# Multiobjective Optimization Neighborhood Exploration

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## Section 1

Module: Neighborhood Exploration

## Requirements

#### The requirements for this class are:

- Data Structures and Algorithmic Complexity
  - Graph concepts
- Programming in Python or C/C++
- Module 1 Fundamentals
- Module 2 Greedy

**Topics** 

## Section 2

Neighborhood Exploration

# Some Definitions (remember from Module 2)

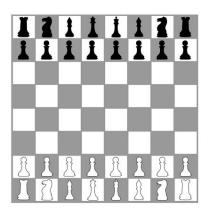
Recall basic definitions for an optimization problem, such as solutions and evaluations, and classic NP-hard problems such as the Knapsack Problem and Traveling Salesman Problem. More precisely:

- The XS denotes a Solution Space, where XE is an Evaluation Space (or Objective Space)
  - The pair  $XES = \langle XS, XE \rangle$  denotes the XESolution space
  - A SO optimization problem is defined by the triple  $\langle XS, XE, f \rangle$
- The space XE can be partioned into  $XE = XFeasible \cup XInfeasible$ , where XFeasible  $\cap$  XInfeasible  $= \emptyset$
- XS denotes all valid representations of a solution, that are structurally correct
  - it may include infeasible solutions s, that are valid, but with infeasible evaluation  $f(s) \in XInfeasible$
  - it depends on how the problem is modeled, but it's not uncommon to have XInfeasible  $\neq \emptyset$
- The optimal solution  $s^*$  is always feasible  $f(s^*) \in XFeasible$ , unless the problem is impossible

# Neighborhood

Given a solution  $s \in XS$ , we define a *neighbor solution*  $s' \in XS$  as:

- a neighborhood (or neighborhood structure)  $\mathcal{N}(s)$  is a set of solutions reachable by some move function/operator  $m: XS \mapsto XS$
- ullet we say that  $s' \in \mathcal{N}(s) \iff \exists m \; such \; that \; s' = m(s)$ 
  - ullet or, typically denoted by operator  $\oplus$  notation:  $s'=s\oplus m$



# Reachability of Solutions and Move Composition

We recall an instance of the Knapsack Problem with 5 items and consider solutions  $s_1 = (01001)$  and  $s_2 = (11010)$  from XS

- We consider the following move definition  $M^{(I)} = \{m_1, m_2, ..., m_i\} = \{m_1, m_2, ..., m_i\}$ {change the value of the bit i}
- We can find moves  $m_1, m_4, m_5 \in M^{(I)}$  such that  $s_2 = ((s_1 \oplus m_1) \oplus m_4) \oplus m_5$ 
  - this changes the values of the first, fourth and fifth bits
  - the following intermediate solutions are visited in this path:  $s_1 = (01001) \rightarrow (11001) \rightarrow (11011) \rightarrow (11010) = s_2$
- Alternatively, a composite move  $m_{1.4.5}$  could be built with function composition:  $m_{1,4,5} = m_5 \circ m_4 \circ m_1$ ; or  $m_{1,4,5} = \bigcap_{m \in (m_1, m_4, m_5)} m$  or by using  $\mapsto$  sequential notation:  $m_{1.4,5}=m_1\mapsto m_4\mapsto m_5$ 
  - In other words,  $m_{1.4.5}(s) = m_5(m_4(m_1(s)))$
- Now we consider moves  $M^{(II)}$  where two bits i and j are simultaneously changed (**Exercise**: What is the size of this neighborhood?)
  - Solution  $s_2$  could never be reachable by  $s_1$  in such neighborhood!

