Heuristic Optimization Methods

Lecture 03 – Simulated Annealing

Simulated Annealing

- A metaheuristic inspired by statistical thermodynamics
  - Based on an analogy with the cooling of material in a heat bath
- Used in optimization for 20 years
- Very simple to implement
- A lot of literature
- Converges to the global optimum under weak assumptions (- usually slowly)

Simulated Annealing - SA

- Metropolis’ algorithm (1953)
  - Algorithm to simulate energy changes in physical systems when cooling
- Kirkpatrick, Gelatt and Vecchi (1983)
  - Suggested to use the same type of simulation to look for good solutions in a COP

SA - Analogy

Thermodynamics

1. Configuration of particles
2. System state
3. Energy
4. State change
5. Temperature
6. Final state

Discrete optimization

1. Solution
2. Feasible solution
3. Objective Function
4. Move to neighboring solution
5. Control Parameter
6. Final Solution

Simulated Annealing

- Can be interpreted as a modified random descent in the space of solutions
  - Choose a random neighbor
  - Improving moves are always accepted
  - Deteriorating moves are accepted with a probability that depends on the amount of the deterioration and on the *temperature* (a parameter that decreases with time)
- Can escape local optima

Move Acceptance in SA

- We assume a minimization problem
- Set Δ = Obj(random neighbor) – Obj(current solution)
- If Δ < 0 → accept (we have an improving move)
- Else accept if

$$Random(0,1) < e^{-\frac{\Delta}{t}}$$

- If the move is not accepted: try another random neighbor

SA - Structure

- Initial temperature t_0 high
  - (if $\infty \rightarrow$ random walk)
- Reduce t regularly
  - need a *cooling schedule*
  - if too fast $\rightarrow$ stop in some local optimum too early
  - if too slow $\rightarrow$ too slow convergence
- Might restart
- Choice of neighborhood structure is important

SA

- Statistical guarantee that SA finds the global optimum
- In practice this requires exponential (or ∞) running time
- The cooling schedule is vitally important
  - Much research on this
  - Static schedules: specified in advance
  - Adaptive schedules: react to information from the search

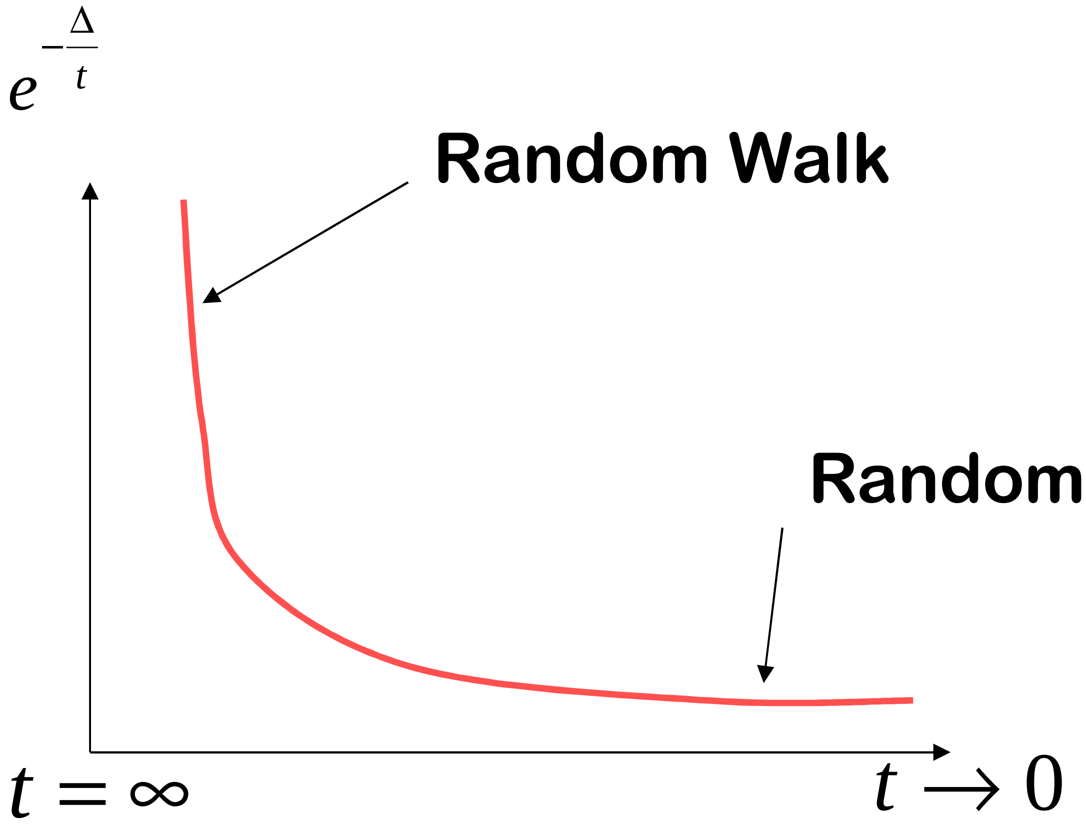
Simulated Annealing

input: starting solution, s_0
input: neighborhood operator, N
input: evaluation function, f
input: the cooling schedule, t_k
input: the number of iterations for each temperature, M_k
$current \Leftarrow s_0$
$k \Leftarrow 0$
while stopping criterion not met **do**
    $m \Leftarrow 0$
    while $m < M_k$ **do**
        $s \Leftarrow$ randomly selected solution from $N(current)$
        if $f(s) \leq f(current)$ **then**
            $current \Leftarrow s$
        else
            $\Delta \Leftarrow f(s) - f(current)$
            $\xi \Leftarrow$ a random number, uniformly drawn from $[0, 1]$
            if $\xi \leq e^{-\Delta/t_k}$ **then**
                $current \Leftarrow s$
            end if
        end if
        $m \Leftarrow m + 1$
    end while
    $k \Leftarrow k + 1$
end while

