Non-convex Multi-objective Optimization
Multi-objective Optimization

▶ Real-world optimization problems usually involve more than one criteria – multi-objective optimization.
▶ Such a kind of optimization problems are important in various fields of industry and research.
▶ In most cases it is impossible to minimize all objectives at the same time, so there is no single optimal solution to a given multi-objective optimization problem. Therefore non-dominated “Pareto-optimal” solutions are searched.
▶ Many methods convert the multi-objective optimization problem into a set of single-objective problems. The most known methods are the linear scalarization where objectives are aggregated with positive weights and the $\varepsilon$-constraint method where one objective is minimized while the others are converted to constraints.
Multi-objective optimization problem

A multi-objective optimization problem with $d$ objectives $f_1(x), f_2(x), \ldots, f_d(x)$ is to minimize the objective vector $f(x) = (f_1(x), f_2(x), \ldots, f_d(x))$:

$$\min_{x \in \mathbb{A}} f(x),$$

where $x$ is the decision vector and $\mathbb{A}$ is the search space.

Decision space

Objective space
Pareto front

- The decision vector $\mathbf{a}$ dominates the decision vector $\mathbf{b}$ if:
  \[ \forall i \in \{1, 2, \ldots, d\} : f_i(\mathbf{a}) \leq f_i(\mathbf{b}) \land \exists j \in \{1, 2, \ldots, d\} : f_j(\mathbf{a}) < f_j(\mathbf{b}). \]

- Non-dominated decision vector are called **Pareto optimal** and a set of those vectors is called **Pareto set**. The set of corresponding objective vectors is called **Pareto front** $\mathbb{P}(\mathbf{f})_O$.

- When it is difficult to determine the **Pareto front** an approximation of Pareto front is sought.
Scalarization in multi-objective optimization

- Scalarization is formulation of a single-objective optimization problem such that its optimal solutions are Pareto optimal solutions to the multi-objective optimization problem.

- Linear scalarization

  $$\min_{x \in A} \sum_{i=1}^{d} w_i f_i(x),$$

  where the positive weights $w_i$ are the parameters of the scalarization.

- ε-constraint method

  $$\min \quad f_j(x)$$
  s.t. \quad $x \in A$
  \quad $f_i(x) \leq \varepsilon_j \text{ for } i \in \{1, \ldots, d\} \setminus \{j\},$

  where $\varepsilon_j$ are parameters and $f_j$ is the objective to be minimized.
Example of linear scalarization

- Choose weights $w_i$:

$$\min 0.4 f_1(x) + 0.6 f_2(x),$$

$$\min 0.8 f_1(x) + 0.2 f_2(x),$$

...
Example of non-convex multi-objective optimization

\[
\begin{align*}
\min_{x \in [-1, 1]} \ f(x), \\
f_1(x) &= (x + 0.5)^2 - \cos(18(x + 0.5)), \\
f_2(x) &= (x - 0.5)^2 - \cos(18(x - 0.5)).
\end{align*}
\]
Non-convex multi-objective optimization

- If objective functions are non-convex, even the scalarized single-objective optimization problem is not easily solved – global optimization must be used.
- Special care must be taken in the case of non-convex Pareto front.

\[
0.5f_1(x) + 0.5f_2(x)
\]
Global optimization

Find \( f^* = \min_{x \in \mathbb{A}} f(x) \) and \( x^* \in \mathbb{A}, f(x^*) = f^* \), where \( \mathbb{A} \subseteq \mathbb{R}^n \).

Example:
- \( n = 1; \)
- \( \mathbb{A} = [0, 10]; \)
- Objective function
  \[
  f(x) = -\sum_{j=1}^{5} j \sin((j+1)x+j); 
  \]
- \( f^* = -12.0312; \)
- \( x^* = 5.7918. \)
Local optimization

- A point $\mathbf{x}^*$ is a local minimum point if $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for $\mathbf{x} \in N$, where $N$ is a neighborhood of $\mathbf{x}^*$.

- A local minimum point can be found stepping in the direction of steepest descent.

- Without additional information one cannot say if the local minimum is global.

- How do we know if we are in the deepest hole?
Algorithms for global optimization

- With guaranteed accuracy:
  - Lipschitz optimization,
  - Branch and bound algorithms.

