CSCI 435: Algorithms and Complexity
4. Local Search

- *gradient descent*
- *Metropolis algorithm*
- *Hopfield neural networks*
- *maximum cut*

Local search

Local search. Algorithm that explores the space of possible solutions in sequential fashion, moving from a current solution to a "nearby" one.

Neighbour relation. Let $S \sim S'$ be a neighbour relation for the problem.

Gradient descent. Let S denote the current solution. If there is a neighbour S' of S with a strictly lower cost, replace S with the neighbour whose cost is as small as possible. Otherwise, terminate the algorithm.

A funnel

a jagged funnel

Gradient descent: vertex cover

Vertex cover. Given a graph $G = (V, E)$, find a subset of nodes S of minimal cardinality such that for each $(u, v) \in E$, either u or v (or both) are in S.

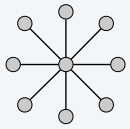
Neighbour relation. $S \sim S'$ if S' can be obtained from S by adding or deleting a single node. Each vertex cover S has at most n neighbours.

Gradient descent. Start with $S = V$. If there is a neighbour S' that is a vertex cover and has lower cardinality, replace S with S'.

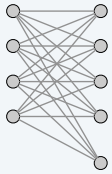
Remark. Algorithm terminates after at most n steps since each update decreases the size of the cover by one.

Gradient descent: vertex cover

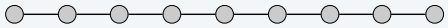
Local optimum. No neighbour is strictly better.



optimum = center node only
local optimum = all other nodes



optimum = all nodes on left side
local optimum = all nodes on right side



optimum = even nodes
local optimum = omit every third node

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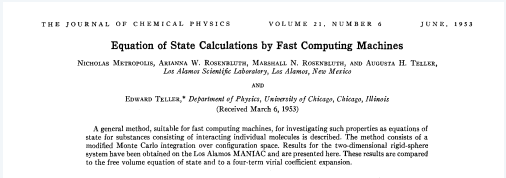
Metropolis algorithm

Key idea.

- Simulate the behaviour of a physical system according to principles of statistical mechanics.
- Globally biased toward "downhill" steps, but occasionally makes "uphill" steps to break out of local minima.

Nicholas Metropolis



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

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(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

Thermodynamics

Gibbs-Boltzmann function. The probability of finding a physical system in a state with energy E is proportional to

$$e^{-E/(kT)},$$

where $T > 0$ is temperature and k is the Boltzmann constant.

- For any temperature $T > 0$, the G-B function is a monotone decreasing function of energy E.
- System is more likely to be in a lower energy state than a higher one.
  - T large $\Rightarrow$ high- and low-energy states have roughly same probability.
  - T small $\Rightarrow$ low-energy states are much more probable.

Thermodynamics

Metropolis algorithm.

- Given a fixed temperature T, maintain the current state S.
- Randomly perturb the current state S to a new state $S' \in N(S)$.
- If $E(S') \leq E(S)$, update the current state to S'.
  Otherwise, update the current state to S' with probability $e^{-\Delta E/(kT)}$, where $\Delta E = E(S') - E(S) > 0$.

Theorem. Let $f_S(t)$ be the fraction of the first t steps in which the simulation is in state S. Then, assuming some technical conditions, with probability 1:

$$\lim_{t \to \infty} f_S(t) = \frac{1}{Z} e^{-E(S)/(kT)},$$

$$\text{where } Z = \sum_{S \in N(S)} e^{-E(S)/(kT)}.$$

Intuition. Simulation spends roughly the right amount of time in each state, according to the Gibbs-Boltzmann equation.

Simulated annealing

Consider how we might approximate the global optimum of some function.

Key idea.

- T large $\Rightarrow$ probability of accepting an uphill move is large.
- T small $\Rightarrow$ uphill moves are almost never accepted.
- Solution: turn a "knob" to control T.
- Cooling schedule: $T = T(i)$ at iteration i.

Physical analog: annealing.

- Take room-temp steel and heat it to a high temperature; we do not expect its molecules to maintain a nice crystal structure.
- Take glowing steel and cool it very abruptly; we do not expect its molecules to maintain a nice crystal structure.
- Anneal the steel by cooling it gradually from a high temperature, allowing it to reach equilibrium via a succession of intermediate lower temperatures.

Simulated annealing

Finding a local maximum.

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Hopfield neural networks

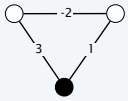
Hopfield networks. Simple model of an associative memory, in which a large collection of units are connected by an underlying network, and neighbouring units try to correlate their states.

