

Random Sampling

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Engineering Systems and Design

Optimization Methods

- Exhaustive search methods are ineffective when solving very large optimization problems
- Exact methods of Optimization solve complex problems without the need to exhaustively search for all possible solutions of a problem. These methos ensure that the solution obtained is the optimal one.
- Several exact methods of optimization in the previous lecture (Simplex ; Branch and Bound; Dynamic Programming ; etc)
- However, as the size of your problem grows, the computation requirements to solve optimization increases considerably.
- In many instance, the solution space for solutions is so large that exact methods of optimization cannot even find feasible solutions for a problem.
- In those situations using exact methods of optimization is impractical

Exact Methods - CPU Performance

	P-1	Median		Travelling Salesman			Vehicle Routing				
n	Fac.	CPU Time	Opt. Value	n	CPU Time	Opt. Value	n	Veh.	Cap.	CPU Time	Opt. Value
10	1	0.12 s	8061276	10	1.29 s	34993	10	2	180	1.22	32846
20	3	0.16	9814108	20			20	3	230	697	58996
25	4	0.14 s	9359061	25	1.21 s	39224	25	4	250	>6000	64362 (11.2%)
50	8	0.17 s	9870230	50	49 s	57546	-	-	-	-	-
75	12	0.25 s	15617651	75	91 s	70395	-	-	-	-	-
100	15	0.32 s	18954163	100	178 s	78357	-	-	-	-	-
200	20	1.25 s	35825600	200	2625 s	105404	-	-	-	-	-
500	30	11.18 s	74794047	500	>6000 s	220704 (25.9%)	-	-	-	-	-
1000	30	147.61 s	161388969	-	-	-	-	-	-	-	-
5000	100	>6000	No Solution Found	-	-	-	-	-	-	-	-

Random Sampling

- The most "naïve" metaheuristic approach consists on randomly sampling solutions from the solution space.
 - **1.** Initialize: Generate random initial solution, $p_{best} = p_{initial}$
 - 2. While (termination criteria is not met, e.g. CPU time)
 - 3. Create random candidate solution p_{new}
 - 4. If p_{new} is better than p_{best} , than $p_{best} = p_{new}$
 - 5. Go back to 2, until termination criteria is met

P-Median Example

 Location planning involves specifying the physical position of facilities that provide demanded services.



Number of candidate locations n=100

Number of locations to open fac=15

Random Sampling: Randomly generate a _ binary vector at each iteration



P-Median – Generate Instance



Demand for each location is generated randomly

P-Median – Initial Solution



P-Median – Random Sampling Search Procedure

Random Algorithm

Random Sampling



P-Median – Random Sampling Search Procedure

Random Sampling



P-Median – Random Sampling Solution (n=100 ; fac=15)



Optimum= 18,954,163.57 (0.7 seconds)

What is the probability of finding the optimal solution through random sampling?

$$\frac{1}{2^{100}} = 1 \text{ in } 1.27 \times 10^{21}$$

P-Median – Random Sampling Solution (n=1000 ; fac=30)

Random Sampling



Obj. Value = 194,419,346.65 (Gap = 16.9%)

Optimum= 161,393,599.84 (321 seconds)

P-Median – Random Sampling Solution (n=5000 ; fac=100)



Obj. Value = 561,681,400.18 Optimum=?

Needle in the Haystack

- Random Sampling keeps randomly generating new candidate solutions
- If we imagine a large space, with, say, millions of points, it is clear that it will take very long until we find the optimal solution for the problem
- It may even take extremely long to find anything remotely good
- Random Sampling is like exhaustive search – not really used in optimization



Using random sampling is like finding a needle in the haystack



Introduction to Local Search

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Local Search

- Local Search is the oldest and simplest metaheuristics method. Also often designated as hill climbing ; steepest descent; iterative improvement, etc.
- At each iteration, the heuristic replaces the current solution by a neighbour that improves the objective function
- A neighbour solution can be reached by applying a move operator
- The search stops when not better solutions can be found



Source: <u>https://buildingai.elementsofai.com/</u> <u>Getting-started-with-AI/hill-climbing</u>