## Move Cost

Given a move m and function f, we can compute the  $move\ cost\ \bar{m}^f$  (or simply  $\bar{m}$ ) in the following way:

- given an evaluation function  $f: XS \mapsto XE$ , and e = f(s) denoting the evaluation of a solution s (when f is known, it can be ommitted)
- given a *neighbor* s' = m(s) the *move cost*  $\bar{m}(s)$  is defined by  $\bar{m}(s) = \bar{m}^f(s) = f(s') f(s)$
- naturally, any  $e \in XE$  space must support add and subtract basic arithmetics
- we **do not** require XE to be a *total order*, although this is true for single objective optimization, i.e., minimization or maximization
- we say that moves  $M=(m_1,m_2,...)$  are independent if composite move  $m'=\bigcap_{m\in M}m$  has a fixed cost  $\bar{m}'(s)=\sum_{m\in M}\bar{m}(s), \ \forall s\in XS$ 
  - this is an important property for newer neighborhood strategies in literature!

# Example for the Traveling Salesman Problem (euclidean)

Let's think of a neighborhood structure for the TSP. What is a move? How much does it cost?



#### Section 3

Neighborhood Exploration Primitives

# Neighborhood Exploration: Basic Primitives

Given a solution  $s \in XS$ , a neighborhood  $\mathcal N$  and its associated *move set*  $\mathcal M = \{m_1, m_2, m_3, ...\}$  such that  $\mathcal N = \{m_1(s), m_2(s), m_3(s), ...\}$ , we define two basic neighborhood exploration primitives: RandomMove and AllMoves.

- the RandomMove returns a random move  $\{m\}$  from move set  $\mathcal{M}$
- ullet the AllMoves returns a sequence  $\mathcal{M}^P=(m_1,m_2,...)$  of move set  $\mathcal{M}$

Typically, two complementary primitives are built on top of AllMoves: FirstMove and NextMove.

- FirstMove( $\mathcal{N}, s$ ) returns  $\{m_1\}$ , where  $m_1$  is the first move from  $\mathcal{M}^P$
- $NextMove(\mathcal{N}, s, m_i)$  returns  $\{m_{i+1}\}$ , where  $m_i$  is a move from  $\mathcal{M}^P$

Note that returned moves may not exist, so one must check it! (typical *optional* behavior...)

# Neighborhood Exploration: Find Primitives

Given a neighborhood  $\mathcal N$  and solution  $s\in XS$ , we define three neighborhood exploration primitives: FindAny, FindFirst and FindBest.

- ullet the FindAny tries to find any move m' with  $s'=m'(s)\in\mathcal{N}(s)$  that improves s
  - we assume a more restricted neighborhood  $\mathcal{N}_{\leq \kappa} \subseteq \mathcal{N}$ , where  $|\mathcal{N}_{\leq \kappa}| \leq k$
  - ullet assuming *minimization*, if such  $s' \in \mathcal{N}_{\leq \kappa}(s)$  exists, then f(s') < f(s)
- the FindFirst tries to find the first move  $m_i$  with
  - $s_i = m_i(s) \in \mathcal{N}(s) = \{s_1, ..., s_i, ...\}$  that improves current solution s
    - assuming minimization, if such  $s_i \in \mathcal{N}(s)$  exists, then i is the smallest value such that  $f(s_i) < f(s)$
- the FindBest tries to find the best move  $m^*$  with  $s^* = m^*(s) \in \mathcal{N}(s)$  that improves current solution s
  - assuming *minimization*, if such  $s^* \in \mathcal{N}(s)$  exists, then  $f(s^*) < f(s)$  and  $f(s^*) \le f(s')$ ,  $\forall s' \in \mathcal{N}(s)$

# Pseudocode for Find Primitives: FindAny

The FindAny considers, without loss of generality, a minimization function f, a neighborhood  $\mathcal{N}$ , a value  $\kappa_{max}$ , a pseudorandom function  $\xi(.)$ , stop criteria stop(.) and current solution s. It can be implemented in the following way:

```
procedure FINDANY(f(.), \mathcal{N}(.), \kappa_{max}, \xi(.), stop(.), s)
    k \leftarrow 0
    while k < \kappa_{max} and not stop(time(), f(s)) do
         m \leftarrow RandomMove(\mathcal{N}, s, \xi)
        if \bar{m}^f(s) < 0 then
             return \{m\}
         else
             k \leftarrow k + 1
         end if
    end while
    return {}
end procedure
```

