Multiobjective Optimization

Neighborhood Exploration

Igor Machado Coelho

20/09/2024-27/09/2024

8 Agradecimentos

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)

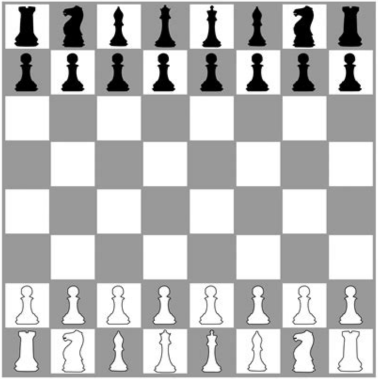
Recall basic definitions for an optimization problem, such as solutions and evaluations, and classic NP-hard problems such as the Knapsack Problem and Traveling Salesman Problem. More precisely:

- The XS denotes a *Solution Space*, where XE is an *Evaluation Space* (or *Objective Space*)
  - The pair $XES = < XS, XE >$ denotes the *XESolution* space
  - A *SO optimization problem* is defined by the triple $< XS, XE, f >$
- 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 $m : XS \mapsto XS$
- we say that $s' \in \mathcal{N}(s) \iff \exists m$ *such that* $s' = m(s)$
  - 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 $M^{(I)} = \{m_1, m_2, ..., m_i\} = \{ \texttt{change the value of the bit } i\}$
- 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: $s_1 = (01001) \to (11001) \to (11011) \to (11010) = s_2$
- 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 $m_{1,4,5} = \bigcirc_{m \in (m_1, m_4, m_5)} m$ 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 ommited)
- 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* $m' = \bigcirc_{m \in M} m$ has a fixed cost $\overline{m'}(s) = \sum_{m \in M} \bar{m}(s), \forall s \in XS$
    - this is an important property for newer neighborhood strategies in literature!

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 $< m(s), m' >$, 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 $< m(s), f(m(s)) >$.

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?

Figure 2: https://simple.wikipedia.org/wiki/Travelling_salesman_problem

Section 3

Neighborhood Exploration Primitives

Neighborhood Exploration: Basic Primitives

Given a neighborhood $\mathcal{N}$ and solution $s \in XS$, we define two basic neighborhood exploration primitives: `RandomMove` and `AllMoves`.

- the `RandomMove` returns a *random move* from neighborhood $\mathcal{N}$
- the `AllMoves` returns sequence $(m_1, m_2, \ldots)$ from neighborhood $\mathcal{N}$

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

- `FirstMove` returns m_1, where m_1 is the first move from `AllMoves`
- `NextMove` returns m_{i+1}, where m_i is a move from `AllMoves`

Neighborhood Exploration: Find Primitives

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

- 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 $|\mathcal{N}_{\leq\kappa}| \leq k$
  - 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 $f(s^*) \leq f(s')$, $\forall s' \in \mathcal{N}(s)$

Pseudocode for Find Primitives: FindAny

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

procedure $\textsc{FindAny}(f(.), \mathcal{N}(.), \kappa_{max}, \xi(.), stop(.), s)$
    $k \leftarrow 0$
    while $k < \kappa_{max}$ **and not** $stop(time(), f(s))$ **do**
        $m \leftarrow \texttt{RandomMove}(\mathcal{N}, s, \xi)$
        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 $\textsc{FindFirst}(f(.), \mathcal{N}(.), stop(.), s)$
    $m \leftarrow \texttt{FirstMove}(\mathcal{N}, s)$
    while $\exists m$ **and not** $stop(time(), f(s))$ **do**
        if $\bar{m}^f(s) < 0$ **then**
            return $\{m\}$
        else
            $m \leftarrow \texttt{NextMove}(\mathcal{N}, s, m)$
        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 $\textsc{FindBest}(f(.), \mathcal{N}(.), stop(.), s)$
  $m \leftarrow \texttt{FirstMove}(\mathcal{N}, s)$
  if $\nexists m$ **then return** $\{\}$
  $\langle e^*, m^* \rangle \leftarrow \left\langle \bar{m}^f(s), m \right\rangle$
  while $\exists m$ **and not** $stop(time(), f(s))$ **do**
    if $\bar{m}^f(s) < e^*$ **then**
      $\langle e^*, m^* \rangle \leftarrow \left\langle \bar{m}^f(s), m \right\rangle$
    end if
    $m \leftarrow \texttt{NextMove}(\mathcal{N}, s, m)$
  end while
  if $e^* < 0$ **then return** $\{m^*\}$ **else return** $\{\}$
end procedure