Local Search Algorithm



Replacement Phase

- First Descent: This strategy consists in choosing the first improving neighbour that is better than the current solution. Then, an improving neighbour is immediately selected to replace the current solution.
- Best Descent: In this strategy, the best neighbour (i.e., neighbour that improves the most the cost function) is selected. The neighbourhood is evaluated in a fully deterministic manner. Hence, the exploration of the neighbourhood is exhaustive
- Random selection: In this strategy, a random selection is applied to those neighbours improving the current solution

Solution Representation

- Designing any iterative metaheuristic needs an encoding of a solution
- The encoding plays a major role in the efficiency and effectiveness of a metaheuristic procedure and constitutes an essential step in designing any metaheuristic.
- Many straightforward encodings may be applied for some traditional families of optimization problems. Those representations may be combined or underlying new representations.



Neighbourhood and Move Operator

- The definition of the neighbourhood is a required common step for the design of any Local Search metaheuristic. It plays a crucial role in the performance
- A neighbour solution is obtained by the application of a search operator that performs a small perturbation to the solutions



The circle represents the neighborhood of *s* in a continous problem with two dimensions.

- Nodes of the hypercube represent solutions of the problem.
- The neighbors of a solution (e.g., (0,1,0)) are the adjacent nodes in the graph.

Size of the neighbourhood

- Binary encoding: the neighbourhood of a binary solution consists in flipping one bit of the solution. For a binary vector of size n, the size of the neighbourhood will be n.
- Discrete encoding: The neighbourhood for binary encodings may be extended to any discrete vector representation using a given alphabet (1,2,...k; a,b,...k). For a discrete vector of size n, and alphabet with k characters, the size of the neighbourhood will be (k-1)n.
- Permutation encoding: A usual neighbourhood is based on the "swap" operator that consists in exchanging (or swapping) the location of two elements. For a permutation of size n, the size of this neighbourhood is n(n - 1)/2



Current



- Local Search iteratively applies a generation and a replacement procedure;
- In the generation phase, a set of candidate solutions is generated from the current solution by applying a move operator;
- In the replacement phase, the best solution from the set of candidate solutions is selected and compared with the current solution. If the solution obtained is better than the current solution, then the current solution is replaced.
 - **1.** Initialize: Generate random initial solution, $p_{best} = p_{initial}$
 - 2. While (termination criteria is not met, e.g. CPU time)
 - 3. Generate a new solution (or a set of new solutions) p_{new} by applying a small perturbation (move operator) to p_{best}
 - 4. If p_{new} is better than p_{best} , than $p_{best} = p_{new}$
 - 5. Go back to 2, until termination criteria is met









Local Search in Python

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P-Median Example

- Solution Representation: Binary Encoding (*we could have used discrete encoding)
- Move Operator: Open 1 random location and close 1 random location
- Replacement Procedure: First Descent







Number of candidate locations n=100

Number of locations to open fac=15

P-Median – Hill Climbing Generation Phase

Hill Climbing Algorithm



of locations

Hill Climbing

iteration=iteration+1

objvalue=sum(objvalue open)

assignment open=np.argmin(distancelct open, axis=0)

objvalue open=distancelct open.min(axis=0)*demandlct

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P-Median – Hill Climbing Replacement Phase

#If objective values improves
if objvalue<np.min(objvalue_i):</pre>



#Update locations
yi=copy.deepcopy(yi_i)
yi_open=copy.deepcopy(yi_open_i)

#Compute links

linkindex_p1=range(n)
linkindex_p2=assignment_open
yi_open_index = np.array(yi_open)
linkindex p2 = yi open index[linkindex p2]

#Plot results

def connectpoints(x,y,p1,p2):
 x1, x2 = x[p1], x[p2]
 y1, y2 = y[p1], y[p2]
 plt.plot([x1,x2],[y1,y2],'k-')



```
plt.plot(coordlct_x, coordlct_y, 'o', color='black');
```

```
for i_index in range(len(yi_open)):
    plt.plot(coordlct_x[yi_open[i_index]], coordlct_y[yi_open[i_index]], 'o', color='red');
```

```
#Update vector of objective values and CPU Time
objvalue_i=np.append(objvalue_i, objvalue)
```

```
now = time.time()
cputime_i=np.append(cputime_i, now-program_starts)
```

```
clear_output(wait=True)
plt.draw()
plt.pause(0.1)
plt.clf()
```

