Monte Carlo for Optimization

- Idea use sampling to compute the global minimum of a function
- Remember that most optimization methods converged to a local minimum
- For some problems a surrogate convex problem can be defined … these are better solved using that approach
- Turns out that there are some very hard "combinatorial optimization" problems, for which a sampling approach works very well

Algorithm 17.1 Simulated Annealing

Given an initial point x, initialize T to some large number and choose a number α between 0 and 1 and a positive number ϵ close to 0.

while $T > \epsilon$,

Generate a random move from the current x to a new $\widehat{x}$.

If $t \equiv f(\widehat{x}) - f(x) < 0$, then our new point improves the function value and we accept the move, setting $x = \widehat{x}$.

If the function value did not improve, then we accept the move, setting $x = \widehat{x}$, with probability $e^{-t/T}$, where T is the current temperature. With probability $1 - e^{-t/T}$ we reject the move and leave x unchanged.

Decrease the temperature, replacing T by αT.

end

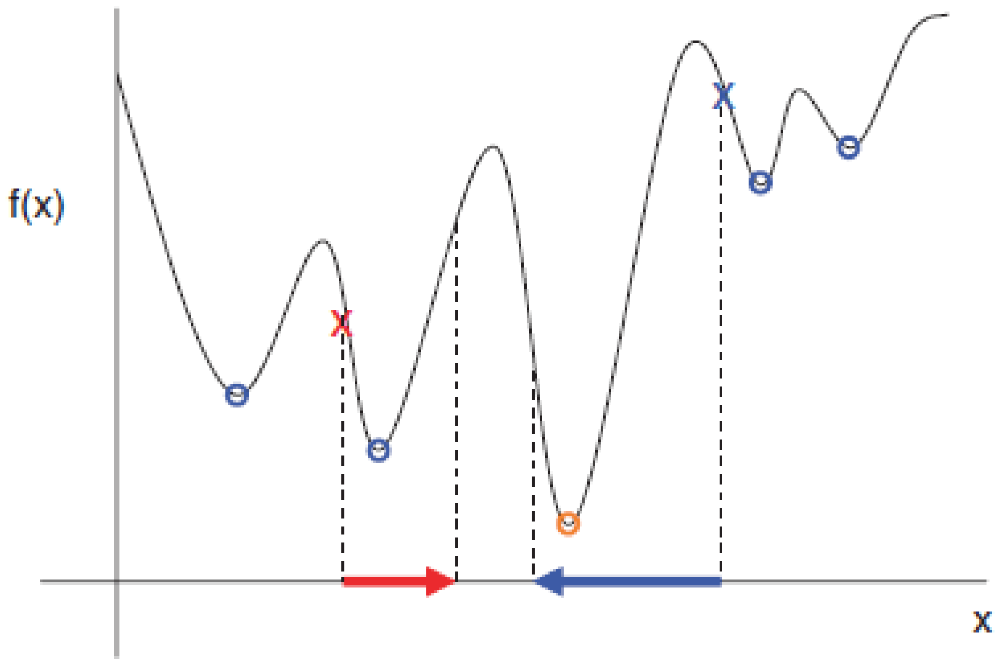


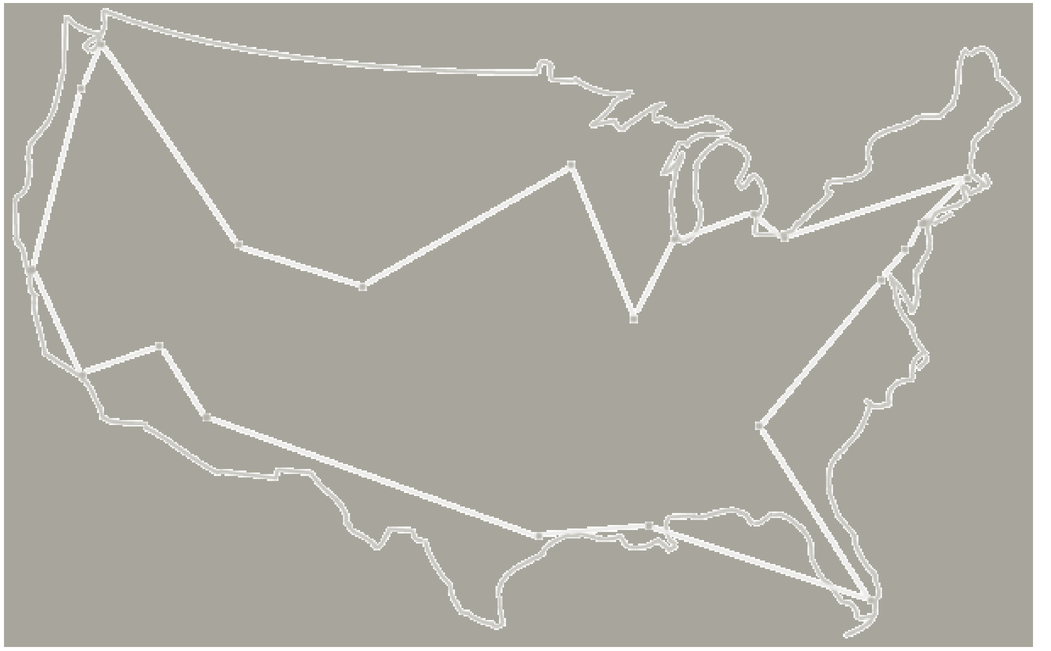
Figure 17.2. *In simulated annealing, we allow moves that increase the function value, such as that illustrated by the shorter arrow. At high temperature, such moves are likely to be accepted, while at low temperature they are likely to be rejected. At high temperature, we also might allow longer moves (horizontally), such as that illustrated by the left-pointing arrow, and these two features can enable us to escape from valleys that do not contain the global minimum.*