- Randomized algorithms and heuristics:
  - Random search,
  - Multi-start,
  - Clustering methods,
  - Generalized descent methods,
  - Simulated annealing,
  - Evolutionary algorithms (genetic algorithms, evolution strategies),
  - Swarm-based optimization (particle swarm, ant colony).
Branch and bound algorithm

- The main concept of branch and bound is to detect sets of feasible solutions which cannot contain optimal solutions.
- The search process can be illustrated as a tree with branches corresponding to subsets of the search space.
- An iteration of the classical branch and bound algorithm processes a node in the search tree that represents an unexplored subset of feasible solutions.
- The iteration has three main components: selection of the subset to be processed, branching corresponding to subdivision of the subset, and bound calculation.
- In single objective optimization, the subset cannot contain optimal solutions and the branch of the search tree corresponding to the subset can be pruned, if the bound for the objective function over a subset is worse than the known function value.
Multi-objective branch and bound algorithm

- In multi-objective optimization, the subset cannot contain Pareto optimal solutions if each bounding vector $\mathbf{b} \in B$ in bounding front $B$ is dominated by at least one already known decision vector $\mathbf{a} \in S$:

$$\forall \mathbf{b} \in B \exists \mathbf{a} \in S : \forall i \in \{1, 2, \ldots, d\} : f_i(\mathbf{a}) \leq b_i \land \exists j \in \{1, 2, \ldots, d\} : f_j(\mathbf{a}) < b_j.$$

- The simplest bounding front consists of a single ideal vector composed of lower bounds for each objective function.
Optimization problem: cell formation

- Cell formation suggests grouping of machines into manufacturing cells and parts into product families so that each family is processed mainly within one cell.
- Cell formation may be interpreted as a network problem and solved as machine/part-machine graph partitioning or using network flow formulation.
- Practical implementation of cellular manufacturing systems involves conflicting objectives.
- We consider two models for bi-objective cell formation problem. The goal of the problem is to find groupings of machines simultaneously optimizing two objectives. The objectives conflict, therefore a single solution minimizing both objectives does not generally exist.
Cell formation problems: notations

- The number of machines is denoted by \( m \), the number of parts by \( n \) and the number of cells by \( k \).
- \( X \) is an \( m \times k \) cell membership matrix where 1 in \( i \)-th row and \( j \)-th column means that \( i \)-th machine is assigned to \( j \)-th cell.
- Each machine can only be assigned to one cell: \( Xe_k = e_m \), where \( e_t \) is a \( t \)-element column vector of ones.
- Minimal (\( L \)) and maximal (\( U \)) number of machines in each cell may be restricted.
- The data is an \( m \times n \) machine-part incidence matrix \( W \) specifying which part needs processing on which machine (1 in \( i \)-th row and \( j \)-th column means that \( j \)-th part needs processing on \( i \)-th machine) or specifying workload on each machine induced by each part.
We will represent a subset of feasible solutions as a partial solution where only some \((m')\) first machines are considered.

In this case the partial solution is represented by an \(m' \times k\) cell membership matrix \(X'\).

Instead of operating with zero-one matrix \(X\) we will operate with the integer \(m\)-element vector \(c\) defining labels of cells to which machines are assigned.

The vector \((1,1,2,3,\ldots)\) means that the first and the second machines are assigned to the first cell, the third machine is assigned to the second cell and the fourth machine is assigned to the third cell.

The matrix \(X\) can be easily built from \(c\):

\[
x_{ij} = \begin{cases} 
1, & c_i = j, \\
0, & \text{otherwise,}
\end{cases} \quad i = 1, 2, \ldots, m.
\]
An example of the search tree for cell formation problem

\( m = 4 \)

▶ In order to avoid equivalent solutions some restrictions are set:

\[
\begin{align*}
\min i < \min_i, \\
\text{c}_i = j, & \quad \text{c}_i = j + 1
\end{align*}
\]

Such restrictions correspond to arrangement of \( X \) so that

\[
\begin{align*}
\min i < \min_i \iff j < l. \\
x_{ij} = 1, & \quad x_{il} = 1
\end{align*}
\]

