## SIMULATED ANNEALING

## Motivation

Finding a good solution to an optimization problem.
Good does not mean perfect.
Trying to minimize the cost of travelling is a good example

## Hill climbing

Our first approach will be the rather naïve Hill Climbing algorithm.

- The basic idea of Hill Climbing is:

1. Choose a starting point.
2. Try to improve solution
3. If no further improvements are possible then stop.

## Hill climbing

It is like the algorithm is climbing a hill and tries to find the top, where the best solution is.
It can only take steps to take it uphill.

- This means it can stop before finding the best solution.


Image source: http://katrinaeg.com/simulated-annealing

## Hill climbing

The biggest hill is the global maximum.
The top of any other hill is a local maximum.


## Hill climbing

$\square$ We need to define the initial solution:

- Randomly generate a sequence o cities.
city $(a, 45,95)$.
city $(b, 90,95)$.
city $(c, 15,85)$.
city (d,40,80).
city $(e, 70,80)$.
city (f,25,65).
city $(\mathrm{g}, 65,65)$.
city $(h, 45,55)$.
city $(i, 5,50)$.
city $(\mathrm{i}, 80,50)$.
city $(1,65,45)$.
city(m,25,40).
city( $n, 55,30$ ).
city (o,80,30).
city $(\mathrm{p}, 25,15)$.
city $(q, 80,15)$.
city $(r, 55,10)$.



## Hill climbing

- We need to define the initial solution:
- Randomly generate a sequence of cities.
initialSolution(Orig,L):-
findall( $\mathrm{X},(\operatorname{city}(\mathrm{X}, \ldots, \quad), \mathrm{X} \backslash=$ Orig),L1), random_permutation(L1,L).
?-initialSolution( $\mathrm{a}, \mathrm{L}$ )



## Hill climbing

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```
    ?-initialSolution(a,L)
```

$$
L=[b, r, c, d, f, l, g, p, n, e, i, m, h, j, q, o]
$$



## Hill climbing

Now, we need to evaluate the solution:

- Compute the total distance.

```
distance(C1,C2,Dist):-
    city(C1,X1,Y1),
    city(C2,X2,Y2),
    DX is X1-X2,
    DY is Y1-Y2,
    Dist is sqrt(DX*DX+DY*DY).
```



## Hill climbing

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        DX is X1-X2,
        DY is Y1-Y2,
        Dist is sqrt(DX*DX+DY*DY).
```

    ?-distance(a,n,D).
    \(D=65.76\)
    

## Hill climbing

Now, we need to evaluate the solution:

- Compute the total distance.
totalDistance([],0).
totalDistance([_],0).
totalDistance( $[\mathrm{X}, \mathrm{Y} \mid \mathrm{L}], \mathrm{T})$ :-
distance (X,Y,CI), totalDistance ([Y|L],T1), T is $\mathrm{Tl}+\mathrm{Cl}$.



## Hill climbing

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totalDistance( $[\mathrm{X}, \mathrm{Y} \mid \mathrm{L}], \mathrm{T})$ :-
distance (X,Y,CI),
totalDistance ( $[\mathrm{Y} \mid \mathrm{L}], \mathrm{T} 1$ ),
T is $\mathrm{Tl}+\mathrm{Cl}$.
?-totalDistance([a,b,r,c,d,f,l,g,p,n,e,i,m,h,i,q,o,a],D).
D $=761$



## Hill climbing

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## Hill climbing

- Compute adjacent solutions:
- Lets swap two random elements

```
newAdjacent(S 1,Sn):-
    length(S 1,T1),
    random_between(1,T1,Pos1),
    random_between(1,T1,Pos2),
    nthl(Posl,S1,E1),
    nth1(Pos2,S1,E2),
    removeElementPos(Pos1,S1,S2),
    insertElementPos(Pos1,E2,S2,S3),
    removeElementPos(Pos2,S3,S4),
    insertElementPos(Pos2,E1,S4,Sn).
```



## Hill climbing

## Compute adjacent solutions:

- Lets swap two random elements
newAdjacent(S1,Sn):-
length(S1,T1), random_between(1,T1,Pos1), random_between(1,T1,Pos2), nthl(Pos $1, \mathrm{~S} 1, \mathrm{E} 1$ ), nthl(Pos2,S1,E2), removeElementPos(Pos 1,S1,S2), insertElementPos(Pos1,E2,S2,S3), removeElementPos(Pos2,S3,S4), insertElementPos(Pos2,E1,S4,Sn).
?-newAdjacent([b,r,c,d,f,l,g,p,n,e,i,m,h,j,q,o],NA).
$N A=[b, r, c, d, h, l, g, p, n, e, i, m, f, i, q, o]$



