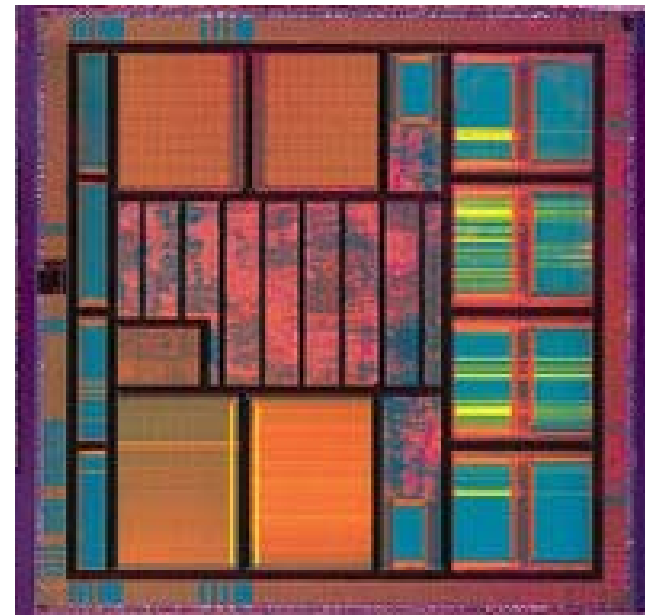
# SA Results: Traveling Salesman continued...

- c) Results at  $T = 1.2$  ( $\alpha = 2.0567$ )
- d) Results at  $T = 0.8$  ( $\alpha = 1.515$ )



# Physical Design of Computers

- Optimization problems in Comp. design
  - Partitioning circuits into groups to fit on chip
  - Placement of circuits on chip
  - Wiring of circuits on chip
- Goal to optimize performance of system without compromising any design stage



# Physical Design of Computers

## continued...

- Partitioning
  - Number of circuits in each partition must fit into package
  - Number of signals crossing boundaries minimized
- Placement
  - Minimize length of connections (reduce signal propagation time)
  - Minimize congestion (overcrowding)
- Wiring
  - Minimize wire lengths used
  - Minimize source of noise

# SA: Placement Problem

- **Problem:** Placement of 98 chips on IBM 3081 processor with 100 sites (10 x 10 grid)
- Re-arrangement moves involve switch between two chips or switch between chip and vacancy
- Histograms used to keep track of congestion and wire length by scoring boundary crossing on grid
  - Minimum one wire per boundary crossed
  - Sum of horizontal bins gives lower bound of horizontal length
  - Sum of vertical bins gives lower bound of vertical length
  - Construction of objective function

# SA: Placement Problem continued...

- Chips are numbered from 1 to 99 (without chip 20)
- Dark squares represent adder chips
- Squares with ruled lines represent chips that supply data to adder chips
- Lightly dotted squares represent chips that perform logical arithmetic (and, or, etc.)
- Open squares represent general-purpose register chips

# SA: Placement Problem continued...

Initial position

	1	2	3	4	5	6	7	8	9	10
262										
	11	12	13	14	15	16	17	18	19	
421										
	21	22	23	24	25	26	27	28	29	30
613										
	31	32	33	34	35	36	37	38	39	40
824										
	41	42	43	44	45	46	47	48	49	50
826										
	51	52	53	54	55	56	57	58	59	60
797										
	61	62	63	64	65	66	67	68	69	70
662										
	71	72	73	74	75	76	77	78	79	80
556										
	81	82	83	84	85	86	87	88	89	90
366										
	91	92	93	94	95	96	97	98	99	

a            366    428    555    759    879    945    990    672    210

# SA Results: Placement Problem

T = 10000

555	5	75	53	52	19			22	21
944	73	23	64	95	41	14	81	77	36
1193		70	16	91	8	31	9	43	56
1378	25	33	15	83				76	
1323	48	57	48	84	79	88	13	96	50
1375	6	39	90	97	94	11	58	29	27
1170		93	55		10	67	72		
535	7	80	75	30	29	59	85	67	49
434	3	24	69	86	51	18	32		1
		59	93	74	12	28	99	92	71

b

513 920 1091 1266 1349 1327 1147 853 503

# SA Results: Placement Problem continued...

T = 1250

568	99	92	40	92	83		72	53	62	87
750	93	95	55	84	52	25	32	88	22	82
809	<del>86</del>	97	69	71	<del>96</del>	64	<del>75</del>	42	<del>61</del>	<del>93</del>
700	90	53	57	<del>83</del>	<del>77</del>	<del>76</del>	94	73	<del>47</del>	<del>31</del>
718		89	27	67	78	21	23	12	10	11
717	29	41	15	16	1	91	2	80	33	4
785	51	50	<del>17</del>	30	49				74	
695	28	18	79	5	13	36	24			
499	9	39	60	19			14	58	38	
	3	6	3	7	<del>57</del>	<del>56</del>	70	<del>59</del>	<del>68</del>	<del>45</del>
C	477	700	892	732	820	932	909	736	439	



# SA Results: Placement Problem continued...

T=0

405	71	92	93	94	87	63	62	92	65	
563	83	84	97	85	77	73	77	97	31	88
559	95	99	93	96	86	52	61	32	12	23
560	5	15	90	98	76	75	82	14	13	2
591	16	25	78	55	69	10	3	21	11	1
595	79	89	27	67	53	64	74	7	7	4
562	3	19	18	29	49	57	59	17	7	4
558	6	39	30	60	51	7	68	48	7	7
395	7	9	50	70	41	7	7	47	56	7
	30	28		40	91	36	7	54	56	33

d

373 471 569 613 580 625 632 590 334

# SA Results: Placement Problem

continued...

- Observed decrease in congestion as T was decreased in SA
- Observed decrease in wire length as T was decreased in SA (minimization of wire length)

# Conclusion

- Simulated annealing with Metropolis algorithm is effective heuristic technique
- Require known initial configuration, objective function, random number generator, and temperature schedule (annealing)
- Success with finding near-optimal solutions for NP-C problems (Traveling salesman)
- Success with optimizing computer design

# References

- Kirkpatrick, S; Gelatt, C. D., Vecchi, M. P. *Optimization by Simulated Annealing*. **Science**. 220 (1983): 671-679.
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- Leach, A. R. *Molecular Modeling: Principles and Applications, 6<sup>th</sup> Edition*. Prentice Hall (2001): 414-418.