▶ Taking into account such restrictions a search tree of the problem with \( m = 4 \) is shown in the figure. Only numerals are shown to save space.
Branch and bound algorithm for bi-objective cell formation

1. Start with $c = (1, 1, \ldots, 1)$, $m' \leftarrow m$

2. If the current solution is complete ($m' = m$)
   - If no solutions in the solution list dominate the current solution, add it to the solution list
   - If there are solutions in the solution list dominated by the current solution, remove them from the solution list
   - Change $c$ by removing from the tail all numbers appearing only once in $c$ and increasing the last remaining number, set $m'$ accordingly

3. Otherwise (partial solution)
   - If no solutions in the solution list dominate the bound vector of the current set of solutions represented by the current partial solution, append 1 to the tail of $c$ and increase $m'$
   - Otherwise change $c$ by removing from the tail all numbers appearing only once in $c$ and increasing the last remaining number, set $m'$ accordingly

4. If $c$ is not empty, return to Step 2
Cell formation Model 1

Decision variables are not only machine-cell membership matrix \( X \), but also \( n \times k \) part-cell membership matrix \( Y \) where 1 in \( i \)-th row and \( j \)-th column means that \( i \)-th part is assigned to \( j \)-th cell. Each part can only be assigned to one cell: \( Ye_k = e_n \).

The data of the problem is an \( m \times n \) machine-part incidence matrix \( W \) where 1 in \( i \)-th row and \( j \)-th column means that \( j \)-th part needs processing on \( i \)-th machine.

\[
\begin{array}{cccccccccccccccc}
W_1 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 17 \\
1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\
2 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
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10 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0
\end{array}
\]
Cell formation Model 1: objectives

- Minimization of the number of exceptional elements: The number of times the parts are processed outside their own cells is minimized.
  The number of exceptional elements is computed as
  \[
  f_1(X, Y) = \langle W, E - XY^T \rangle,
  \]
  where \( \langle , \rangle \) denotes the inner product of matrices and \( E \) is an \( m \times n \) matrix of ones.

- Minimization of the number of voids: The number of times the part is not processed inside its own cell is minimized.
  The number of voids is computed as
  \[
  f_2(X, Y) = \langle E - W, XY^T \rangle.
  \]
Cell formation Model 1: example

- There are $m = 8$ machines and $n = 4$ parts in this problem.
- Additional restrictions are used: two cells, minimum 2 and maximum 6 machines in each cell ($K = 2$, $L = 2$, $U = 6$).
- All three solutions have the same grouping of the machines to cells, but different assignments of the parts to cells.
Cell formation Model 1: bounds

- The bounding front of objective functions of Model 1 may be computed taking non-dominated vectors from the set

\[
\left\{ \left( \sum_{i=1}^{n} \sum_{j=1}^{m'} (w_{ji} - w_{ji}x'_{jl}), \sum_{i=1}^{n} \sum_{j=1}^{m'} (x'_{jl} - w_{ji}x'_{jl}) \right) : l_i \in \{1, 2, \ldots, k\} \right\}.
\]

- A less computationally expensive bounding set of objective functions may be computed as a single vector of separate bounds

\[
b_1(X') = \sum_{i=1}^{n} \min_{l=1, \ldots, k} \sum_{j=1}^{m'} (w_{ji} - w_{ji}x'_{jl}),
\]

\[
b_2(X') = \sum_{i=1}^{n} \min_{l=1, \ldots, k} \sum_{j=1}^{m'} (x'_{jl} - w_{ji}x'_{jl}).
\]

Assignment of other machines to cells later on during the search process can only increase objective functions since already assigned machines will not change and additional non-negative elements will be added to the rightmost sums.
Cell formation Model 2

- Decision variables are machine-cell membership matrix $X$.
- The data is an $m \times n$ machine-part incidence matrix $W$ specifying workload on each machine induced by each part and an $n$-element vector $p$ of production requirements of parts.

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$p_{155 150 148 160 144 158 152 155 164 148 140 144 145 162 217 014 0 156 132 217 216 4 144158155152140166 148145144170}$
Cell formation Model 2: objectives

- Minimization of the total intercell moves: The number of cells processing each part is minimized. Intercell moves are computed as

\[ f_1(X) = p^T (\Phi(W^T X)e_k - e_n), \]

where the function \( \Phi \) changes the nonzero elements of matrix to ones.