## Hill climbing

## Compute adjacent solutions:

- Lets swap two random elements
newAdjacent(S1,Sn):-
length(S $1, \mathrm{~T} 1$ ), random_between(1,T1,Pos1), random_between(1,T1,Pos2), nth $1(\operatorname{Pos} 1, S 1, E 1)$, nthl(Pos2,S1,E2), removeElementPos(Pos 1,S1,S2), insertElementPos(Pos1,E2,S2,S3), removeElementPos(Pos2,S3,S4), insertElementPos(Pos2,E1,S4,Sn).
?-newAdjacent([b,r,c,d,f,l,g,p,n,e,i,m,h,i,q,o],NA).
$N A=[b, r, c, d, h, l, g, p, n, e, i, m, f, j, q, o]$



## Hill climbing

- Compute adjacent solutions:
- Now we can compute some adjacents (let's do it 10 times)
[b,r,c,d,h,l,g,p,n,e,i,m,f,i,q,o] [b,r,c,d,l,f,g,p,n,e,i,m,h,i,q,o] [b,r,c,d,f,l,g,p,n,e,i,h,m,i,q,o] [b,r,c,d,f,q,g,p,n,e,i,m,h,i,l,o] [b,r,l,l,d,f,c,g,p,n,e,i,m,h,i,q,o] [b,r,c,d,f,l,g,p,n,e,i,m,h,i,q,o] [b,r,c,d,f,l,g,h,n,e,i,m,p,i,q,o] [b,r,c,g,f,l,d,p,n,e,i,m,h,i,q,o] [b,h,c,d,f,l,l,g,p,n,e,i,m,r,i,q,o] [b,r,c,c,n, $, l, g, p, f, e, i, m, h, i, q, o]$



## Hill climbing

- Compute adjacent solutions:
- And add the origin/destination
[a,b,r,c,c,d,h,l,g,p,n,e,i,m,f,i,q,o,a] [a,b,r,c,c,l,l,f,g,p,n,e,i,m,h,i,q,o,a] $[a, b, r, c, d, f, l, g, p, n, e, i, h, m, i, q, o, a]$ $[a, b, r, c, d, f, q, g, p, n, e, i, m, h, i, l, o, a]$ $[a, b, r, l, l, d, f, c, g, p, n, e, i, m, h, i, q, o, a]$ $[a, b, r, c, d, f, l, g, p, n, e, i, m, h, i, q, o, a]$ [a,b,r,r,c,d,f,l,g,h,n,e,i,m,p,i,q,o,a] [a,b,r,c,g,f,l,d,p,n,e,i,m,h,i,q,o,a] [a,b,h,c,d,f,f,l,g,p,n,e,i,m,r,i,q,q,o,a] $[a, b, r, c, d, n, l, l, g, p, f, e, i, m, h, i, q, o, a]$



## Hill climbing

- Compute adjacent solutions:
- Are they better than my original path (761)?
[ (764,[a,b,r,c,d,h,l,g,p,n,e,i,m,f,i,q,o,a]), (803,[a,b,r,c,c,d,l,f,g,p,n,e,i,m,h,i,q,o,a]), (799,[a,b,r,c,d,f,l,g,p,n,e,i,h,m,i,q,o,a]), ( $810,[a, b, r, c, d, f, q, g, p, n, e, i, m, h, i, l, o, a]$ ), ( $741,[a, b, r, l, d, f, c, g, p, n, e, i, m, h, i, q, o, a])$, ( $761,[a, b, r, c, d, f, l, g, p, n, e, i, m, h, i, q, o, a]$ ), (742,[a,b,r,c,d,f,l,g,h,n,e,i,m,p,i,q,o,a]), ( $834,[\mathrm{a}, \mathrm{b}, \mathrm{r}, \mathrm{c}, \mathrm{g}, \mathrm{f}, \mathrm{l}, \mathrm{d}, \mathrm{p}, \mathrm{n}, \mathrm{e}, \mathrm{i}, \mathrm{m}, \mathrm{h}, \mathrm{i}, \mathrm{q}, \mathrm{o}, \mathrm{a}]$ ), ( $716,[a, b, h, c, d, f, l, g, p, n, e, i, m, r, i, q, o, a])$, (777,[a,b,r,c,d,n,l,g,p,f,e,i,m,h,i,q,o,a])]



## Hill climbing

- If we have a better solution we move.

$$
(716,[a, b, h, c, d, f, l, g, p, n, e, i, m, r, i, q, o, a])
$$

- We define a total number of iterations to stop or we stop when no neighbor is a better solution!
- But not finding a better solution in the neighborhood doesn't mean it does not exist.



## Simulated Annealing

$\square$ Tries to overcome this problem by (sometimes) not accepting to move to best neighbors.