John Hopfield

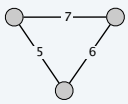
Input. Graph $G = (V, E)$ with integer (positive or negative) edge weights w.

Output. Node assignment (or configuration) $s_u = \pm 1$.

Intuition. If $w_{uv} < 0$, then u and v want to have the same state; if $w_{uv} > 0$, then u and v want different states.



Note. In general, no configuration respects all constraints.



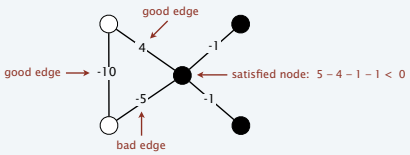
Hopfield neural networks

Def. With respect to a configuration S, an edge $e = (u, v)$ is good if $w_e \times s_u \times s_v < 0$. That is, if $w_e < 0$, then $s_u = s_v$; if $w_e > 0$, then $s_u \neq s_v$.

Def. With respect to a configuration S, a node u is satisfied if the weight of incident good edges ≥ the weight of incident bad edges.

$$\sum_{v:\, e=(u,v) \in E} w_e s_u s_v \;\leq\; 0$$

Def. A configuration is stable if all nodes are satisfied.



Goal. Find a stable configuration, if such a configuration exists.

State-flipping algorithm

Goal. Find a stable configuration, if such a configuration exists.

Idea. Repeatedly flip the state of an unsatisfied node.

HOPFIELD-FLIP *(G, w)*

$S \leftarrow$ arbitrary configuration

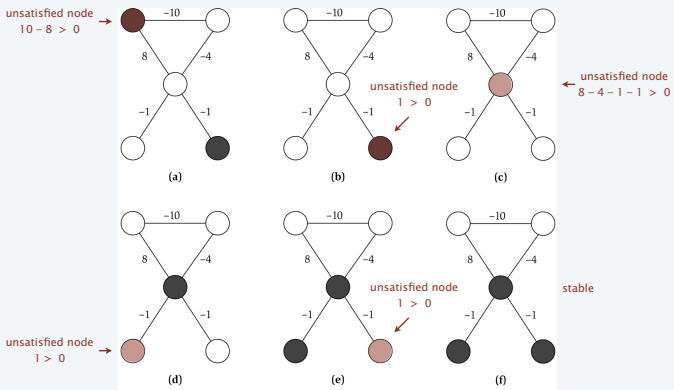
WHILE (current configuration is not stable)

  $u \leftarrow$ unsatisfied node

  $s_u \leftarrow -s_u$

RETURN S

State-flipping algorithm: example



State-flipping algorithm: proof of correctness

Theorem. The state-flipping algorithm terminates with a stable configuration after at most $W = \Sigma_e |w_e|$ iterations.

Pf attempt.

Consider measure of progress $\Phi(S) = \#$ satisfied nodes.

State-flipping algorithm: proof of correctness

Theorem. The state-flipping algorithm terminates with a stable configuration after at most $W = \Sigma_e |w_e|$ iterations.

Pf.

Consider measure of progress $\Phi(S) = \Sigma_{e \text{ good}} |w_e|$.

- Clearly, $0 \le \Phi(S) \le W$.
- We show $\Phi(S)$ increases by at least 1 after each flip.

  When u flips state:
  - all good edges incident to u become bad
  - all bad edges incident to u become good
  - all other edges remain the same

$$\Phi(S') = \Phi(S) - \sum_{\substack{e:\, e=(u,v)\in E \\ e \text{ is bad}}} |w_e| + \sum_{\substack{e:\, e=(u,v)\in E \\ e \text{ is good}}} |w_e| \;\ge\; \Phi(S) + 1$$

u is unsatisfied

Complexity of Hopfield neural networks

Hopfield network search problem. Given a weighted graph, find a stable configuration if one exists.

Hopfield network decision problem. Given a weighted graph, does there exist a stable configuration?

Remark. The decision problem is trivially solvable (always yes), but there is no known poly-time algorithm for the search problem.

polynomial in n and $\log(W)$

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Maximum cut

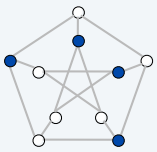
Maximum cut. Given an undirected graph $G = (V, E)$ with positive integer edge weights w_e, find a cut (A, B) such that the total weight of edges crossing the cut is maximized.

$$w(A, B) := \sum_{u \in A,\, v \in B} w_{uv}$$

Toy application.

