Mathematical optimization/programming problem

\[
\max\{g(x) \mid f_j(x) \leq 0, x \in D\} \text{ or } \min\{g(x) \mid f_j(x) \leq 0, x \in D\}
\]

with \( D \subseteq \mathbb{R}^n \), \( g, f_j : D \to \mathbb{R} \), \( j = 1, \ldots, m \).
- **Mathematical optimization/programming problem**

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\end{align*}
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with \( D \subseteq \mathbb{R}^n \), \( g, f_j : D \rightarrow \mathbb{R} \), \( j = 1, \ldots, m \).

- **Feasible solution:** \( x^* \in D \) with \( f_j(x^*) \leq 0 \), for all \( j \).
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Feasible solution: \( x^* \in D \) with \( f_j(x^*) \leq 0, \) for all \( j. \)

Optimal solution: Feasible solution such that

\[
g(x^*) = \max\{g(x) \mid f_j(x) \leq 0, \text{ for all } j, \ x \in D\}.
\]
Mathematical optimization/programming problem

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Optimal solution: Feasible solution such that

\[ g(x^*) = \max \{ g(x) \mid f_j(x) \leq 0, \text{ for all } j, \ x \in D \} . \]

Feasible/optimal solutions

- need not exist,
- need not be unique.
\[
\begin{align*}
\text{max} & \quad c_1 x_1 + \cdots + c_n x_n \\
\text{w.r.t.} & \quad a_{11} x_1 + \cdots + a_{1n} x_n \leq b_1, \\
& \quad \vdots \\
& \quad a_{m1} x_1 + \cdots + a_{mn} x_n \leq b_m, \\
& \quad x_1, \ldots, x_n \in \mathbb{R}.
\end{align*}
\]
Linear optimization

\[
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\end{align*}
\]
\[
\quad x_1, \ldots, x_n \in \mathbb{R}.
\]

In matrix notation:

\[
\max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \},
\]

with \( A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m, c \in \mathbb{R}^n \).
A. Bockmayr, 26 May 2016
Geometric illustration

Polyhedron

$\Delta P = \{ x \in \mathbb{R}^n | Ax \leq b \} \rightarrow \text{feasible region}$

Linear optimization problem (LP): max

$\{ c^T x | Ax \leq b, x \in \mathbb{R}^n \}$
Geometric illustration

Polyhedron $P = \{ x \in \mathbb{R}^n \mid Ax \leq b \} \mapsto$ feasible region

Linear optimization problem (LP): $\max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \}$
Geometric illustration

Polyhedron $P = \{ x \in \mathbb{R}^n | Ax \leq b \} \Rightarrow$ feasible region

Linear optimization problem (LP): max $\{ c^T x | Ax \leq b, x \in \mathbb{R}^n \}$
Polyhedron $P = \{ x \in \mathbb{R}^n \mid Ax \leq b \} \leadsto$ feasible region

Linear optimization problem (LP): $\max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \}$
Linear optimization problem

\[
\max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \} \quad \text{(LP)}
\]
Linear optimization problem

\[ \max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \} \]  

(SLP)

Simplex-Algorithm (Dantzig 1947)

1. Find a vertex of the polyhedron \( P \).
2. Proceed from vertex to vertex along edges of \( P \) such that the objective function \( g = c^T x \) increases.
3. Either a vertex will be reached that is optimal, or an edge will be chosen which goes off to infinity and along which \( g \) is unbounded.
All known variants of the Simplex algorithm have worst-case exponential running time.
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In practice, the Simplex algorithm is very efficient.
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In practice, the Simplex algorithm is very efficient.

There exist polynomial-time algorithms for linear optimization

- Ellipsoid method (Khachiyan 1979)
- Interior point methods (Karmarkar 1984)
Integer linear optimization

- **Linear optimization/programming (LP)** polynomial

  \[
  \max \{ c^T x \mid Ax \leq b, \, x \in \mathbb{R}^n \}
  \]

- **Integer linear optimization (IP)** NP-hard

- **Mixed-Integer linear optimization (MIP)** NP-hard

- **Mixed 0-1 linear optimization** NP-hard
Integer linear optimization

- **Linear optimization/programming (LP)**
  \[
  \max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \}
  \]
  polynomial

- **Integer linear optimization (IP)**
  \[
  \max \{ c^T x \mid Ax \leq b, x \in \mathbb{Z}^n \}
  \]
  NP-hard

A. Bockmayr, 26 May 2016
Integer linear optimization

- **Linear optimization/programming (LP)** polynomial
  \[
  \max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \}
  \]

- **Integer linear optimization (IP)** NP-hard
  \[
  \max \{ c^T x \mid Ax \leq b, x \in \mathbb{Z}^n \}
  \]

- **Mixed-Integer linear optimization (MIP)** NP-hard
  \[
  \max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^p \times \mathbb{Z}^q \}
  \]
Integer linear optimization

- **Linear optimization/programming (LP)**, polynomial
  \[ \max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \} \]

- **Integer linear optimization (IP)**, NP-hard
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- **Mixed 0-1 linear optimization**, NP-hard
  \[ \max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^p \times \{0,1\}^q \} \]
\( P = \{ x \in \mathbb{R}^n \mid Ax \leq b \}, \ A \in \mathbb{Z}^{m \times n}, \ b \in \mathbb{Z}^m \) polyhedron

Integer points in \( P \ \implies \ P \cap \mathbb{Z}^n \)
\( P = \{ x \in \mathbb{R}^n \mid Ax \leq b \}, \ A \in \mathbb{Z}^{m \times n}, \ b \in \mathbb{Z}^m \) polyhedron