Neighborhood Exploration: FindNext Primitive (extra)

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

- the `FindNext` tries to find *the next* $s_i \in \mathcal{N}(s) = \{s_j, ..., s_i, ...\}$ 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 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 κ_{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 $\textsc{RandomSelection}(f(.), \mathcal{N}(.), \kappa_{max}, \xi(.), stop(.), s)$
    $m \leftarrow \texttt{FindAny}(f, \mathcal{N}, \kappa_{max}, \xi(.), stop, s)$
    if $\exists m$ **then**
        return $\{m(s)\}$
    else
        return $\{\}$
    end if
end procedure

Refinement Heuristic: First Improvement

Given a neighborhood $\mathcal{N}$, 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 $\textsc{FirstImprovement}(f(.), \mathcal{N}(.), \mathit{stop}(.), s)$
    $m \leftarrow \texttt{FindFirst}(f, \mathcal{N}, \mathit{stop}, s)$
    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 $\textsc{BestImprovement}(f(.), \mathcal{N}(.), stop(.), s)$
    $m \leftarrow \texttt{FindBest}(f, \mathcal{N}, stop, s)$
    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 $\textsc{HillClimbing}(f(.), \mathcal{H}(.), stop(.), s)$
    $s' \leftarrow \mathcal{H}^{f,stop}(s)$
    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 κ_{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 $\textsc{RandomDescentMethod}(f(.), \mathcal{N}(.), \kappa_{max}, \xi, stop(.), s)$
  $kgets0$
  while $k < \kappa_{max}$ **and not** $stop(time(), f(s))$ **do**
    $m \leftarrow \texttt{RandomMove}(\mathcal{N}, s, \xi)$
    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*.

- VND is very sensitive the order of 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 $\{s\}$
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 $\mathrm{RVND}(f(.),\ \mathcal{H}'_k(.),\ \xi,\ stop(.),\ s)$
$\quad \mathcal{H} \leftarrow shuffle^{\xi}(\mathcal{H}')$
$\quad i \leftarrow 1$
$\quad$ **while** $i \leq k$ **and not** $stop(time(), f(s))$ **do**
$\quad\quad s' \leftarrow \mathcal{H}_i^{f,stop}(s)$
$\quad\quad$ **if** $\exists s'$ **then** $\langle s, i \rangle \leftarrow \langle s', 1 \rangle$ **else** $i \leftarrow i + 1$
$\quad$ **end while**
$\quad$ **return** $\{s\}$
end procedure

Section 5

Advanced Topic: Multi Improvement

MultiImprovement: the Idea

Given a solution $s \in XS$, a neighborhood $\mathcal{N}$ and the *move set* $\mathcal{M} = \{m_1, m_2, ...\}$ such that $\mathcal{N} = \{m_1(s), m_2(s), ...\}$, the *Multi Improvement* (MI) heuristic is an implementation of the primitive `FindFirst` or `FindBest` over compound neighborhood $\mathcal{M}^\star$.

The compound neighborhood $\mathcal{M}^\star = 2^{\mathcal{M}}$ can be seen as a set of all move compositions for $\mathcal{M}$, but 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.

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 the *move set* $\mathcal{M} = \{m_1, m_2, ...\}$ such that $\mathcal{N} = \{m_1(s), m_2(s), ...\}$, we can formulate this problem as the following *maximization* problem:

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

$\mathcal{M}^a \in \mathcal{M}^\star = 2^{\mathcal{M}}$

$m^a = \bigcirc_{m \in \mathcal{M}^a} m$

Independence:

$\bar{m}^a(s) = \sum_{m \in \mathcal{M}^a} \bar{m}(s)$

Exploring the Multi Improvement technique

Please read recent articles from our research group!

Section 6

Practical Exercise

Implementing a Local Search (Step 1/3)

- Choose a language: Python or C/C++
- 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

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.

Estendo os agradecimentos aos demais colegas que colaboraram com a elaboração do material do curso de Pesquisa Operacional, que abriu caminho para verificação prática dessa tecnologia de slides.

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/

Exceto expressamente mencionado (com as devidas ressalvas ao material cedido por colegas), a licença será Creative Commons.

Igor Machado Coelho

This Slide Is Intentionally Blank (for goomit-mpx)