TECHNISCHE UNIVERSITÄT DRESDEN

Artificial Intelligence, Computational Logic

PROBLEM SOLVING AND SEARCH IN ARTIFICIAL INTELLIGENCE

Lecture 3 Metaheuristic Algorithms

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DRESDEN concept Exzellenz aus Wissenschaft und Kultur

Agenda

Hill-climbing Methods

- Hill climbing methods use an iterative improvement technique.
- Technique is applied to a single point - the current point - in the search space.
- During each iteration, a new point is selected from the neighborhood of the current point.
- If new point provides better value (in light of evaluation function) the new point becomes the current point.
- Otherwise, some other neighbor is selected and tested against the current point.
- The method terminates if no further improvement is possible, or we run out of time.

Iterated Hill-Climber

Algorithm iterated hill-climber

$t \leftarrow 0$
initialize $best$
repeat
    $local \leftarrow$ FALSE
    select a current point v_c at random
    evaluate v_c
    repeat
        select all new points in the neighborhood of v_c
        select the point v_n from the set of new points with the best value of evaluation function $eval$
        if $eval(v_n)$ is better than $eval(v_c)$ **then**
            $v_c \leftarrow v_n$
        else
            $local \leftarrow$ TRUE
        end if
    until $local$
    $t \leftarrow t + 1$
    if v_c is better than $best$ **then**
        $best \leftarrow v_c$
    end if
until $t = MAX$

Weaknesses of Hill-climbing Algorithms

1. They usually terminate at solutions that are only locally optimal.
2. No information about how much the local optimum deviates from the global optimum, or from other local optima.
3. The obtained optimum depends on the initial configuration.
4. In general, it is not possible to provide an upper bound for the computation time.

But, they are easy to apply. All that is needed is:

- the representation,
- the evaluation function, and
- a measure that defines the neighborhood around a given solution.

Balance Between Exploration and Exploitation

Effective search techniques provide a mechanism for balancing two conflicting objectives:

- exploiting the best solutions found so far, and
- at the same time exploring the search space.

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Exploit the best available solution for possible improvement but neglect exploring a large portion of the search space.

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Hill-climbing Techniques

Exploit the best available solution for possible improvement but neglect exploring a large portion of the search space.

Random Search

Explores the search space thoroughly (points are sampled from the search space with equal probabilities) but foregoes exploiting promising regions.

Balance Between Exploration and Exploitation

Effective search techniques provide a mechanism for balancing two conflicting objectives:

- exploiting the best solutions found so far, and
- at the same time exploring the search space.

There is no way to choose a single search method that can serve well in every case!

Local Search

1. Pick a solution from the search space and evaluate its merit. Define this as the current solution.
2. Apply a transformation to the current solution to generate a new solution and evaluate its merit.
3. If the new solution is better than the current solution then exchange it with the current solution; otherwise discard the new solution.
4. Repeat sets 2 and 3 until no transformation in the given set improves the current solution.

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  - Then, current solution has no effect on the probabilities of selecting any new solution.
  - The search becomes essentially enumerative.
  - Could be even worse: one might resample points that have already been tried.

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  - Then, current solution has no effect on the probabilities of selecting any new solution.
  - The search becomes essentially enumerative.
  - Could be even worse: one might resample points that have already been tried.
- Another extreme would be to always return the current solution - **this gets you nowhere!**

Local Search ctd.

- Searching within some local neighborhood of current solution is a useful compromise.
- Then, current solution imposes a bias on where we can search next.
- If we find something better, we can update the current point to new solution and retain what we have learned.
- If the size of the neighborhood is small, the search might be very quick, but we might get trapped at local optimum.
- If the size of neighborhood is very large, there is less chance to get stuck, but the efficiency may suffer.
- **The type of transformation we apply determines the size of neighborhood.**

Local Search and the SAT

Local search algorithms are surprisingly good at finding satisfying assignments for certain classes of SAT formulas. GSAT is one of the best-known (randomized) local search algorithms for SAT.

