Exact Optimization in Spin-Glass Physics

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Outline

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1. Spin Glasses
2. Complexity Theory in a Nutshell
3. Branch-and-Bound
4. Branch-and-Cut for Ising Spin Glasses
5. Branch-and-Cut for Potts Spin Glasses

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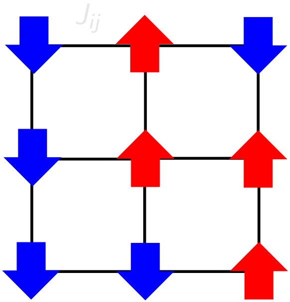
e.g. $Rb_2Cu_{1-x}Co_xF_4$
experiments (Cannella & Mydosh 1972) reveal:
at low temperatures: $\rightarrow$ phase transition spin glass state

Edwards Anderson Model (1975)

- short-range model
- interactions randomly chosen
  - $J_{ij} \in \{+1, -1\}$ or
  - Gaussian distributed
- $H(S) = -\sum_{<i,j>} J_{ij} S_i S_j$, with spin variables S_i



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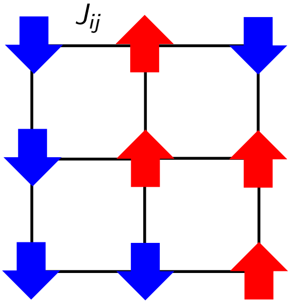

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Why Exact Ground States?

in contrast to Monte-Carlo Simulations or genetic algorithms:
we want to compute **exact solutions**
disadvantages of heuristic methods:

- might become stuck in local minima and do not know anything about the quality of the solution $\longrightarrow$ physical analysis might be biased.
- configurations with almost the same energy might be very different $\longrightarrow$ not clear whether results of spin-spin correlation functions can yield relevant information.

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Cologne Spin-Glass Ground-State Server

- An exact ground state can be computed via our server on the web
  `www.informatik.uni-koeln.de`
- submit jobs via a command-line client (or via www-interface) and get exact results via email. (will be extended in the future.)
- current focus: compute exact results for **hard** instances of the problem.
  - 2d spin glasses
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‘This is a Hard Problem’ means...

- NP-hard, i.e. we cannot expect to find an algorithm that solves it in time growing polynomial in the size of the input
- e.g., $2d$ Ising spin glasses with an external field or $3d$ lattices
- whereas $2d$, no field, free boundaries: ‘easy’

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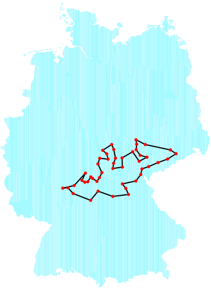
General Concepts

many problems can be formulated on **graphs** $G = (V, E)$ with node set V and edge set E.

Edge weights $c_e \in \mathcal{R}$ might be present.

Examples (from ABC^2's TSPbook):



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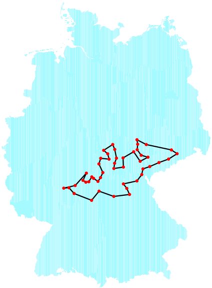

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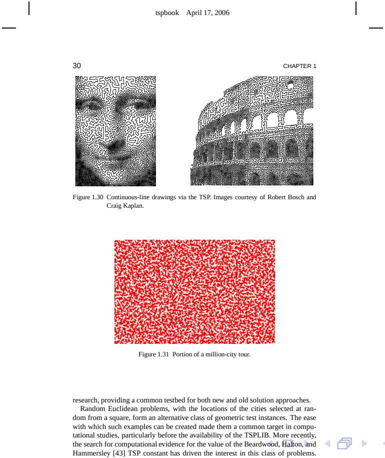

Figure 1.30 Continuous-line drawings via the TSP. Images courtesy of Robert Bosch and Craig Kaplan.

Figure 1.31 Portion of a million-city tour.

research, providing a common testbed for both new and old solution approaches.