- Minimization of within-cell load variation: The differences between workload induced by a part on a specific machine and the average workload induced by this part on the cell are minimized. Within-cell load variation is computed as

\[ f_2(X) = \langle W - M(X), W - M(X) \rangle, \]

where the matrix \( M(X) \) is an \( m \times n \) matrix with average cell loads: the element in \( i \)-th row and \( j \)-th column specifies the average load of \( j \)-th part in the cell where \( i \)-th machine is assigned.
Cell formation Model 2: example

- Model 2 provides grouping of the machines to cells only.
- One can interpret that the part is supposed to be assigned to one of the cells where it needs processing (boxed).
- Intercell moves are required if the part needs processing in several cells, the labels of such parts are shown in bold.
- When workloads of the same part vary in the same cell we show them in bold font.

<table>
<thead>
<tr>
<th></th>
<th>(0,6.75)</th>
<th></th>
<th>(1,3)</th>
<th></th>
<th>(2,0)</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
</tbody>
</table>

(0,6.75)  (1,3)  (2,0)
Cell formation Model 2: bounds

- The bounds of objective functions may be computed as

\[ b_1(X') = p^T (\Phi(W'^T X')e_k - \Phi(W'^T X')e_k) \]

\[ b_2(X') = \langle W' - M(X'), W' - M(X') \rangle \]

where \( W' \) denotes a matrix composed of \( m' \) first rows of matrix \( W \).

- Assignment of other machines to cells later on during the search process cannot reduce intercell moves since already assigned machines will not change and the newly assigned machines can only introduce new intercell moves.

- The cell load variation will remain the same if the other machines are assigned to new separate cells and cannot decrease after assignment of other machines.
Results from the literature solving $W_0$ (Arkat et al., 2011)

- **$\varepsilon$-constraint method**

<table>
<thead>
<tr>
<th>Round</th>
<th>$f_1$</th>
<th>$f_2$</th>
<th>Efficiency</th>
<th>$t$, s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>2</td>
<td>Efficient</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
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<td>1</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td></td>
<td>Infeasible</td>
<td>1</td>
</tr>
</tbody>
</table>

- Genetic algorithm: 20 individuals, 20 generations, 10 runs, 3 seconds.
Results of branch and bound algorithm solving $W_0$

$m = 8, \, n = 4$

<table>
<thead>
<tr>
<th>$K$</th>
<th>$L$</th>
<th>$U$</th>
<th>$t$, s</th>
<th>NFE</th>
<th>$t$, s</th>
<th>NFE</th>
<th>$t$, s</th>
<th>NFE</th>
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<table>
<thead>
<tr>
<th>$\epsilon$-CM GA (Arkat et al., 2011)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t$, s</td>
</tr>
<tr>
<td>6</td>
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Results from the literature solving $W_1$ (Arkat et al., 2011)

- $\varepsilon$-constraint method

<table>
<thead>
<tr>
<th>Round</th>
<th>$f_1$</th>
<th>$f_2$</th>
<th>Efficiency</th>
<th>$t$, h:min</th>
<th>Round</th>
<th>$f_1$</th>
<th>$f_2$</th>
<th>Efficiency</th>
<th>$t$, h:min</th>
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<td></td>
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<td>0:11</td>
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</table>

Total run time 22:56

- Genetic algorithm: 100 individuals, 200 generations, 15 runs, 5 minutes.
Results of branch and bound algorithm solving $W_1$

$m = 10, n = 17$

<table>
<thead>
<tr>
<th>$K$</th>
<th>$L$</th>
<th>$U$</th>
<th>$t$, s</th>
<th>NFE</th>
<th>$t$, s</th>
<th>NFE</th>
<th>$t$, h:min</th>
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5
6
7
8
9
Pareto front for $\mathbf{W}_1$ with Model 1

$K = 3$ (o), $K = 3$, $L = 2$, $U = 5$ (x) and $K = 3$, $L = 2$, $U = 6$ (+)
Experimental comparison on $W_2$ with Model 2