Algorithm GSAT

```
for i ← 1 step 1 to MAX-TRIES do
    T ← a randomly generated truth assignment
    for j ← 1 step 1 to MAX-FLIPS do
        if T satisfies the formula then
            return(T)
        else
            make a flip
        end if
    end for
    return("no satisfying assignment found")
end for
```

Local Search and the SAT

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            make a flip
        end if
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    return("no satisfying assignment found")
end for
```

- "make a flip" flips the variable in T that results in the largest decrease in the number of unsatisfied clauses.
- MAX-TRIES, determines the number of new search sequences.
- MAX-FLIPS, determines the maximum number of moves per try.

Local Search and the SAT ctd.

- GSAT begins with randomly generated truth assignment.
- If assignment satisfies the problem, the algorithm terminates.
- Else, it flips each of the variables from TRUE to FALSE or FALSE to TRUE and records the decrease in the number of unsatisfied clauses.
- After trying all possible flips, it updates current solution to solution with largest decrease in unsatisfied clauses.
- If this new solution satisfies the problem, we are done.
- Otherwise, the algorithm starts flipping again.

Local Search and the SAT ctd.

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Interesting feature of the algorithm:

- Best available flip might **decrease** the number of unsatisfied clauses.
- Selection is only made from neighborhood of current solution. If every neighbor (defined as being one flip away) is worse than current solution, then GSAT takes the one that is the least bad.
- Has the chance to escape local optimum!
  - But, it might oscillate between points and never escape from some plateaus.
  - One can assign a weight to each clause, and increase the weight for those who remain unsatisfied.

Local Search and the TSP

- There are many local search algorithms for TSP.
- The simplest is called $2\text{−}opt$.
- Starts with random permutation of cities (call this tour T) and tries to improve it.
- Neighborhood of T is defined as the set of all tours that can be reached by changing two nonadjacent edges in T.
- This move is called a $2\text{−}interchange$.

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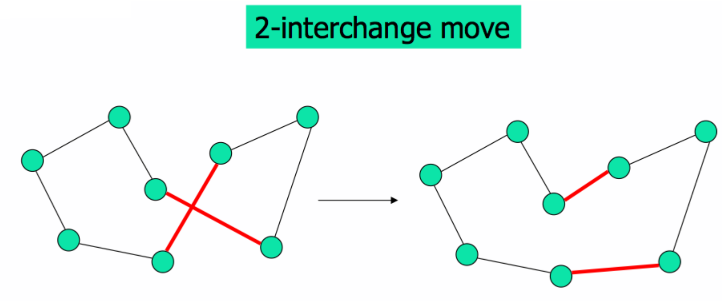

$2\text{−}opt$ Algorithm

- A new tour T' replaces T if it is better.
  - Note: we replace the tour every time we find an improvement.
  - Thus, we terminate the search in the neighborhood of T when the first improvement is found.
- If none of the tours in neighborhood of T is better, then T is called $2\text{−}optimal$ and algorithm terminates.
- As GSAT, algorithm should be restarted from several random permutations.

$2-opt$ Algorithm

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  - Note: we replace the tour every time we find an improvement.
  - Thus, we terminate the search in the neighborhood of T when the first improvement is found.
- If none of the tours in neighborhood of T is better, then T is called $2-optimal$ and algorithm terminates.
- As GSAT, algorithm should be restarted from several random permutations.
- Can be generalized to $k-opt$, where either k or upto k edges are selected.
- Trade-off between size of neighborhood and efficiency of the search:
  - If k is small the entire neighborhood can be searched quickly, but increases likelihood of suboptimal answer.
  - For larger values of k, the number of solutions in neighborhood become enormous (grows exponentially with k). Seldomly used for $k > 3$.

Escaping Local Optima

- Traditional problem-solving strategies either
  - guarantee discovering global solution, but are too expensive, or
  - have a tendency of "getting stuck" in local optima.
- There is almost no chance to speed up algorithms that guarantee finding global solution.
  - Problem of finding polynomial-time algorithms for real problems (as they are NP-hard).
- Remaining option is to design algorithms capable of escaping local optima.

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Simulated Annealing

Additional parameter (called temperature) that change the probability of moving from one point of the search space to another.

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Tabu Search

Memory, which forces the algorithm to explore new areas of the search space.

Local Search Revisited

Algorithm local search

$x =$ some initial starting point in $\mathcal{S}$
while improve(x) $\neq$ "no" **do**
  $x =$ improve(x)
end while
return(x)

Local Search Revisited

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- improve(x) returns new point y from neighborhood of x, i.e., $y \in N(x)$, if y is better than x,
- otherwise, returns a string "no". In that case, x is a local optimum in $\mathcal{S}$.

Simulated Annealing

Algorithm simulated annealing

$x =$ some initial starting point in $\mathcal{S}$
while not termination-condition **do**
  $x =$ improve?(x, T)
  update(T)
end while
return(x)

Simulated Annealing vs. Local Search

There are three important differences:

1. How the procedure halts.
   - Simulated annealing is executed until some external termination condition is satisfied.
   - Local search is performed until no improvement is found.
2. improve?(x, T) doesn't have to return a better point from the neighborhood of x. It returns an accepted solution $y \in N(x)$, where acceptance is based on the current temperature T.
3. Parameter T is updated periodically, and the value of T influences the outcome of the procedure "improve?".

Iterated Hill-Climber Revisited

Algorithm iterated hill-climber