- The basic idea:

1. Generate an initial random solution.
2. Calculate its cost $\mathrm{c}_{\text {old }}$.
3. Generate a random neighbor
4. Calculate the new solution's cost $\mathrm{c}_{\text {new }}$
5. Compare them:
6. If $c_{\text {new }}<c_{\text {oldd }}$ move to the new solution
7. If $c_{\text {new }}>c_{\text {old }}$ : maybe move to the new solution
8. Repeat steps 3-5 above until an acceptable solution is found or you reach some maximum number of iterations.

## Simulated Annealing

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 acceptable solution is found or you reach some maximum number of iterations.

## Simulated Annealing

## If $\mathrm{c}_{\text {new }}>\mathrm{c}_{\text {old }}$ : maybe move to the new solution

- Hill climbing can get caught at local maxima.
- To avoid that problem, Simulated Annealing sometimes chooses to keep the worse solution.
- To decide, the algorithm calculates an acceptance probability and then compares it to a random number.


## Simulated Annealing

The acceptance probability function takes $\mathrm{c}_{\text {old }}$, $\mathrm{c}_{\text {new }}$ and a temperature $T$.

- Temperature?
- Yes, Simulated Annealing is based on metalworking.
- Temperature is usually started at 1.0
- It decreases at the end of each iteration by multiplying by a constant $\alpha$ (usually a value between 0,80 and 0,99 )
- Experience shows that higher is better!


## Simulated Annealing

- Temperature?
- We also need to decide how many neighbour generations and comparisons we make at each temperature.
- One can use a fixed value (the higher the better between 100 and 1000)
- An alternative is to dynamically change the number of iterations as the algorithm progresses.
- At lower temperatures it is important that a large number of iterations are done so that the local optimum can be fully explored.
- At higher temperatures, the number of iterations can be less.


## Simulated Annealing

- Going back...
- The acceptance probability function takes $\mathrm{c}_{\text {old }} \mathrm{c}_{\text {new }}$ and a temperature $T$.
- The acceptance probability generates a number between 0 and 1 , which is a sort of recommendation on whether or not to jump to the new solution. For example:
- 1.0: switch (the new solution is better)
- 0.0: do not switch (the new solution is infinitely worse)

Once the acceptance probability is calculated, it's compared to a randomly-generated number between 0 and 1 .
If the acceptance probability is larger than the random number, switch to the new solution.

## Simulated Annealing

$\square$ The acceptance probability function takes $\mathrm{c}_{\text {old }} \mathrm{c}_{\text {new }}$ and a temperature $T$.
And how do we compute it?
Usually with the following formula:

$$
A p=e^{\frac{c_{o l d}-c_{n e w}}{T}}
$$

(Stuart Russell and Peter Norvig. 2009. Artificial Intelligence: A Modern Approach (3rd ed.). Prentice Hall Press, Upper Saddle River, NJ, USA.)

## Simulated Annealing

$$
A p=e^{\frac{c_{o l d}-c_{n e w}}{T}}
$$

- The probability decreases exponentially with the "badness" of the move. $\left(c_{\text {old }}-c_{\text {new }}\right)$.
$\square$ The probability also decreases as the "temperature" $T$ goes down:
- "bad" moves are more likely to be allowed at the start when $T$ is high, and they become more unlikely as T decreases.
$\square$ If the algorithm lowers T slowly enough, it will find a global optimum with probability approaching 1.


## Simulated Annealing

$$
A p=e^{\frac{c_{\text {old }}-c_{n e w}}{T}}
$$

$\square$ Examples:
$\square T=1, c_{\text {old }}=99$ and $c_{\text {new }}=100, A p \approx 0,38(38 \%)$
$\square \mathrm{T}=0.9, \mathrm{c}_{\text {old }}=100$ and $\mathrm{c}_{\text {new }}=98, \mathrm{Ap} \approx 9$ (more than 1, we consider 100\%)
$\square \mathrm{T}=0.9, \mathrm{c}_{\text {old }}=98$ and $\mathrm{c}_{\text {new }}=100, \mathrm{Ap} \approx 0,11(11 \%)$
(Recall $e=2,71828$ )

## Simulated Annealing

The complete idea:
Generate an initial random solutions.
Calculate its cost $c_{\text {old }}$.
While $T>0$ and not reached a maximum number of iterations
While the total number of iterations per temperature is not exceeded
Generate a random neighbour s'
Calculate the new solution's cost $c_{\text {new }}$
If $\mathrm{c}_{\text {naw }}<\mathrm{c}_{\text {old }}$
$\mathrm{s}=\mathrm{s}$ '
else

$$
\begin{aligned}
& A p=e^{\frac{c_{\text {old }}-c_{\text {new }}}{T}} \\
& \text { if Ap }>\text { random }(0,1) \\
& s=s^{\prime} \\
& c_{\text {od }}=c_{\text {new }}
\end{aligned}
$$

