Topics in Optimization

João Pedro Gonçalves Dionísio

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Course Structure

- 6 weeks?
- 1h lecture + 30min exercises

Github Page

https://github.com/Joao-Dionisio/Minicurso

- Slides (unfinished)
- Lecture Notes (unfinished)
- Some Code (unfinished)
- Competition Details

Competition

Course Contents

- Convexity Theory
- 2 Linear Programming
- Complexity Theory
- Integer Programming
- Decomposition Methods

Convex sets

Definition

A set $X \in \mathbb{R}^n$ is said to be convex if

$$\forall x, y \in X, (1-t)x + ty \in X, t \in [0,1]$$

Convex sets

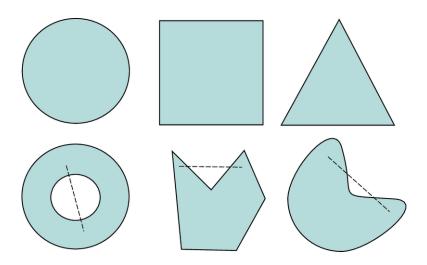


Figure: Examples of convex and non-convex sets

Convex Functions

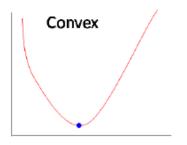
Definition

A function $f: \mathbb{R}^n \to \mathbb{R}$ is said to be convex if

$$\forall x, y \in \mathbb{R}^n, \forall \lambda \in [0, 1]$$
 we have

$$f((1-\lambda)x + \lambda y) \le (1-\lambda)f(x) + \lambda f(y)$$

Convex Functions



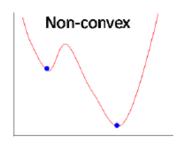


Figure: Examples of convex and non-convex functions

Epigraph

Definition

We call the epigraph of a function $f: X \to \mathbb{R}$, denoted by epi(f), to the following set:

$$epi(f) = \{(x, y) \in X \times \mathbb{R} \mid f(x) \le y\}$$

Epigraph

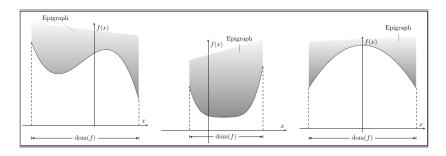


Figure: Examples of epigraph

Convex sets and convex functions

Proposition

The following two statements are equivalent:

- f is convex;
- 2 epi(f) is a convex set.

Convex Optimization

Definition

A convex optimization problem is

$$\min_{x} f(x)$$
s.t. $g_i(x) \ge 0, i \in [m]$

 $f, g_i, i = 1..., m$ convex functions. It implies that $\bigcap_{i \in [m]} \operatorname{epi}(g_i)$ forms a convex set.

Sufficient Optimality Condition

Theorem

Let \mathcal{P} be a convex optimization problem, and without loss of generality, assume it is a minimization problem. Then, if x^* is a local minimizer, then x^* is a global minimizer.

Bibliography



Linear Programming

The feasible region is a polyhedron.

Small Example

Dunder Mifflin can produce two types of industrial-sized sheets, type A and type B. Type A can be produced at a ratio of **200m** per hour, while type B can be produced at a ratio of **140m** per hour. The profits from each type of paper are **25** cents per meter and **30** cents per meter, respectively. Taking the market demand into account, next week's production schedule cannot exceed **6000m** for paper of type A and **4000m** for paper of type B. If on that week there is a *limit of* **40** production hours, how many meters of each product should be produced to maximize the profit?

Small Example

$$\max_{A,B} 25A + 30B$$
s.t. $A/200 + B/140 \le 40$
 $A \le 6000$
 $B \le 4000$
 $A, B \ge 0$

Example - Max flow

Suppose you have a network of pipes and receive money based on the amount of a valuable liquid that reaches a single destination, coming from a single source. Assume that the pipes have limited capacity and none of the liquid is gained or lost along the way. This is the max-flow problem, whose linear programming model follows.