\( \triangleright \) Integer points in \( P \leadsto P \cap \mathbb{Z}^n \)
\[ P = \{ x \in \mathbb{R}^n \mid Ax \leq b \}, \quad A \in \mathbb{Z}^{m \times n}, \quad b \in \mathbb{Z}^m \text{ polyhedron} \]

\[ \text{Integer points in } P \mapsto P \cap \mathbb{Z}^n \]

\[ P_I = \text{conv}(P \cap \mathbb{Z}^n) \text{ integer hull} \]
\( P = \{ x \in \mathbb{R}^n \mid Ax \leq b \}, \quad A \in \mathbb{Z}^{m \times n}, \quad b \in \mathbb{Z}^m \) polyhedron

- Integer points in \( P \) \( \leadsto \) \( P \cap \mathbb{Z}^n \)

- \( P_I = \text{conv}(P \cap \mathbb{Z}^n) \) integer hull

- \( P_I \) is a polyhedron: \( P_I = \{ x \in \mathbb{R}^n \mid \tilde{A}x \leq \tilde{b} \}, \quad \tilde{A} \in \mathbb{Z}^{k \times n}, \quad \tilde{b} \in \mathbb{Z}^k \)
$P = \{ x \in \mathbb{R}^n \mid Ax \leq b \}, \quad A \in \mathbb{Z}^{m \times n}, b \in \mathbb{Z}^m$ polyhedron

- Integer points in $P \rightsquigarrow P \cap \mathbb{Z}^n$

- $P_I = \text{conv}(P \cap \mathbb{Z}^n)$ integer hull

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\[
\max\{ c^T x \mid Ax \leq b, x \in \mathbb{Z}^n \} = \max\{ c^T x \mid \tilde{A}x \leq \tilde{b}, x \in \mathbb{R}^n \}
\]
$P_I$ is very hard to compute $\leadsto$ approximation by cutting planes (Gomory 1958)
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- Solve the linear relaxation
  $$\max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \}$$
  and find an optimal solution $x^\ast$. 
$P_I$ is very hard to compute $\leadsto$ approximation by cutting planes (Gomory 1958)

▷ Solve the linear relaxation
\[
\max \{ c^T x \mid Ax \leq b, x \in \mathbb{R}^n \}
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and find an optimal solution $x^*$. 

▷ If $x^* \in \mathbb{Z}^n$, the integer linear program has been solved.
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- If $x^* \notin \mathbb{Z}^n$, generate a cutting plane
  $a^T x \leq \beta$, which is satisfied by all integer points in $P$, but which cuts off the non-integer vertex $x^*$. 

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- If $x^* \notin \mathbb{Z}^n$, generate a cutting plane $a^T x \leq \beta$, which is satisfied by all integer points in $P$, but which cuts off the non-integer vertex $x^*$.

- Add the inequality $a^T x \leq \beta$ to the system $Ax \leq b$ and solve the relaxation again.
Chvátal-Gomory cutting plane

Gomory 58, Chvátal 73
Gomory 58, Chvátal 73
Chvátal-Gomory cutting plane

Gomory 58, Chvátal 73

A. Bockmayr, 26 May 2016
Chvátal-Gomory cutting plane

Gomory 58, Chvátal 73
Chvátal-Gomory cutting plane

Gomory 58, Chvátal 73

\[ \begin{align*}
Ax & \leq b \\
\mathbf{u}^T Ax & \leq \left\lfloor \mathbf{u}^T b \right\rfloor
\end{align*} \]

if \( \begin{cases} 
\mathbf{u} \geq 0 \\
\mathbf{u}^T A \in \mathbb{Z}^n
\end{cases} \)
Branch-and-Bound

Land/Doig 1960

- Divide the set of feasible solutions into subsets ("branch")
- Compute bounds for the objective function on these subsets ("bound") \(\leadsto\) linear relaxation!
- Use these bounds to discard some subsets from further consideration.
Branch-and-Bound

Divide the set of feasible solutions into subsets ("branch")
Compute bounds for the objective function on these subsets ("bound") $\leadsto$ linear relaxation!
Use these bounds to discard some subsets from further consideration.

Basic principle
$S = S^0 \cup S^1$
Local upper bound: $\max\{c^T x \mid x \in S^0\} \leq UB^0$
Global lower bound (feasible solution): $x^* \in S$, with $c^T x^* = LB > UB^0$
$\leadsto x_{opt} \in S^1$. 
Grötschel, Padberg, Rinaldi, ... , 1980’s

- Combine branch-and-bound with cutting plane generation.

- Improve upper bounds by tightening the linear relaxation using cutting planes.

- Study the facets of the integer hull $P$ to find strong cutting planes ("polyhedral combinatorics").

- Many results on strong cuts for particular problems (e.g. knapsack, traveling salesman, alignment, ...)

- Strong cuts for general problems: Gomory’s mixed integer cuts, lift-and-project cuts, ...

- Software: CPLEX, Gurobi, SCIP, ...
Branch-and-Cut

Grötschel, Padberg, Rinaldi, . . . , 1980’s

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Linear optimization
  ▶ Polyhedra
  ▶ Simplex algorithm, interior point methods
Linear optimization
- Polyhedra
- Simplex algorithm, interior point methods

(Mixed-)integer linear optimization
- Integer hull and linear relaxation
- Cutting planes
- Branch-and-bound
- Branch-and-cut

NP-hard

polydivial
Summary

- Linear optimization
  - Polyhedra
  - Simplex algorithm, interior point methods

- (Mixed-)integer linear optimization
  - Integer hull and linear relaxation
  - Cutting planes
  - Branch-and-bound
  - Branch-and-cut

- Many applications in bioinformatics and systems biology
  - Flux balance analysis
  - Elementary flux modes

polynomial

NP-hard

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