## Pseudocode for Find Primitives: FindFirst

The FindFirst considers, without loss of generality, a minimization function f, a neighborhood  $\mathcal{N}$ , stop criteria stop(.) and current solution s. It can be implemented in the following way:

```
procedure FINDFIRST(f(.), \mathcal{N}(.), stop(.), s)
    m \leftarrow FirstMove(\mathcal{N}, s)
    while \exists m and not stop(time(), f(s)) do
        if \bar{m}^f(s) < 0 then
             return \{m\}
        else
             m \leftarrow NextMove(\mathcal{N}, s, m)
        end if
    end while
    return {}
end procedure
```

## Pseudocode for Find Primitives: FindBest

The FindBest considers, without loss of generality, a minimization function f, a neighborhood  $\mathcal{N}$ , stop criteria stop(.) and current solution s. It can be implemented in the following way:

```
procedure FINDBEST(f(.), \mathcal{N}(.), stop(.), s)
     m \leftarrow FirstMove(\mathcal{N}, s)
     if \exists m then return \{\}
     \langle e^*, m^* \rangle \leftarrow \langle \bar{m}^f(s), m \rangle
     while \exists m and not stop(time(), f(s)) do
          if \bar{m}^f(s) < e^* then
               \langle e^*, m^* \rangle \leftarrow \langle \bar{m}^f(s), m \rangle
          end if
          m \leftarrow NextMove(\mathcal{N}, s, m)
     end while
     if e^* < 0 then return \{m^*\} else return \{\}
end procedure
```

#### Section 4

Local Search and Refinement Heuristics

# Heuristics for Neighborhood Exploration and Local Optima

Given a neighborhood  $\mathcal{N}$  and a solution s, we can explore it, in order to improve solution s by finding a better neighbor s'

Some heuristics for neighborhood exploration are classic, mainly three: random selection (RS); first improvement (FI); and best improvement (BI). We have also proposed a multi improvement (MI) strategy that will be studied later.

These are also called *refinement heuristics* and are the foundations for several local search (LS) algorithms.

Differently from a global search (GS) algorithm, that tries to find an optimal solution, a local search tries to find a locally optimal solution regarding some specific neighborhood  $\mathcal{N}$ .

- So, recalling the basic definitions with XE as a total order, we define local optima  $s^* \in XS$ , given neighborhood  $\mathcal{N}$  and a solution  $s \in XS$ :
  - For minimization, we have that  $f(s^*) \leq f(s'), \forall s' \in \mathcal{N}(s)$
  - For maximization, we have that  $f(s^*) \geq f(s'), \forall s' \in \mathcal{N}(s)$

## Some Refinement Heuristics and Local Search

In the same way that constructive heuristics are able to generate initial solutions, the Refinement Heuristics can try to improve them. In special, local search algorithms are refinment heuristics that try to reach some local optima related to one or many neighborhoods.

We have seen some neighborhood exploration primitives that try to generate an *improving move* over  $\mathcal{N}$  for solution  $s \in XS$ . Now, the refinement heuristic  $\mathcal{H}$  will try to return an improving neighbor  $s' = \mathcal{H}(s) \in XS$ (naturally, if  $\exists s'$  then f(s') < f(s) for minimization).

We begin with classic refinement heuristics: Random Selection, First Improvement and Best Improvement.

