A combinatorial branch-and-bound algorithm for box search

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A practical problem posed by the steel industry

A problem inspired by data mining

Galvanization consists in applying a protective zinc coating on steel. This is a very complicated process depending on many parameters.

Idea of the problem: Based on the data gathered in the past, find a set of parameters that lead to an average high quality product.

Or, based on a set of runs, find the parameters that explain why these runs led to bad quality products.
A mathematical statement
This can be transformed into a discrete optimization problem.

Data

- **D**-dimension normalized space (e.g. \([0, 1]^D\))
- **M** points characterized by:
  - coordinates \(x^i\)
  - classification:

\[
c^i = \begin{cases} 
\text{success} = 1 \\
\text{or} \\
\text{failure} = -1 \\
\text{or} \\
y^i \in \mathbb{R}
\end{cases}
\]
A mathematical statement

Definition

A box $S$ is defined by
- two extreme points: $l$ and $u$

Implicitly it defines
- the sets of **included** success and failure points
- the sets of **non-included** success and failure points
A mathematical statement

Definition

The quality or value of a box is defined as the number of success points minus the number of failure points included in the box or more precisely

\[ f(B) = \sum_{i \in B} c^i, \]

where \( c^i \) is the value of point \( i \).

Problem statement

Find the box \( B \) with the maximal score

Alternative (easier) problem

Find the box \( B \) with the maximal number of success points without any failure points.

Tackled by [Eckstein, Hammer, Liu, Nediak, Simeone 2002]
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Some comments

Why boxes?
Because they are easy to interpret and to use for the operator!

Easy problem?
Finding the best homogeneous box (without any failure) is NP-hard which implies that our problem is NP-hard.
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Easy problem?
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A mixed-integer programming formulation

Variables

\[ l_d \in [0, 1]^D \]  The lower bounds of the box
\[ u_d \in [0, 1]^D \]  The upper bounds of the box

\[ z^i \in \{0, 1\} \]
- \[ = 1 \] if \( i \) belongs to the box
- \[ = 0 \] if \( i \) does not belong to the box

\[ v^i_t \in \{0, 1\} \]
- \[ = 1 \] if failure point \( i \) satisfies the lower bound in dim \( t \)
- \[ = 0 \] otherwise

\[ w^i_t \in \{0, 1\} \]
- \[ = 1 \] if failure point \( i \) satisfies the upper bound in dim \( t \)
- \[ = 0 \] otherwise
A mixed-integer programming formulation

maximize \( \sum_{i=1}^{M} c^i z^i \) subject to

for \( d = 1, \ldots, D \):

\[ l_d \leq u_d \quad (1) \]

for \( i \) success point, \( d = 1, \ldots, D \):

\[ l_d \leq x_d^i + (1 - z^i) \quad (2) \]

\[ x_d^i z^i \leq u_d \quad (3) \]

for \( i \) failure point, \( d = 1, \ldots, D \):

\[ v_d^i \geq (x_d^i - l_d) + \epsilon \quad (4) \]

\[ w_d^i \geq (u_d - x_d^i) + \epsilon \quad (5) \]

for \( i \) failure point:

\[ z^i \geq \sum_{d=1}^{D} (v_d^i + w_d^i) - 2D + 1/2 \quad (6) \]
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Is it a good formulation?

**Pro**

A quite **compact** formulation:

- \( M + 2D + 2|\text{failure} | \) variables

- \( (2|\text{success} | + 1)D + |\text{failure} |(1 + 2D) \) constraints

**Cons**

- The linear relaxation is very weak
- The formulation is numerically unstable
Is it a good formulation?

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**Cons**

- The linear relaxation is *very weak*
- The formulation is *numerically instable*
A combinatorial branch-and-bound

We propose to branch on the decision: “is a point included or excluded of the box”? 

- Failure point
- Unfixed success point
- Included success point
- Excluded success point
Inference of the inclusion/exclusion of points

- Unfixed success point
- Included success point
- Excluded success point

Automatically included

Automatically excluded
Inference of the inclusion/exclusion of points

- Unfixed success point
- Included success point
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Inference of the inclusion/exclusion of points

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Finding a primal bound

Definition

We define the operational box as a box with

\[ l_t = \min_{i=1,\ldots,M} x^i_t \]
\[ u_t = \max_{i=1,\ldots,M} x^i_t \]

Using the inference of included points, we can define a primal solution.
Finding an upper bound

The maximum number of success points that might be included is the size of the biggest partition (↕).

Dimension: 1 2 3

- Box
- Included success point
- Excluded success point

The maximum number of success points that might be included is the size of the biggest partition (↕).
**Definition**

For each excluded point $i$ and dimension $t$, we define $\Delta^i_t$ to be

- 0 if $i$ is in the operational box for that specific dimension $t$

- the sum of the values of the positive points that are on the right side of $i$ compared with the operational box for that specific dimension $t$

**Lemma**

$\Delta^i_t$ is an upper bound on the number of additional success points that can be included in the box if $i$ is excluded in dimension $t$.

**Lemma**

For a specific fixing, the maximum number of additional success points that can be added to the box is given by

$$\min_{i \in \mathcal{E}} \left\{ \max_{t=1,\ldots,D} \Delta^i_t \right\}$$
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Branching strategies

What is branching in this case?

Select the point that will be included/excluded.

⇒ **Aim** : compute the least number of nodes needed in the branch-and-bound tree

Which one should we choose?

Branching candidates : unfixed points
Strong branching

Principle

- Try branching on every $\ominus$
- Choose the greatest $\searrow$ of upper bound.

Results

Low number of nodes, but high computational cost

$\Rightarrow$ like LP-based B&B
**Strong branching**

**Principle**
- Try branching on every $\emptyset$
- Choose the greatest $\downarrow$ of upper bound.

**Results**
Low number of nodes, but high computational cost
⇒ like LP-based B&B
Reliability branching

Principle

- Introduced by T. Achterberg, T. Koch, A. Martin in 2004
- Selected 5 times OK ⇒ globally OK
- Branched less than 5 times ⇒ not reliable
Scattered branching

Principle

- Problem specific
- Build a scattered order
- Select the next in the line
  ⇒ Cheap computational cost
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- Problem specific
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- Select the next in the line
  ⇒ Cheap computational cost
Least local branching

 Principle

- $\forall \emptyset$, compute an approximation of the $\downarrow$ of upper bound.
  - **Included**: Compute the score of the new box
  - **Excluded**: Compute the partition for this point

- Branch on the greatest expected $\downarrow$ of upper bound.
## Computational results

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<th>D</th>
<th>M</th>
<th>PP-St</th>
<th>PP-R</th>
<th>PP-LL</th>
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Conclusions

- The algorithm performs quite well on relatively small instances.
- The algorithm is too slow for practical performances: We use a heuristic based on starting with the whole set and peeling the box in one dimension at each iteration.
- In practice, we like to define the box on few dimensions for it to be even more easy to interpret. The problem is more complicated to formulate and solve.