#Update last objective value

objvalue_i=np.append(objvalue_i, min(objvalue_i))
now = time.time()
cputime_i=np.append(cputime_i, now-program_starts)



Keep trace of the objective values obtained over time

Replacement Phase (First Descent)

Hill Climbing

Plot

If objective value is worse than the

iterations, then nothing happens;

best objective value found in previous

otherwise we update the best solution

P-Median – Hill Climbing Solution (n=100 ; fac=15)

Hill Sampling



Obj. Value Rand. Sampling = 21,321,318.07 (Gap = 11.1%) Obj. Value Hill Climbing = 18,983,919.72 (Gap = 0.16%) Optimum= 18,954,163.57 (0.7 seconds)

P-Median – Hill Climbing Solution (n=1000 ; fac=30)

Hill Climbing



Obj. Value Rand. Sampling = 194,419,346.65 (Gap = 16.9%) Obj. Value Hill Climbing = 162,325,709.91 (Gap = 0.57%) Optimum= 161,393,599.84 (321 seconds)

P-Median – Hill Climbing Solution (n=5000 ; fac=100)

Hill Climbing



TSP Example

- Solution Representation: Premutation Encoding
- Move Operator: Swap 2 locations
- Replacement Procedure: First Descent



no. locations



Number of candidate locations n=100

TSP – Generate Instance



TSP – Initial Solution



TSP – Random Sampling Search Procedure

Random Algorithm

random.seed(3) iteration=0 ObjValueOpt=ObjValue Objvalue list=ObjValue program starts = time.time() cputime i=[0,0] while cputime i[-1]<6000: iteration=iteration+1 #Random permutation Solution i=random.sample(list(range(n), n) dfSolution i=pd.DataFrame(Solution i) dfSolution i dflinkindex p1=dfSolution i dflinkindex p2=dfSolution i.shift(-1) dflinkindex p2.loc[n-1]=dflinkindex p1.loc[0] linkindex p1=dflinkindex p1.to numpy() linkindex p2=dflinkindex p2.to numpy() linkindex p1=linkindex p1.astype(int) linkindex p2=linkindex p2.astype(int) linkindex p1=linkindex p1.transpose()[0] linkindex p2=linkindex p2.transpose()[0]

#Compute Objective Value ObjValue=sum(distancelct[linkindex_p1,linkindex_p2])

Random Sampling

Generate new random permutation of locations

Compute Objective Value

TSP – Random Sampling Search Procedure

#Update Optimal Solution
if ObjValue<ObjValueOpt:
 ObjValueOpt=copy.deepcopy(ObjValue)
 OptSolution=copy.deepcopy(Solution_i)</pre>



Objvalue_list=np.append(Objvalue_list, ObjValueOpt)
now = time.time()
cputime_i=np.append(cputime_i, now-program_starts)

```
#print(ObjValueOpt)
```

```
#def connectpoints(x,y,p1,p2):
```

```
# x1, x2 = x[p1], x[p2]
```

```
# y1, y2 = y[p1], y[p2]
```

```
# plt.plot([x1,x2],[y1,y2],'k-')
```

```
#for i_index in range(len(linkindex_p2)):
# connectpoints(coordlct_x,coordlct_y,linkindex_p1[i_index],linkindex_p2[i_index])
```

```
#plt.plot(coordlct_x, coordlct_y, 'o', color='black');
```

```
#clear_output(wait=True)
#plt.draw()
#plt.pause(0.1)
#plt.clf()
```

#Update Last objective value Objvalue_list=np.append(Objvalue_list, min(Objvalue_list)) now = time.time() cputime_i=np.append(cputime_i, now-program_starts)

Random Sampling

If objective value is worse than the best objective value found in previous iterations, then nothing happens; otherwise we update the best solution