```
t ← 0
initialize best
repeat
    local ← FALSE
    select a current point v_c at random
    evaluate v_c
    repeat
        select all new points in the neighborhood of v_c
        select the point v_n from the set of new points with the best value of evaluation function eval
        if eval(v_n) is better than eval(v_c) then
            v_c ← v_n
        else
            local ← TRUE
        end if
    until local
    t ← t + 1
    if v_c is better than best then
        best ← v_c
    end if
until t = MAX
```

Modification of Iterated Hill-Climber

- Instead of checking all strings in the neighborhood of v_c and selecting the best one, select only one point, v_n from this neighborhood.
- Accept this new point, i.e., $v_c \leftarrow v_n$ with some probability that depends on the relative merit of these two points, i.e., the difference between the values returned by the evaluation function for these two points.

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$\Rightarrow$ **Stochastic hill-climber**

Stochastic Hill-Climber

Algorithm stochastic hill-climber

$t \leftarrow 0$
select a current point v_c at random
evaluate v_c
repeat
  select the string v_n from the neighborhood of v_c
  select v_n with probability $\frac{1}{1+e^{\frac{eval(v_c)-eval(v_n)}{T}}}$
  $t \leftarrow t+1$
until $t = MAX$

Analyzing Stochastic Hill-Climber

- Probabilistic formula for accepting a new solution is based on maximizing the evaluation function.
- It has only one loop. No repeated calls from different random points.
- Newly selected point is accepted with probability p. Thus, the rule of moving from current point v_c to new neighbor, v_n, is probabilistic.
- New accepted point can be worse than current point.
- $p = \frac{1}{1+e^{\frac{eval(v_c)-eval(v_n)}{T}}}$
- Probability of acceptance depends on the difference in merit between these two competitors, i.e., $eval(v_c) - eval(v_n)$, and on the value of an additional parameter T.
- T remains constant during the execution of the algorithm.

Role of Parameter T

Example:

- $eval(v_c) = 107$ and $eval(v_n) = 120$
- $eval(v_c) - eval(v_n) = -13$, new point v_n is better then v_c

Role of Parameter T

Example:

- $eval(v_c) = 107$ and $eval(v_n) = 120$
- $eval(v_c) - eval(v_n) = -13$, new point v_n is better then v_c
- What is probability of accepting new point based on different values of T?

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- $eval(v_c) - eval(v_n) = -13$, new point v_n is better then v_c
- What is probability of accepting new point based on different values of T?

T	$e^{\frac{-13}{T}}$	p
1	0.000002	1.00
5	0.0743	0.93
10	0.2725	0.78
20	0.52	0.66
50	0.77	0.56
10^{10}	0.9999 ...	0.5 ...

Role of Parameter T

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- The greater T, the smaller the importance of the relative merit of the competing points!
- If T is huge (e.g., $T = 10^{10}$), the probability of acceptance approaches 0.5. **The search becomes random!**
- If T is very small (e.g., $T = 1$), we have an ordinary hill-climber!

Role of new String

Suppose $T = 10$ and $eval(v_c) = 107$. Then, probability of acceptance depends only on the value of the new string.

$eval(v_n)$	$eval(v_c) - eval(v_n)$	$e^{\frac{eval(v_c)-eval(v_n)}{T}}$	p
80	27	14.88	0.06
100	7	2.01	0.33
107	0	1.00	0.50
120	-13	0.27	0.78
150	-43	0.01	0.99

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- If new point has same merit as current point, i.e., $eval(v_c) = eval(v_n)$, the probability of acceptance is 0.5.
- If new point is better, the probability of acceptance is greater than 0.5.
- The probability of acceptance grows together with the (negative) difference between these evaluations.

Simulated Annealing

- Main difference to stochastic hill-climber is that simulated annealing changes the parameter T during the run.
- Starts with high values of T making procedure more similar to random search, and then gradually decreases value of T.
- Towards end of the run, values of T are quite small, like an ordinary hill-climber.
- In addition, new points are always accepted if they are better than current point.

Simulated Annealing ctd.

Algorithm simulated annealing

$t \leftarrow 0$
initialize T
select a current point v_c at random
evaluate v_c
repeat
    repeat
        select new point v_n in the neighborhood of v_c
        if $eval(v_c) < eval(v_n)$ **then**
            $v_c \leftarrow v_n$
        else if $random[0,1) < e^{\frac{eval(v_c) - eval(v_n)}{T}}$ **then**
            $v_c \leftarrow v_n$
        end if
    until (termination-condition)
    $T \leftarrow g(T, t)$
    $t \leftarrow t + 1$
until (halting-criterion)

Simulated Annealing ctd.

- Is also known as Monte Carlo annealing, statistical cooling, probabilistic hill-climbing, stochastic relaxation, and probabilistic exchange algorithm.
- Based on an analogy taken from thermodynamics.
  - To grow a crystal, the row material is heated to a molten state.
  - The temperature of the crystal melt is reduced until the crystal structure is frozen in.
  - Cooling should not be done two quickly, otherwise some irregularities are locked in the crystal structure.

Analogies Between Physical System and Optimization Problem

Physical System	Optimization Problem
state	feasible solution
energy	evaluation function
ground state	optimal solution
rapid quenching	local search
temperature	control parameter T
careful annealing	simulated annealing

Problem-Specific Questions

As with any search algorithm, simulated annealing requires answers for the following problem-specific questions.

- What is a solution?
- What are the neighbors of a solution?
- What is the cost of a solution?
- How do we determine the initial solution?

Answers yield the structure of the search space together with the definition of a neighborhood, the evaluation function, and the initial starting point.

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Further Questions

- How do we determine the initial "temperature" T?
- How do we determine the cooling ration $g(T, t)$?
- How do we determine the termination condition?
- How do we determine the halting criterion?

STEP 1:

$T \leftarrow T_{max}$
select v_c at random

STEP 2:

pick a point v_n from the neighborhood of v_c
if $eval(v_n)$ is better than $eval(v_c)$ **then**
    select if $(v_c \leftarrow v_n)$
else
    select it with probability $e^{\frac{-\Delta eval}{T}}$
end if
repeat
    this step
until k_T times

STEP 3:

set $T \leftarrow rT$
if $T \geq T_{min}$ **then**
    goto STEP 2
else
    goto STEP 1
end if

Where, T_{max} initial temperature, k_T number of iterations, r cooling ratio, and T_{min} frozen temperature.

SA for SAT

Algorithm SA-SAT