Example - Max Flow

Definition

Let G(V, E) be a graph with $s, t \in V$ being defined as the source and target. The **max-flow problem** is the following LP:

$$\begin{aligned} & \max & & \sum_{v:(s,v)\in E} f_{sv} \\ & \text{s.t.} & & f_{uv} \leq c_{uv}, \forall (u,v) \in E \\ & & \sum_{u} f_{uv} - \sum_{w} f_{vw} = 0, \forall v \in V \setminus \{s,t\} \end{aligned}$$

PySCIPOpt

Supporting hyperplane theorem

Theorem (Supporting Hyperplanes)

Let $C \subset \mathbb{R}^n$ be a convex set, and $x \in \partial C$. Then, there exists a hyperplane H, s.t. $x \in H \cap C$ and C is contained in one of the half-spaces bounded by H.

It justifies the importance of LPs in the more general Convex Optimization.

Supporting hyperplane theorem

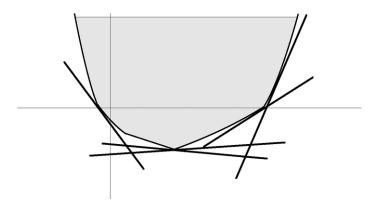


Figure: Visual representation

Duality

How can we know if we are close to the optimal solution? Can we derive bounds?

Duality

Definition

The dual problem of an LP of the form 16 (which we now call the primal) is:

$$\max_{y} b^{\mathsf{T}} y$$
s.t. $A^{\mathsf{T}} y \ge c$

$$y \ge 0$$

Every primal constraint has an associated dual variable, and vice-versa.



Strong Duality

Theorem (Strong Duality for LPs)

Let P be an LP, D the corresponding dual, and x^*, y^* be the respective optimal solutions. We have that $b^Ty^* = c^Tx^*$.

Interpretations of the Dual

The maximum amount of money that the decision maker will be willing to spend to buy an additional resource.

Optimal solution at vertex

Theorem

Consider the following LP:

Suppose it has at least one vertex. Then, if an optimal solution exists, there is also an optimal solution at a vertex.

Preliminaries

Definition

A point x of a convex set C is an **extreme point** (vertex) if $\nexists y, z \in C, \lambda \in]0,1[|x=\lambda y+(1-\lambda)z]$.

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A polyhedron P contains a **line** if $\exists d \in \mathbb{R}^n, x \in P \mid \forall \lambda \in \mathbb{R}, x + \lambda d \in P$.

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Definition

A polyhedron P contains a **line** if $\exists d \in \mathbb{R}^n, x \in P \mid \forall \lambda \in \mathbb{R}, x + \lambda d \in P$.

Lemma

P has a line \iff P does not have an extreme point.

P has an extreme point $\implies P$ has no line.

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Proof Sketch

P has an extreme point $\Longrightarrow P$ has no line. Q the set of optimal points has no line $(Q \subseteq P)$, so it has an extreme point. Let x^* be an extreme point of Q. We want to show that it is an extreme point of P. We assume it is not, and write it as $x^* = \lambda y + (1 - \lambda)z$. We then multiply both sides by c^{T} on the left. Some reasoning gives us that y and z are also optimal points.

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Algorithm for solving LPs

With this theorem, we have can create an algorithm to solve LPs. How?

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João, say stuff about Dantzig, Von Neumann, and WWII.

Simplex visualization

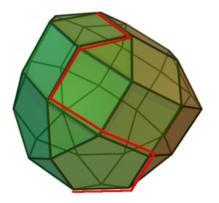


Figure: Example of simplex - only moves forward

Simplex Complexity

For the vast majority of problems, the Simplex Method runs in polynomial time, but so-called pathological examples have been found that ensure that the Simplex Method has to visit an exponential number of vertices.