## Refinement Heuristic: Random Selection

Given a neighborhood  $\mathcal{N}$  and a parameter  $\kappa_{max}$ , the Random Selection (RS) heuristic is an implementation of the primitive FindAny:

- RS tries to find any solution  $s' \in \mathcal{N}(s)$  that improves current solution  $s \in XS$
- RS is limited to  $k_{max}$  tries

```
procedure RANDOMSELECTION(f(.), \mathcal{N}(.), \kappa_{max}, \xi(.), stop(.), s)
    m \leftarrow FindAny(f, \mathcal{N}, \kappa_{max}, \xi(.), stop, s)
    if \exists m then
         return \{m(s)\}
    else
         return {}
    end if
end procedure
```

## Refinement Heuristic: First Improvement

Given a neighborhood N, the First Improvement (FI) heuristic is an implementation of the primitive FindFirst:

• FI tries to find the first solution  $s' \in \mathcal{N}(s)$  that improves current solution  $s \in XS$ 

```
procedure FIRSTIMPROVEMENT(f(.), \mathcal{N}(.), stop(.), s)
    m \leftarrow FindFirst(f, \mathcal{N}, stop, s)
    if \exists m then
        return \{m(s)\}
    else
        return {}
    end if
end procedure
```

# Refinement Heuristic: Best Improvement

Given a neighborhood  $\mathcal{N}$ , the Best Improvement (BI) heuristic is an implementation of the primitive FindBest:

• FI tries to find the best solution  $s' \in \mathcal{N}(s)$  that improves current solution  $s \in XS$ 

```
procedure Bestimprovement(f(.), \mathcal{N}(.), stop(.), s)
    m \leftarrow FindBest(f, \mathcal{N}, stop, s)
    if \exists m then
        return \{m(s)\}
    else
        return {}
    end if
end procedure
```

# Classic Local Search techniques

We now explore some classic local search techniques, such as: Hill Climbing (HC), Random Descent Method (RDM) and Variable Neighborhood Descent (VND).

#### Combining refinement heuristics

Each of these local search methods can be combined with all previous refinement heuristics.

#### Reaching local optimality

Not all of these local search methods can guarantee local optimality, but they will try!.

# Local Search: Hill Climbing

Given a refinement heuristic  $\mathcal{H}$  that explores some neighborhood and a solution  $s \in XS$ , the *Hill Climbing* (HC) is an iterative algorithm that finds a *local optimum*. HC is very simple and popular (see wiki).

- HC is also known as Simple Hill Climbing, when integrated with FI
- HC is also known as *Steepest Ascent/Descent Hill Climbing*, when integrated with *BI*
- HC is also known as Stochastic Hill Climbing, when integrated with RS

```
procedure HILLCLIMBING(f(.), \mathcal{H}(.), stop(.), s)
s' \leftarrow \mathcal{H}^{f,stop}(s)
while \exists s' and not stop(time(), f(s')) do
s \leftarrow s'
s' \leftarrow \mathcal{H}^{f,stop}(s)
end while
return \ \{s\}
end procedure
```

## Local Search: Random Descent Method

Given a neighborhood  $\mathcal{N}$ , a parameter  $\kappa_{max}$  and a solution  $s \in XS$ , the Random Descent Method (RDM) is an iterative algorithm that tries to finds a local optimum. It is very similar to the Stochastic Hill Climbing.

```
procedure RANDOMDESCENTMETHOD(f(.), \mathcal{N}(.), \kappa_{max}, \xi, stop(.), s)
    kgets0
    while k < \kappa_{max} and not stop(time(), f(s)) do
         m \leftarrow RandomMove(\mathcal{N}, s, \xi)
        if \exists m and \bar{m}^f(s) < 0 then
             s \leftarrow m(s)
             k \leftarrow 0
         else
             k \leftarrow k + 1
         end if
    end while
    return \{s\}
end procedure
```

# Local Search: Variable Neighborhood Descent

Given multiple refinement heuristics  $\mathcal{H}_1, \mathcal{H}_2, ..., \mathcal{H}_k$  that explore some neighborhoods and a solution  $s \in XS$ , the Variable Neighborhood Descent (VND) is an iterative algorithm that finds a local optimum regarding all neighborhoods.