- n activities, m people.
- Each person wants to participate in two of the activities.
- Schedule each activity in the morning or afternoon to maximize the number of people that can enjoy both activities.

Real applications. Circuit layout, statistical physics.



Maximum cut: local search

Single-flip neighbourhood. Given a cut (A, B), move one node from A to B (or one from B to A) if it improves the solution.

Greedy algorithm.

```
MAX-CUT-LOCAL (G, w)

(A, B) ← random cut
WHILE (there exists an improving node v)
  IF (v ∉ A)
    A ← A ∪ { v }
    B ← B − { v }
  ELSE
    B ← B ∪ { v }
    A ← A − { v }
RETURN (A, B)
```

Maximum cut: local search analysis

Theorem. Let (A, B) be a locally optimal cut and let (A^*, B^*) be an optimal cut. Then $w(A, B) \geq \frac{1}{2} \sum_e w_e \geq \frac{1}{2} w(A^*, B^*)$.

weights are nonnegative

Pf.

- Local optimality implies that for all $u \in A$: $\sum_{v \in A} w_{uv} \leq \sum_{v \in B} w_{uv}$
  Adding up all these inequalities yields:

$$2 \sum_{\{u,v\} \subseteq A} w_{uv} \leq \sum_{u \in A,\, v \in B} w_{uv} = w(A, B)$$

- Similarly, we have that $2 \sum_{\{u,v\} \subseteq B} w_{uv} \leq \sum_{u \in A,\, v \in B} w_{uv} = w(A, B)$
- Now,

each edge counted once

$$\sum_{e \in E} w_e = \underbrace{\sum_{\{u,v\} \subseteq A} w_{uv}}_{\leq \frac{1}{2} w(A, B)} + \underbrace{\sum_{u \in A,\, v \in B} w_{uv}}_{w(A, B)} + \underbrace{\sum_{\{u,v\} \subseteq A} w_{uv}}_{\leq \frac{1}{2} w(A, B)} \leq 2w(A, B) \quad \blacksquare$$

Maximum cut: big improvement flips

Local search. Within a factor of 2 for MAX-CUT, but not poly-time!

Big-improvement-flip algorithm. Only choose a node which, when flipped, increases the cut value by at least $\frac{2\varepsilon}{n} w(A, B)$.

Claim. Upon termination, big-improvement-flip algorithm returns a cut (A, B) such that $(2 + \varepsilon)\, w(A, B) \geq w(A^*, B^*)$.

Pf idea. Add $\frac{2\varepsilon}{n} w(A, B)$ to each inequality in the original proof. ▪

Claim. Big-improvement-flip algorithm terminates after $O(\varepsilon^{-1} n \log(W))$ flips, where $W = \sum_e w_e$.

Pf idea.

- Each flip improves the cut value by at least a factor of $(1 + \varepsilon / n)$.
- After n / ε iterations, the cut value improves by a factor of 2.
- Cut value can be doubled at most $\log_2(W)$ times. ▪

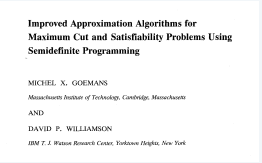
if $x \geq 1$, $(1 + 1/x)^x \geq 2$

Maximum cut: context

Theorem. [Sahni-Gonzales, 1976] There exists a ½-approximation algorithm for MAX-CUT.

Theorem. [Goemans-Williamson, 1995] There exists a 0.878-approximation algorithm for MAX-CUT.

Theorem. [Håstad, 2001] Unless **P** = **NP**, there does not exist any 0.942-approximation algorithm for MAX-CUT.



Improved Approximation Algorithms for Maximum Cut and Satisfiability Problems Using Semidefinite Programming

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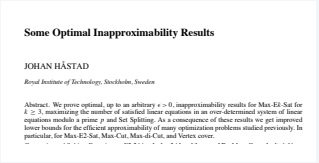

Some Optimal Inapproximability Results

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Abstract. We prove optimal, up to an arbitrary $\epsilon > 0$, inapproximability results for Max-Ek-Sat for $k \geq 3$, maximizing the number of satisfied linear equations in an over-determined system of linear equations modulo a prime p and Set Splitting. As a consequence of these results we get improved lower bounds for the efficient approximability of many optimization problems studied previously. In particular, for Max-E2-Sat, Max-Cut, Max-di-Cut, and Vertex cover.