IPM Motivation

Can be used on general NLPs.

$$\min_{x} c^{\mathsf{T}} x
\text{s.t.} c_{i}(x) \ge 0, i = 1, \dots, m$$

IPM Motivation

We replace the constraints with what is called a *barrier function*, most commonly a logarithm, to discourage solutions close to the border of the feasible region.

$$\min_{x} c^{\mathsf{T}}x - \mu \sum_{i=1}^{m} \log(c_{i}(x))$$

Successive iterations decrease the value of μ .

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Successive iterations decrease the value of μ . IPM has a

polynomial running time ($O(n^{3.5}log(1/\varepsilon))$), in fact).

IPM visualization

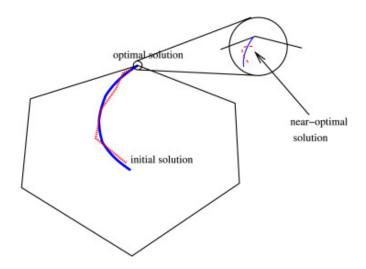
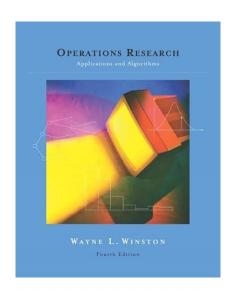


Figure: Example of IPM iterations

Bibliography



Exercises

Big-O

Definition

Given functions $f,g:\mathbb{R}^n \to \mathbb{R}$, we say that $f \in O(g(x))$ if

$$\forall x \geq x_0, |f(x)| \leq Mg(x)$$

Algorithmic complexity

- Writing every number from 1 to n requires us to write O(n) numbers. What about 1 to 2n?
- Writing every element of the power set of size n require us to write $O(2^n)$ numbers. What about 2n?

Complexity Classes

Skipping over a lot of details, (time) complexity classes are sets of problems characterized by the difficulty (time) of solving them.

E.g.: **P**, **EXP**, ...

P and NP

P is the set of problems for which an algorithm that runs in polynomial time solves it. **NP** is the set of problems for which an algorithm that runs in polynomial time can verify if a given candidate solution is indeed a solution.

Min Vertex-Cover

Given a graph G(V, E) find the minimum number of vertices that cover all edges

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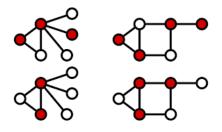


Figure: Example of Vertex Cover solutions

Min Vertex-Cover formulation

min
$$\sum_{v \in V} x_v$$

s.t. $x_u + x_v \ge 1, \forall (uv) \in E$
 $x_v \in \{0, 1\}$

PySCIPOpt

Max Knapsack

Given items with value and weight, fit them into a bag such that the total weight does not exceed W and the value is maximized.

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Given items with value and weight, fit them into a bag such that the total weight does not exceed W and the value is maximized.

$$\max \sum_{i=1}^{n} v_i x_i$$
s.t.
$$\sum_{i=1}^{n} w_i x_i \le W$$

$$x_i \in \{0, 1\}$$

Traveling-Salesman

Given a graph G(V, E) with weighted edges, find the least costly Hamiltonian cycle.

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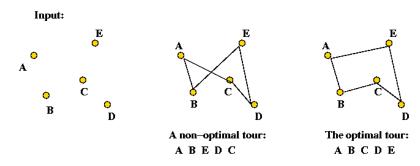


Figure: TSP example

TSP formulation

min
$$\sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} c_{ij} x_{ij}$$
s.t.
$$\sum_{i \neq j, i=1}^{n} x_{ij} = 1, j \in [n]$$

$$\sum_{i \neq j, j=1}^{n} x_{ij} = 1, i \in [n]$$

$$\sum_{i \in Q} \sum_{j \neq i, j \in Q} x_{ij} \le |Q| - 1, \forall Q \subsetneq \{1, \dots, n\}, |Q| \ge 2$$

$$x_{ij} \in \{0, 1\}$$

Cutting-Stock

Minimize the number of sheets of metal that, when cut into smaller sheets, satisfies a demand.