• typically, start from smaller then explore the larger procedure  $\mathrm{VND}(f(.),\,\mathcal{H}_k(.),\,stop(.),\,s)$   $i\leftarrow 1$  while  $i\leq k$  and not stop(time(),f(s)) do  $s'\leftarrow\mathcal{H}_i^{f,stop}(s)$  if  $\exists s'$  then  $\langle s,i\rangle\leftarrow\langle s',1\rangle$  else  $i\leftarrow i+1$  end while return  $\{s\}$ 

VND is very sensitive the order of neighborhoods

end procedure

# Local Search: Randomized Variable Neighborhood Descent

In 2010, our research group proposed a randomized version of VND, called Randomized Variable Neighborhood Descent (RVND).

In fact, two subgroups independently proposed the same technique (see Souza 2010 and Anand 2010)

RVND is not sensitive the order of neighborhoods

```
procedure RVND(f(.), \mathcal{H}'_{k}(.), \xi, stop(.), s)
     \mathcal{H} \leftarrow shuffle^{\xi}(\mathcal{H}')
     i \leftarrow 1
     while i < k and not stop(time(), f(s)) do
           s' \leftarrow \mathcal{H}_i^{f,stop}(s)
           if \exists s' then \langle s, i \rangle \leftarrow \langle s', 1 \rangle else i \leftarrow i + 1
     end while
     return \{s\}
end procedure
```

## Section 5

Advanced Topic: Multi Improvement

# MultiImprovement: the Idea

Given a solution  $s \in XS$ , a neighborhood  $\mathcal N$  and its associated move set  $\mathcal M$ , the Multi Improvement (MI) heuristic is an implementation of the primitive FindFirst or FindBest over a compound neighborhood  $\mathcal N^\circ$ .

The compound neighborhood  $\mathcal{N}^{\circ}$  is associated to a compound move set  $\mathcal{M}^{\circ} = \{m^{\circ}|m^{\circ} = \bigcirc_{m \in \mathcal{X}} m, \forall \mathcal{X} \in \mathcal{M}^{\star}\}$  that be seen as a set of all move compositions for  $\mathcal{M}^{\star}$ , which is a subset of the powerset  $2^{\mathcal{M}}$  only containing independent moves for s. Note that operator  $\in$  takes a set of the powerset and also performs a permutation, transforming the selected set into a sequence.

Finding a "best" compound move can only be done exactly (and it's even NP-hard for some neighborhoods!). So finding a "first" solution can be feasible on practice, by employing some "greedy" strategy. In this sense, using CPU-GPU hybrid architecture can help deciding how such "FindFirst" operation can work efficiently, by organizing GPU blocks and shared memory in a smart way.

## Some formulation

Given  $s \in XS$ , a neighborhood  $\mathcal{N}$  and its *move set*  $\mathcal{M}$ , we can formulate this problem as the following *maximization* problem:

$$\max \bar{m}^{\circ}(s)$$

$$\mathcal{X} \in \mathcal{M}^\star \subseteq 2^\mathcal{M}$$

$$m^{\circ} = \bigcap_{m \in \mathcal{X}} m$$

Move Independence:

$$ar{m}^{\circ}(s) = \sum_{m \in \mathcal{P}} ar{m}(s), orall \mathcal{P} \in \Pi(\mathcal{X})$$

Where,  $\Pi(C)$  is the set of all permutations of set C.

# Exploring the Multi Improvement technique

Please read recent articles from our research group!