Random Euclidean problems, with the locations of the cities selected at random from a square, form an alternative class of geometric test instances. The ease with which such examples can be created made them a common target in computational studies, particularly before the availability of the TSPLIB. More recently, the search for computational evidence for the value of the Beardwood, Halton, and Hammersley [43] TSP constant has driven the interest in this class of problems.

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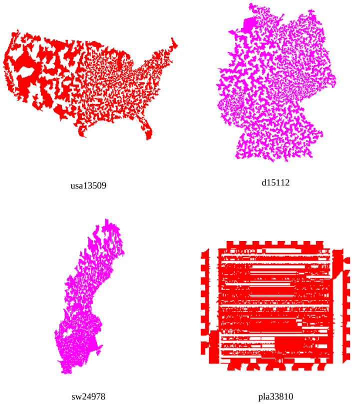

Figure 1.47 Optimal tours.

General Concepts

many problems can be formulated on **graphs** $G = (V, E)$ with node set V and edge set E.
Edge weights $c_e \in \mathcal{R}$ might be present.
Examples:

- shortest paths in networks
- shortest traveling salesman tour (TSP)
- etc.

Some of them are 'easy', some 'hard'.
...in more detail:

Complexity of Decision Problems

A problem $\mathcal{P}$ is a **decision problem**, if the set of all instances $I_{\mathcal{P}}$ of $\mathcal{P}$ is partitioned into the 'yes' and the 'no'-instances. For each instance we ask: Is it a 'yes'- or a 'no'-instance?

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1. instance: $n \in \mathcal{N}$
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2. instance: graph $G = (V, E)$
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Contains all decision problems $\mathcal{P}$ for which there exists a solution algorithm that solves $\mathcal{P}$ within a time polynomially bounded in the size needed to store the input, i.e., number of bits.

polynomially bounded?

- assume: each elementary algorithmic step (summation, assignment, etc.) has cost 1.
- Let input for some problem be stored by m bits. (e.g., for $n \in \mathcal{N}$, $m = \log n$ bits are needed.)
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NP: nondeterministic polynomial
A decision problem is in NP, if for an arbitrary instance and for a given (possible) solution it can be **verified** in polynomial time whether the solution yields a 'yes' or a 'no' answer.
Example:

- for boolean variables $x_1, \ldots, x_n$: given a clause $x_1 \vee \neg x_2 \ldots x_k \wedge x_2 \vee x_4 \ldots x_l$. Is there a true/false assignment of values to the variables satisfying the clause? (SAT)
- given a graph $G = (V, E)$ with edge weights c_e, and $k \in \mathcal{N}$. Is there a tour that visits every node exactly once with length $\leq k$? (TSP)

Here, a candidate solution can be verified by insertion.

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- SAT was the first problem to be proven to be NP-complete (Cook (1971))
- For many other problems *NP*-completeness was proven since then by reduction to and from other *NP*-complete problems

Examples

$\{0,1\}$-integral solution for inequality system ($\exists 01IP$)

instance: $A \in \mathcal{Z}^{m\times n}$, $b \in \mathcal{Z}^m$

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Optimization Problems

an optimization problem is characterized by

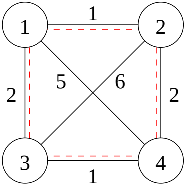
- the set of instances
- information whether we should maximize or minimize
- the set of feasible solutions
- for each instance and each feasible solution, the objective function value of the solution

Example

MINIMUM TRAVELING SALESMAN (TSP)

instance: set of cities $\{1, 2, \ldots, n\}$, distance matrix $D \in \mathcal{Z}_+^{n \times n}$
solution: permutation $\{i_1, i_2, \ldots, i_n\}$ of $\{1, 2, \ldots, n\}$ ('tour' through all cities)
objective function value: $\left(\sum_{k=1}^{n-1} d_{i_k, i_{k+1}}\right) + d_{i_n, i_1}$

$$\begin{array}{c|cccc|} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 2 & 5 \\ 2 & 1 & 0 & 6 & 2 \\ 3 & 2 & 6 & 0 & 1 \\ 4 & 5 & 2 & 1 & 0 \\ \hline \end{array}$$



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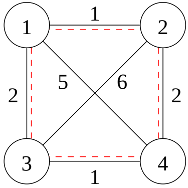

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The Classes NP and NPO

An optimization problem is in *PO*, if there exists a polynomial-time algorithm that for each instance of the problem determines an optimum solution and returns its value.