Simulated Annealing

- Simulated annealing algorithm is slow
- Advantages
  - Compared to standard minimization algorithms, it gives a better probability of finding a global rather than a local minimizer.
  - It does not require derivative values for f . In fact, it does not even require f to be differentiable.
- The art of the method is determining the probability function and the temperature sequence appropriate to the specific problem.

Travelling Salesperson Problem

- Finding the shortest cyclical itinerary for a traveling salesperson who must visit each of N cities in turn.



Discrete/Combinatorial Optimization

- Configuration problems are simple to state but difficult to solve.
- Example is the **traveling salesperson problem (TSP)**.
  - needs to visit n cities exactly once
  - wants to minimize the total distance traveled
  - finish the trip at the starting point.
- Solution: permutation of the list of cities that corresponds to the shortest total distance traveled.
- If the first city is known then solution requires minimum distance from the $(n-1)!$ permutations
  - Enormous number of possibilities for moderate (recall Stirling's formula)
  - not practical to test each of them.
- Therefore, an approximate solution is often found
  - either by generating random permutations and choosing the best (a Monte Carlo algorithm),
  - or using simulated annealing.

Matlab builtin

- Travel
- Randomly picks pair and interchanges them
- Can also be done via simulated annealing

TSP solution via simulated annealing

- Start with an initial ordering of cities and an initial temperature T .
- Randomly choose two cities.
- **if** interchanging those cities decreases the length of the tour **then** interchange them!
- **else**
  - Interchange them with a probability that is an increasing function of temperature and a decreasing function of the change in tour length.
- **end**
- Decrease the temperature.
- Let's experiment with Monte Carlo and simulated annealing solutions to TSP. One specific temperature sequence, the log cooling schedule, is discussed in the answer to the next challenge.

Counting problem on Lattices

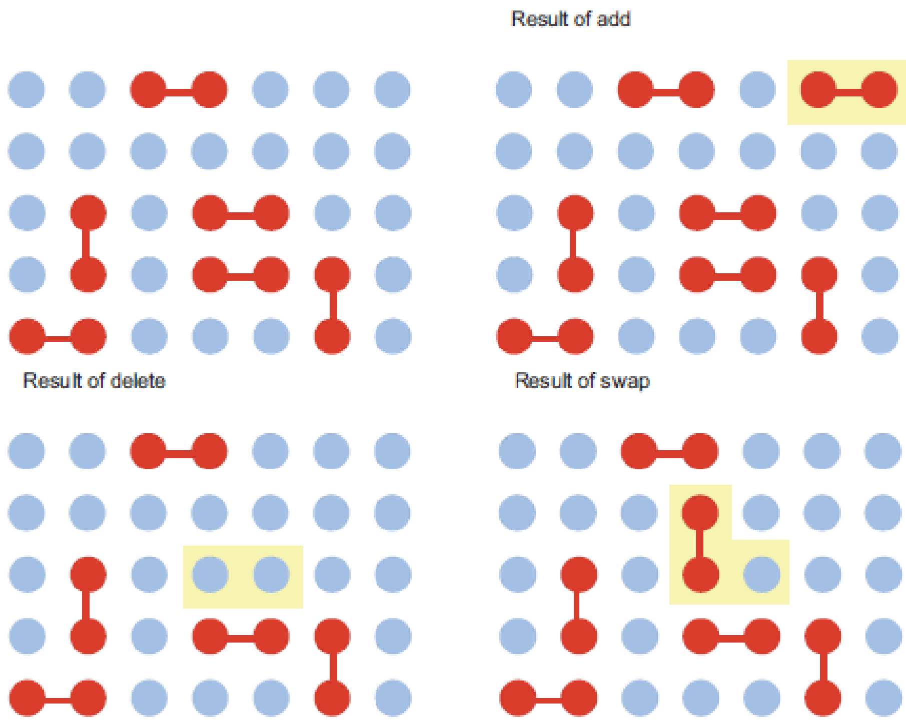


Figure 17.3. *Upper left: a lattice of 6 dimers (red) and 23 monomers (blue), used to illustrate the add, delete, and swap operations. Upper right: adding a dimer in row 1. Bottom left: deleting a dimer in row 3. Bottom right: swapping a horizontally oriented dimer in row three for a vertical one.*