- A benchmark on multi improvement neighborhood search strategies in CPU/GPU systems (2016)
- Exploring parallel multi-GPU local search strategies in a metaheuristic framework (2018)
- A DVND local search implemented on a dataflow architecture for the minimum latency problem (2018)
- Multi Improvement: uma Solução Alternativa para o Problema de Roteamento de Veículos (2019)
- A multi-improvement local search using dataflow and GPU to solve the minimum latency problem (2020)
- Finding the maximum multi improvement on neighborhood exploration (2022)

## Section 6

## Practical Exercise

# Implementing a Local Search (Step 1/3)

- Choose a language: Python or C/C++
- ullet Consider the following data for a Knapsack Problem with n=5 items and capacity Q=10

```
5
10
1 1 1 5 5
1 2 3 7 8
```

- Save it into a file and read it
  - First load the n and Q
  - Then, for each item, load each profit  $p_i$  and weight  $w_i$

# Implementing a Local Search (Step 2/3)

- Model the solution representation as an array (or list) of booleans or binary numbers
- Create a neighborhood structure and two neighborhood exploration techniques (example: best improvement and first improvement)
- Generate multiple initial solutions with some randomness (example, 1000)
- Compute de Average cost and Computational time taken for each of the two refinement heuristics
- Which of these are the best one?

# Implementing a Local Search (Step 3/3)

- Now, choose some Local Search technique, such as Hill Climbing (for BI, FI or RS) or RDM
- Generate multiple initial solutions with some randomness (example, 1000)
- Apply each of the two Local Search on them, for each generated solution
- Compute de Average cost and Computational time taken for each of the two local searches
- Generate bigger instances, to make the problem harder!
- Which one is better?

### Section 7

### **Discussions**

#### Short discussion

#### Current scenario: optimization problems in the university and work

- Do you know of any optimization problem that needs to be solved in the university or your work?
- Can exact methods solve them? Do you need heuristic methods?
- Read the introduction material from prof Marcone (in Portuguese): http://www.decom.ufop.br/prof/marcone/Disciplinas/InteligenciaComput

### Section 8

### **Unused Slides**

### Moves: Basic Primitives

Given a move m, a solution  $s \in XS$  and its evaluation  $e = f(s) \in XE$ , we define three basic move primitives: CanApply, Apply and Cost.

- the CanApply returns true only if  $m(s) \in XS$ , i.e., if the generated neighbor is a valid solution in XS space
  - this can be useful when moves are clearly defined, such as changing a bit
     i in a knapsack problem, but not all moves lead to valid solutions, for
     example, if knapsack capacity would be exceeded after move and that is
     not allowed in XS
- the Apply primitive returns pair  $\langle m(s), m' \rangle$ , where m' is an undo move, such that, s = m'(m(s))
  - only defined if CanApply is true
- the Cost primitive returns evaluation difference value  $e_{diff} = f(m(s)) f(s)$ 
  - only defined if CanApply is true

A fourth non-basic primitive typically used is the ApplyUpdate, that returns both the solution neighbor and its evaluation in a pair  $\langle m(s), f(m(s)) \rangle$ .

## Neighborhood Exploration: FindNext Primitive (extra)

Although not commonly used, one can define a FindNext primitive:

- the FindNext tries to find the next  $s_i \in \mathcal{N}(s) = \{s_i, ..., s_i, ...\}$  that *improves* current solution *s* 
  - assuming minimization, if such  $s_i \in \mathcal{N}(s)$  exists, then i is the smallest value such that  $f(s_i) < f(s)$  and i > j

### Section 9

## Agradecimentos

#### Pessoas

Em especial, agradeço aos colegas que elaboraram bons materiais, como o prof. Raphael Machado, Kowada e Viterbo cujos conceitos formam o cerne desses slides.

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#### Software

Esse material de curso só é possível graças aos inúmeros projetos de código-aberto que são necessários a ele, incluindo:

- pandoc
- LaTeX
- GNU/Linux
- git
- markdown-preview-enhanced (github)
- visual studio code
- atom
- revealjs
- groomit-mpx (screen drawing tool)
- xournal (screen drawing tool)
- . . .

## **Empresas**

Agradecimento especial a empresas que suportam projetos livres envolvidos nesse curso:

- github
- gitlab
- microsoft
- google
- . . .

## Reprodução do material

Esses slides foram escritos utilizando pandoc, segundo o tutorial ilectures:

https://igormcoelho.github.io/ilectures-pandoc/

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