Example:

- shortest paths
- minimum spanning trees
- matching
- etc.

An optimization problem is in *NPO*, if

- the instances can be recognized in polynomial time
- for all instances the size of a feasible solution is polynomially bounded in the size of the input
- for all y that are polynomially bounded it can be verified in polynomial time whether y is a feasible solution
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Example:

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- etc.

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Martin Weigel has already pointed you to several relevant polynomial optimization problems with applications in physics.

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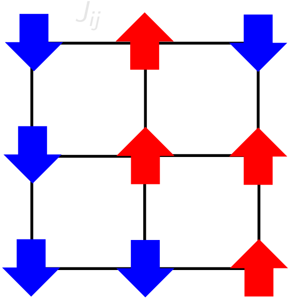

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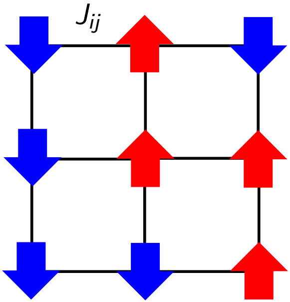

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Exact Ground States of Hard Instances

Spinglass	Graph $G=(V, E)$
↑	● node of G
↑–↓	●–● edge of G
coupling J_{ij}	edge weight c_{ij}
configuration	node partition V^+, V^-

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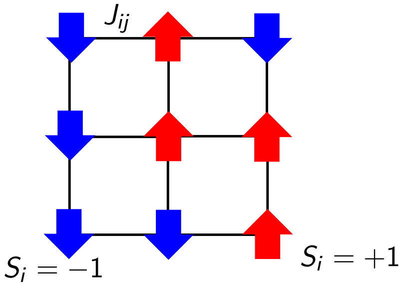

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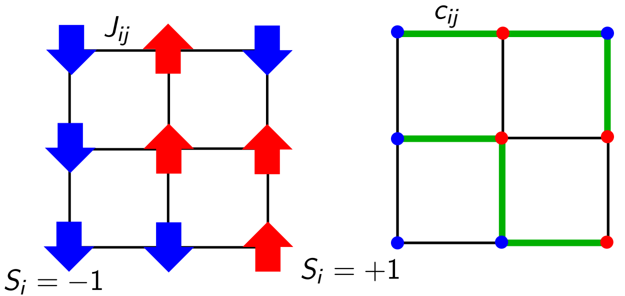

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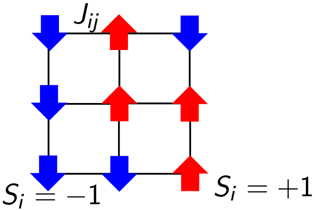
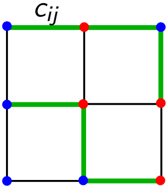
$H = -\sum_{e \in E} J_{ij} S_i S_j$