Choice of Move in SA

- Modified ”Random Descent”
- Select a random solution in the neighborhood
- Accept this
  - Unconditionally if better than current
  - With a certain, finite probability if worse than current
- The probability is controlled by a parameter called the *temperature*
- Can escape from local optima

SA - Cooling



SA – Overall Structure

- Set the initial value of the control variable t (t_0) to a high value
- Do a certain number of iterations with the same temperature
- Then reduce the temperature $t_{i+1} = \alpha(t_i)$
- Need a ”cooling schedule”
- Stopping criterion – e.g. ”minimum temperature”
  - Repetition is possible
- Solution quality and speed are dependent on the choices made
- Choice of neighborhood structure is important

Statistical Analysis of SA

- Model: State transitions in the search space
- Transition probabilities $[p_{ij}]$ (i,j are solutions)
- Only dependent on i and j: homogenous Markov chain
- If all the transition probabilities are finite, then the SA search will converge towards a stationary distribution, independent of the starting solution.
  - When the temperature approaches zero, this distribution will approach a uniform distribution over the global optima
- Statistical guarantee that SA finds a global optimum
- But: exponential (or infinite) search time to guarantee finding the optimum

SA in Practice (1)

- Heuristic algorithm
- Behaviour strongly dependent on the cooling schedule
- Theory:
  - An exponential number of iterations at each temperature
- Practice:
  - A large number of iterations at each temperature, few temperatures
  - A small number of iterations at each temperature, many temperatures

SA in Practice (2)

- Geometric chain
  - $t_{i+1} = \alpha\, t_i$, $i = 0,\ldots,K$
  - $\alpha < 1$ (0.8 - 0.99)
- Number of repetitions can be varied
- Adaptivity:
  - Variable number of moves before the temperature reduction
- Necessary to experiment

SA – General Decisions

- Cooling Schedule
  - Based on maximum difference in the objective function value of solutions, given a neighborhood
  - Number of repetitions at each temperature
  - Reduction rate, α
- Adaptive number of repetitions
  - more repetitions at lower temperatures
  - number of accepted moves, but a maximum limit
- Very low temperatures are not necessary
- Cooling rate most important

SA – Problem Specific Decisons

- Important goals
  - Response time
  - Quality of the solution
- Important choices
  - Search space
    - Infeasible solutions – should they be included?
  - Neighborhood structure
  - Move evaluation function
    - Use of penalty for violated constraints
    - Approximation – if expensive to evaluate
  - Cooling schedule

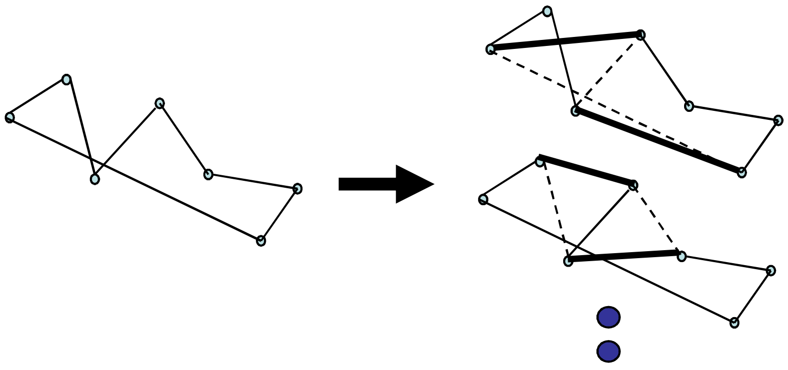
SA – Choice of Neighborhood

- Size
- Variation in size
- Topologi
  - Symmetry
  - Connectivity
    - Every solution can be reached from all the others
- Topography
  - Spikes, Plateaus, Deep local optima
- Move evaluation function
  - How expensive is it to calculate ?

SA - Speed

- Random choice of neighbor
  - Reduction of the neighborhood
  - Does not search through all the neighbors
- Cost of new candidate solution
  - Difference without full evaluation
  - Approximation (using surrogate functions)
- Move acceptance criterion
  - Simplify

SA – Example: TSP



- Search space - (n-1)!/2
- Neighborhood size:
  - 2-opt: n(n-1)/2
- Connected
- Simple representation of moves
- Natural cost function
- Difference in cost between solutions is easy to calculate
- Generalization: k-Opt

SA – Fine Tuning

- Test problems
- Test bench
- Visualization of solutions
- Values for
  - cost / penalties
  - temperature
  - number / proportion of accepted move
  - iterations / CPU time
- Depencies between the SA-parameters
- The danger of overfitting

SA – Summary

- Inspired by statistical mechanics - cooling
- Metaheuristic
  - Local search
  - Random descent
  - Use randomness to escape local optima
- Simple and robust method
  - Easy to get started
- Proof for convergence to the global optimum
  - Worse than complete search
- In practise:
  - Computationally expensive
  - Fine tuning can give good results
  - SA can be good where robust heuristics based on problem structure are difficult to make