$m = 15, n = 30$

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<thead>
<tr>
<th>$K$</th>
<th>Branch and bound</th>
<th>Complete enumeration</th>
<th>Speed-up</th>
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<tbody>
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<td>$t$, s</td>
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Pareto front for $\mathbf{W}_2$ with Model 2

Pareto front found with branch and bound (○) and solutions given in literature: + (Dimopoulos, 2007) and × (Venugopal and Narendran, 1992)
Continuous bi-objective Lipschitz optimization

- A class of Lipschitz objective functions $\Phi(L)$ is considered, i.e. $f(x) = (f_1(x), f_2(x))^T \in \Phi(L)$, where
  \[ |f_k(x) - f_k(t)| \leq L_k \cdot |x - t|, \quad k = 1, 2, \]
  for $x, t \in \Delta = [a, b], \quad L = (L_1, L_2)^T, \quad L_k > 0, \quad k = 1, 2$.

- Functions $g_k(x), \quad k = 1, 2$, define the lower bounds for $f_k(x)$:
  \[ g_k(x) = \max (y_{k,i} - L_k(x - x_{o,i}), y_{k,i+1} - L_k(x_{o,i+1} - x)), \]
  \[ x_{o,i} \leq x \leq x_{o,i+1}, \quad i = 1, \ldots, n - 1, \]
  where $x_{o,i}, \quad i = 1, \ldots, n$, denote increasingly ordered points $x_i$, $y_{k,i}^o$ denote the corresponding values of the objective functions.
Lipschitz lower bound

- The Pareto front of the bi-objective problem

\[
\min_{x_{o_i} \leq x \leq x_{o_i+1}} g(x), \ g(x) = (g_1(x), g_2(x))^T,
\]

is called a local Lipschitz lower bound for \( \mathbb{P}(f)_O \), and it is denoted as \( V_j \). The subset of \( \bigcup_j V_j \) constituted of non-dominated points is denoted by \( V(Y^n) \) and called Lipschitz lower bound for \( \mathbb{P}(f)_O \).
Illustration on Rastrigin functions

\[
\min_{x \in [-1,1]} f(x), \\
\begin{align*}
f_1(x) &= \frac{((x + 0.5)^2 - \cos(18(x + 0.5)))}{21}, \\
f_2(x) &= \frac{((x - 0.5)^2 - \cos(18(x - 0.5)))}{21}.
\end{align*}
\]
Illustration on two dimensional Fonseca problem

\[
\min_{\mathbf{x} \in [-4,4]^2} \mathbf{f}(\mathbf{x}),
\]

\[
f_1(\mathbf{x}) = 1 - e^{-\sum_{i=1}^{n}(x_i - 1/\sqrt{n})},
\]

\[
f_2(\mathbf{x}) = 1 - e^{-\sum_{i=1}^{n}(x_i + 1/\sqrt{n})}.
\]
Illustration on example problem 1 from (Evtushenko, Posypkin, 2013)

\[
\begin{align*}
\min_{\mathbf{x} \in [0,2]^2} f(\mathbf{x}), \\
\quad f_1(\mathbf{x}) &= x_0, \\
\quad f_2(\mathbf{x}) &= \left(\min(|x_0 - 1|, 1.5 - x_0) + x_1 + 1\right)/2.
\end{align*}
\]
Illustration on example problem 2 from (Evtushenko, Posypkin, 2013)

\[
\min_{x \in [0, 1]^2} f(x),
\]

\[
f_1(x) = \frac{(x_0 - 1)x_1^2 + 1}{3},
\]

\[
f_2(x) = x_1.
\]
# Numerical comparison

<table>
<thead>
<tr>
<th>Method</th>
<th>NFE</th>
<th>$\varepsilon$</th>
<th>$np$</th>
<th>$hv$</th>
<th>$ud$</th>
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<td><strong>Problem 1</strong></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Genetic algorithm</td>
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<td>221</td>
<td>3.27</td>
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<tr>
<td>Monte Carlo</td>
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<tr>
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<td>0.310</td>
<td>0.178</td>
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</tbody>
</table>

$$ud = \sqrt{\sum_{i=1}^{np} (d_i - d)^2}, \quad d = \frac{1}{np} \sum_{i=1}^{np} d_i, \quad d_i = \min_{i \neq j} d_{ij}.$$