Computing Exact Ground States



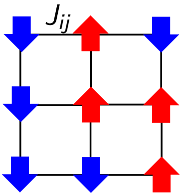


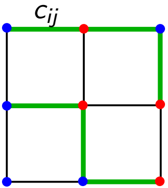
$$H(\underline{S}) + \sum_{(i,j)\in E} J_{ij} = \sum_{(i,j)\in E} J_{ij} \underbrace{(1 - S_i S_j)}$$

$$= \begin{cases} 2 & \text{, if } S_i \neq S_j \\ 0 & \text{, otherwise} \end{cases}$$

$$= 2 \sum_{S_i \neq S_j} J_{ij}$$

Computing Exact Ground States



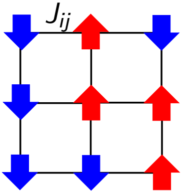


$$H(\underline{S}) + \text{const}$$
$$= 2 \sum_{S_i \neq S_j} J_{ij}$$

$$\text{cut} = \{(i,j) \in E \mid (i,j) = \}$$

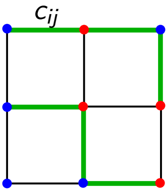
its weight: $\sum_{(i,j)\in \text{cut}} c_{ij}$

Computing Exact Ground States



$$H(\underline{S}) + \text{const} = 2 \sum_{S_i \neq S_j} J_{ij}$$

$\boxed{\text{ground state } \min H(\underline{S})}$



$\text{cut} = \{(i,j) \in E \mid (i,j) = \}$

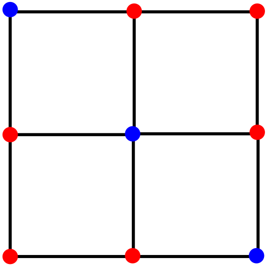
weight $\sum_{(i,j)\in \text{cut}} c_{ij}$

with $c_{ij} = -J_{ij}$:

$\boxed{\text{maximum cut in } G}$

NP-hard in general

Example



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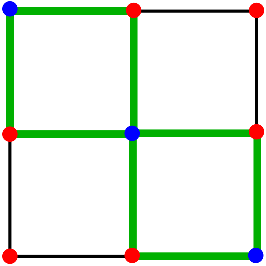

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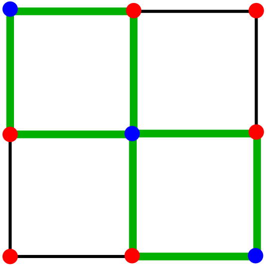

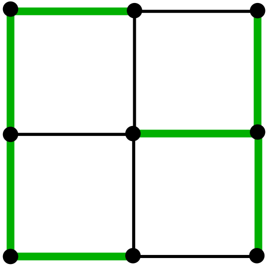

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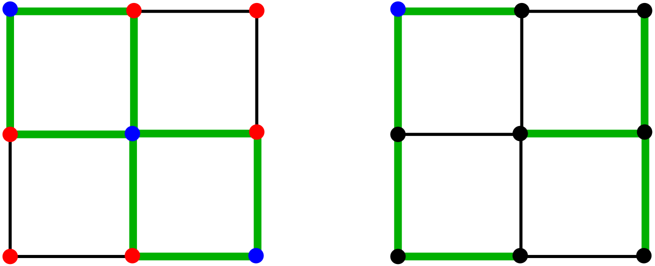

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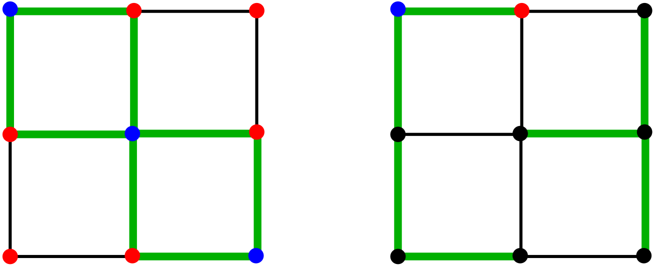

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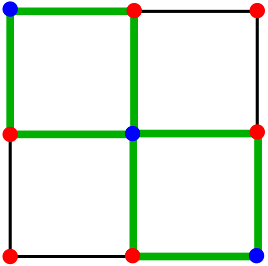