```
tries ← 0
repeat
    v ← random truth assignment
    j ← 0
    repeat
        if v satisfies the clauses then
            return v
            T = T_max · e^(−j·r)
            for k = 1 to the number of variables do
                compute the increase (decrease) δ in the number of clauses made true if v_k was flipped
                flip variable v_k with probability (1 + e^(−δ/T))^(−1)
                v ← new assignment if the flip is made
            end for
            j ← j + 1
        end if
    until T < T_min
    tries ← tries+1
until tries = MAX-TRIES
```

SA for SAT ctd.

- Outermost loop variable called "tries" keeps track of the number of independent attempts to solve the problem.
- T is set to T_{max} at the beginning of each attempt ($j \leftarrow 0$) and a new random truth assignment is made.
- Inner repeat loop tries different assignments by probabilistically flipping each of the Boolean variables.
- Probability of a flip depends on the improvement δ of the flip and the current temperature.
- If the improvement is negative, the flip is unlikely to be accepted and vice versa.
- r represents a decay rate for the temperature, the rate where it drops from T_{max} to T_{min}.
- The drop is caused by incrementing j, as $T = T_{max} \cdot e^{-j \cdot r}$.

SA-SAT vs. GSAT

- Major difference: GSAT can make a backward move (decrease in number of unsatisfied clauses) if other moves are not available.
- GSAT cannot make two backward moves in a row, as one backward move implies existence of next improvement move!
- SA-SAT can make an **arbitrary sequence of backward moves**, thus **escape local optima**!
- SA-SAT appeared to satisfy at least as many formulas as GSAT, with less work.
- Applications of SA: traveling salesman problem, production scheduling, Timetabling problems and image processing

Summary

- Hill-climbing methods face a danger of getting trapped in local optima.
- Local search can make one backward move.
- Simulated annealing is designed to escape local optima and can make uphill moves at any time.
- Hill-climbing, local search and SA work on complete solutions.
- SA has many parameters to worry about (temperature, rate of reductions, ...).
- The more sophisticated the method, the more you have to use your judgment as to hwo it should be utilized.

References

Zbigniew Michalewicz and David B. Fogel.
How to Solve It: Modern Heuristics, volume 2. Springer, 2004.