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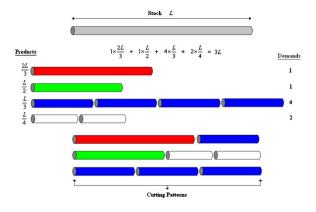


Figure: Cutting stock example

Cutting-Stock Formulation

$$\begin{aligned} & \min & & \sum_{j=1}^{M} y_{j} \\ & \text{s.t.} & & \sum_{j=1}^{M} x_{ij} = d_{i}, & & i \in [n] \\ & & & \sum_{i=1}^{n} l_{i} x_{ij} \leq L, & & j \in [m] \\ & & & x_{ij} \leq d_{i} y_{j}, & & i \in [n], j \in [m] \\ & & & x_{ij} \in \mathbb{Z}^{+}, & & i \in [n], j \in [m] \\ & & & y_{j} \in \{0, 1\}, & & j \in [m] \end{aligned}$$

Reductions

Knowing the solution to some optimization problems can give us the solution to other optimization problems.

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Vehicle routing and TSP

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- Mapsack and Cutting Stock

Exercises

Integer Programming

$$\min_{x,y} c^{\mathsf{T}}(xy)^{\mathsf{T}}$$
s.t. $f(x,y) \leq 0$

$$x \geq 0$$

$$y \in \mathbb{Z}$$

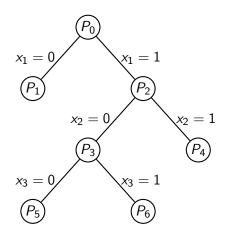
Non-convex

Integer programming is not convex. Which strategies can we employ to solve it?

Linear Relaxations

Relaxing constraints provides a bound on the optimal solution. Can we use this to solve IPs?

Branch-and-Bound



Revisiting Knapsack

$$\max \sum_{i=1}^{n} v_i x_i$$
s.t.
$$\sum_{i=1}^{n} w_i x_i \le W$$

$$x_i \in \{0, 1\}$$

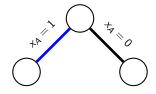
It has an easy LP-relaxation

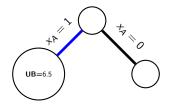
- Sort items by price density (price/weight)
- Pick items until capacity is exceeded
- Remove the excess of the last item

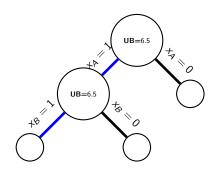
Knapsack instance

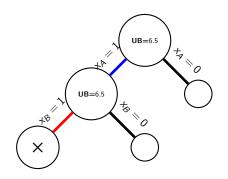
Item	Weight	Value	Value/Weight
Α	3	5	1.67
В	2	3	1.5
С	1	1	1

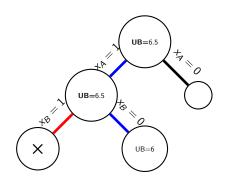
Knapsack capacity: 4

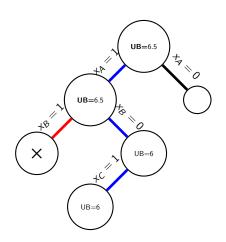


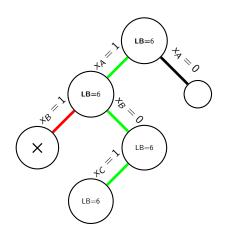


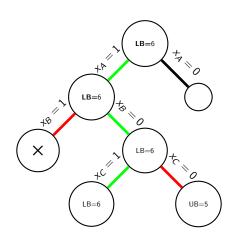


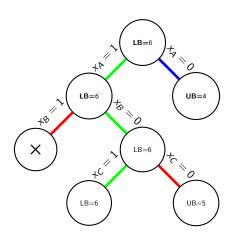


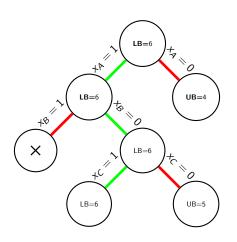












Heuristics

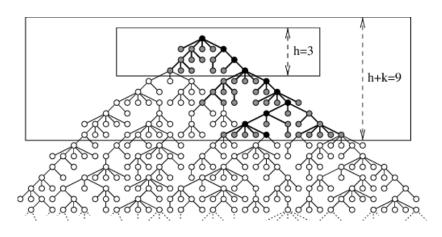
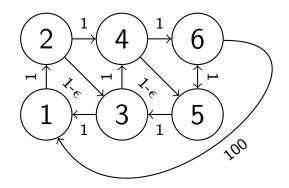