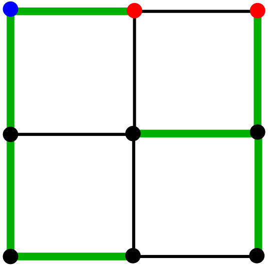

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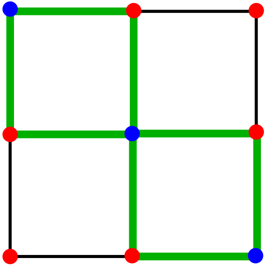

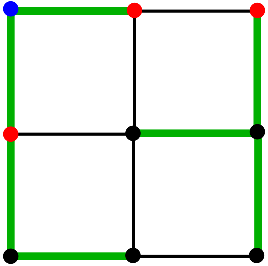

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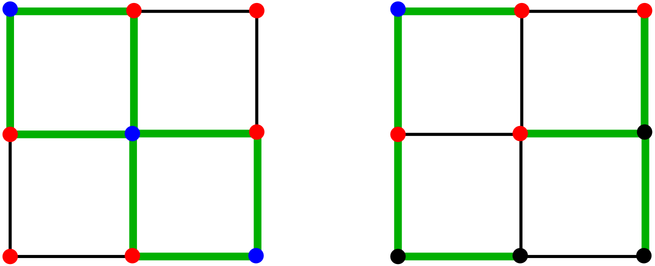

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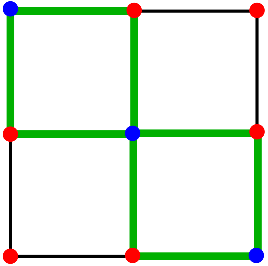

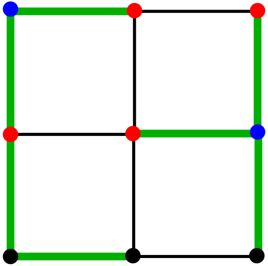

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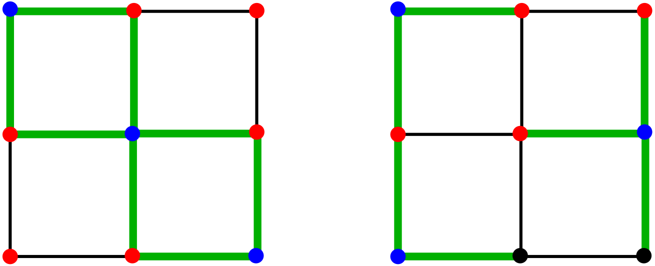

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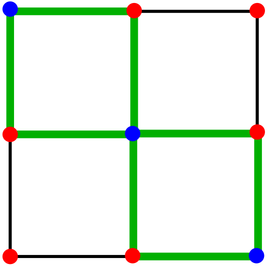

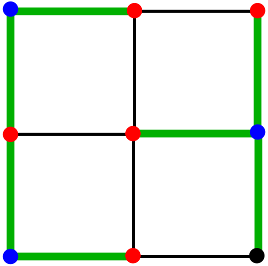

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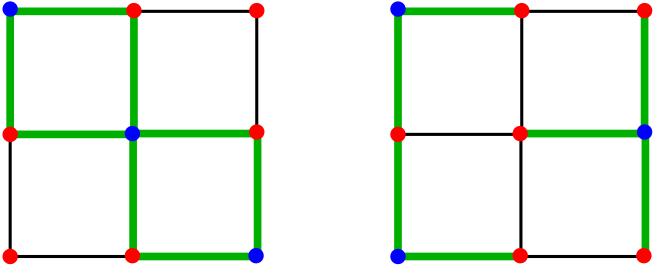

Complexity Status of Maximum Cut

- for general instances NP-hard, i.e. we cannot expect to find an algorithm that solves it in time growing polynomial in the size of the input
- NP-hard for, e.g., $2d$ Ising spin glasses with an external field or $3d$ lattices. more general: on general graphs or on almost planar graphs
- $2d$, no field, free boundaries: polynomial solvable (see M. Weigel's talk)
- Goemans und Williamson found a 0.878-approximation algorithm, i.e.,. a polynomial algorithm, in which the computed solution has a value of at least 0.878 times the value of an optimum cut. However: If P$\neq$NP, there does not exist a polynomial algorithm that computes a solution with value at least 98% of the value of an maximum cut.