TSP – Hill Climbing Generation Phase

random.seed(3)
iteration=0
ObjValueOpt=ObjValue
Objvalue_list=ObjValue
program_starts = time.time()
cputime_i=[0,0]
OptSolution=Solution_i

while cputime_i[-1]<6000:</pre>

iteration=iteration+1
Solution_i=copy.deepcopy(OptSolution)

swap_it=0
while swap_it<no_swap:
 swap_random(Solution_i)
 swap it=swap it+1</pre>

dfSolution_i=pd.DataFrame(Solution_i)
dfSolution_i
dflinkindex_p1=dfSolution_i
dflinkindex_p2=dfSolution_i.shift(-1)
dflinkindex_p2.loc[n-1]=dflinkindex_p1.loc[0]
linkindex_p1=dflinkindex_p1.to_numpy()
linkindex_p2=dflinkindex_p2.to_numpy()
linkindex_p1=linkindex_p1.astype(int)
linkindex_p2=linkindex_p1.transpose()[0]
linkindex_p2=linkindex_p2.transpose()[0]

#Compute Objective Value
ObjValue=sum(distancelct[linkindex_p1,linkindex_p2])

Hill Climbina

#Exchange Operator
def swap_random(seq):
 idx = range(len(seq))
 i1, i2 = random.sample(idx, 2)
 seq[i1], seq[i2] = seq[i2], seq[i1]

Apply swap operator

Select two random locations Swap location in the permutation

Generation Phase (Move Operator Code)

Compute Objective Value

TSP – Hill Climbing Replacement Phase

#Update Optimal Solution
if ObjValue<ObjValueOpt:
 ObjValueOpt=copy.deepcopy(ObjValue)
 OptSolution=copy.deepcopy(Solution_i)</pre>



Objvalue_list=np.append(Objvalue_list, ObjValueOpt)
now = time.time()
cputime_i=np.append(cputime_i, now-program_starts)

```
#def connectpoints(x,y,p1,p2):
```

```
# x1, x2 = x[p1], x[p2]
```

- # y1, y2 = y[p1], y[p2]
- # plt.plot([x1,x2],[y1,y2],'k-')

```
#for i_index in range(len(linkindex_p2)):
```

connectpoints(coordlct_x,coordlct_y,linkindex_p1[i_index],linkindex_p2[i_index])

```
#plt.plot(coordlct_x, coordlct_y, 'o', color='black');
```

```
#clear_output(wait=True)
#plt.draw()
#plt.pause(0.1)
#plt.clf()
```

#Update last objective value

Objvalue_list=np.append(Objvalue_list, min(Objvalue_list))
now = time.time()
cputime i=np.append(cputime i, now-program starts)

Hill Climbing

If objective value is worse than the best objective value found in previous iterations, then nothing happens; otherwise we update the best solution

Plot

Replacement Phase (First Descent)



TSP Solution (n=100)



TSP Solution (n=500)



Design versus Control Problems



Design versus Control Problems

- Design problems: Design problems are generally solved once. They need a very good quality of solutions whereas the time available to solve the problem is important. These problems involve an important financial investment; (e.g. telecommunication network design and processor design, etc.)
- Control problems: Control problems represent the other extreme where the problem must be solved frequently in real time. These problems require very fast heuristics are needed; the quality of the solutions is less critical (e.g. routing messages in a computer network; traffic management in a city; ridesharing operations.
- Planning problems: Between these extremes, one can find an intermediate class of problems represented by planning problems. In this class of problems, a trade-off between the quality of solution and the search time must be optimized; (e.g. scheduling of operations; task assignment, etc.)

Activity 1

- Consider the following problem: Given a set of *n* packages with profit *p_j* and weight *w_j*, and a set of *m* containers with weight capacity *c_i*, select *m* disjoint subsets of packages so that the total profit of the selected packages is maximum, while ensuring the containers' capacity is never exceeded
- Exercise 1: Formulate the problem mathematically
- Exercise 2: Solve the problem using pyomo (instances in the next slide)
- Exercise 3: Propose and apply a random sampling and a local search algorithm for the problem



Activity 1 - Instances

Instance 1

random.seed(1)

n = 100#number of objects

b= 5 #number of bins

cap=50

#Generate random locations
value = random.choices(range(10, 100), k=n)
weights = random.choices(range(5, 20), k=n)

Solution*=2356 CPU time = 0.53 sec

Instance 2

random.seed(1)

n = 10000 #number of packagesb= 200 #number of bins

cap=50

#Generate random locations
profit = random.choices(range(10, 100), k=n)
weights = random.choices(range(5, 20), k=n)

Solution*=117925.0 CPU time = 986 sec