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Applications of Maximum Cut

- quadratic 0-1 optimization: Given $A \in \mathcal{R}^{n \times n}$ and $a \in \mathcal{R}^n$, compute $\min\{x^T A x + a^T x \mid x \in \{0,1\}^n\}$
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Outline

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Branch & Bound

- standard approach for the solution of NP-hard integer and mixed-integer optimization problems
- can be used for a wide class of problems
- basic idea is very simple
- however: practical usefulness depends strongly on good data structures, clever implementation, etc.

known names for Branch & Bound:

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- backtracking

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In the following wlog: consider maximization problems.

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- in case bounds are equal: optimality proven
- otherwise: divide the problem into subproblems so that the combination of the solutions in the sub problems can be combined to the solutions of the original problem
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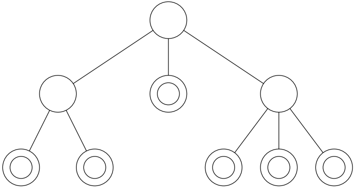
associate to the solution process in a natural way a branch & bound-tree:



- the root is the original problem
- a node represents some sub problem
- a direct child of a node u represents a sub problem of u
- tree leafs represent 'solved' problems

BRANCH & BOUND(A, b, c, N_1) (Dakin) for MIP

Input:
mixed-integer problem (MIP) with rational data

$$
(MIP^{=}) \qquad \begin{array}{rrcl} \max & c^T & & \\ & Ax & = & b \\ & x & \geq & 0 \\ & x_i & & \text{integer } \forall i \in N_1 \end{array}
$$

Output: solution of the problem or proof of infeasibility.

BRANCH & BOUND(A, b, c, N_1) (Dakin) for (MIP)

1. initialize the list of active sub problems with the original problem. opt $= -\infty$
2. **while** list of active sub problems not empty **do**
   begin
3. choose from the list of active problems one. 'Solve' it by:
   1. find optimal solution for the sub problem, or
   2. prove that the sub problem does not have a feasible solution, or
   3. prove by using a relaxation (bound) that there does not exist a feasible solution for the sub problem with a higher objective function value than the up to now best known solution (**fathoming**)
   4. if above not possible: **branch**, i.e., divide the problem into further sub problems, add them to list of active problems.

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4. if (opt $> -\infty$) **return** best known feasible solution as optimum. otherwise: return 'problem infeasible'.

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- important: keep the size of the tree 'small' $\Rightarrow$ need good bounds.
- to 3 (2): if a relaxation of a sub problem is infeasible $\longrightarrow$ sub problem itself is infeasible.
- For fathoming a sub problem in 3 (3): need good upper and lower bounds. Lower bounds: given by feasible solutions calculated by heuristics, or by an optimal solution of a sub problem.
- easiest branching: choose some x_e that needs to be integer, however the optimum in the LP is $x_e^\star \notin \mathbb{Z}$. Replace the current sub problem by two, in one of which one adds the inequality $x_e \leq \lfloor x_e^\star \rfloor$, and in the other $x_e \geq \lceil x_e^\star \rceil$.
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Example

Consider

$$\begin{array}{rrrrrrrrrrrl}
\max & -7x_1 & - & 3x_2 & - & 4x_3 & & & & & & \\
 & x_1 & + & 2x_2 & + & 3x_3 & - & x_4 & & & = & 8 \\
 & 3x_1 & + & x_2 & + & x_3 & & & - & x_5 & = & 5 \\
 & & & & & & & & & x_1, x_2, x_3, x_4, x_5 & \geq & 0 \\
 & & & & & & & & & x_1, x_2, x_3, x_4, x_5 & \in & \mathcal{Z}
\end{array}$$

LP-Optimum

$$x_3 = x_4 = x_5 = 0 \ , \ x_1 = \frac{2}{5} \ , \ x_2 = \frac{19}{5}$$

value $c^* = -\frac{71}{5}$ $(= -14.2)$. upper bound: -15
branch on x_2

$$P_1 = P_0 \cap \{x \mid x_2 \leq 3\}$$
$$P_2 = P_0 \cap \{x \mid x_2 \geq 4\}$$

choose P_1 as next problem.

Example

optimum solution of LP-relaxation LP_1 is

$$x_4 = x_5 = 0\ ,\ x_1 = \frac{1}{2}\ ,\ x_2 = 2\ ,\ x_3 = \frac{1}{2}$$

and $c^* = -\frac{29}{2}$ (upper bound -15).
subdivide P_1, get:

$$P_3 = P_1 \cap \{x \mid x_1 \leq 0\}$$
$$P_4 = P_1 \cap \{x \mid x_1 \geq 1\}$$

active problems are $K = \{P_2, P_3, P_4\}$. solving LP_3 gives

$$x_1 = x_5 = 0\ ,\ x_2 = 3\ ,\ x_3 = 2\ ,\ x_4 = 4$$

and $c^* = -17$. then P_3 is solved , best solution (global lower bound) has value -17.

Example

solve P_4, get:

$$x_4 = 0 \ , \ x_1 = 1 \ , \ x_2 = 3 \ , \ x_3 = \frac{1}{3} \ , \ x_5 = \frac{4}{3}$$

and $c^* = -\frac{52}{3} = -17\frac{1}{3}$. The found upper bound -18 is worse than best solution, and P_4 is fathomed.
Need to solve P_2. We get as a solution of the LP-relaxation

$$x_3 = x_5 = 0 \ , \ x_1 = \frac{1}{3} \ , \ x_2 = 4 \ , \ x_4 = \frac{1}{3}$$

and $c^* = -\frac{43}{3}$. P_2 is not yet solved. Branch on x_1

$$P_5 = P_2 \cap \{x \mid x_1 \leq 0\}$$
$$P_6 = P_2 \cap \{x \mid x_1 \geq 1\}$$

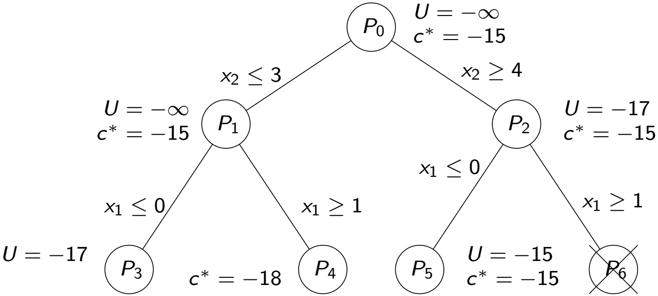
solving LP_5 yields

$$x_1 = x_3 = x_5 = 0 \ , \ x_2 = 5 \ , \ x_4 = 2$$

and $c^* = -15$. This is the new best solution with value -15.
P_5 is then solved.

Example

No need to consider P_6 further, as because of LP_2 no better solution is possible.



Implementation Details

- **branching** can also divide into more than 2 sub problems, or by more complicated inequalities. Good choice of branching variable is important!
- Exploit **logical implications**. E.g. for constraints $\sum_{i \in S} x_i = 1$, $x_i \in \{0, 1\}$: If some $x_j = 1 \rightarrow$ all other variables in S have value 0. $\Rightarrow$ branch with $\sum_{i \in S_1} x_i = 0$ and $\sum_{i \in S_2} x_i = 0$ with $S_1 \cup S_2 = S$
- **primal heuristics**: sometimes it takes long until good feasible solutions are found. $\rightarrow$ additional heuristics
- good strategies for **sub problem selection** strongly influence the total number of sub problems to be solved. It is not easy to devise a strategy that works well for any problem. often used: "'Best first search"'
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Conclusions

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