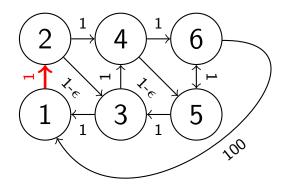
Figure: Branch and Bound trees can get very big. How big?

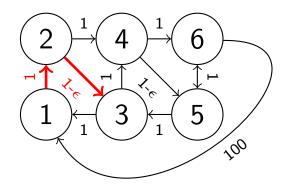
Heuristics

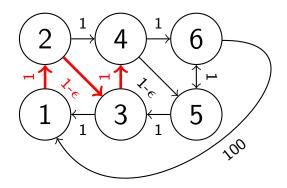
We will focus on heuristics for the TSP.

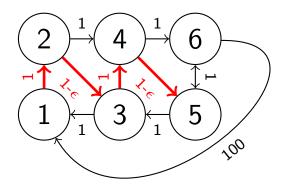
$$\begin{aligned} & \min \quad \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} c_{ij} x_{ij} \\ & \sum_{i \neq j, i=1}^{n} x_{ij} = 1, j \in [n] \\ & \sum_{i \neq j, j=1}^{n} x_{ij} = 1, i \in [n] \\ & \sum_{i \in Q} \sum_{j \neq i, j \in Q} x_{ij} \leq |Q| - 1, \forall Q \subsetneq \{1, \dots, n\}, |Q| \geq 2 \\ & x_{ij} \in \{0, 1\} \end{aligned}$$

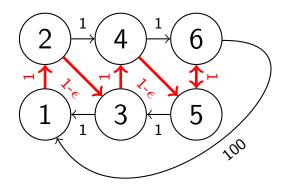


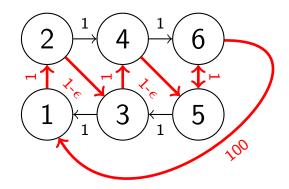


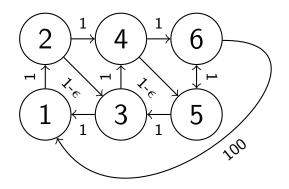


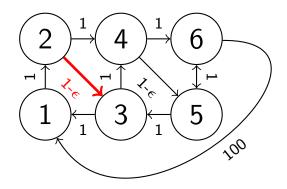


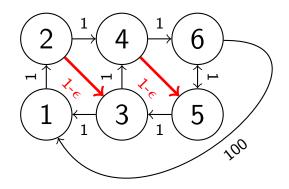


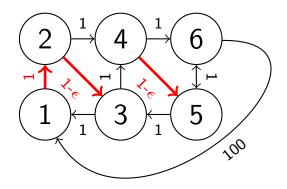


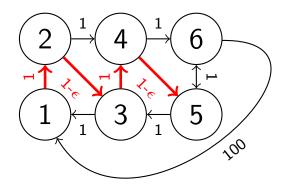


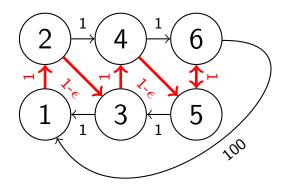




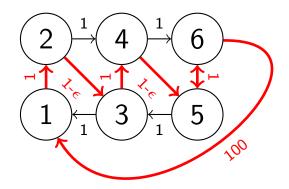








Greedy Algorithm



2-OPT algorithm

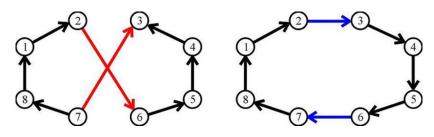


Figure: If two edges cross, we can find a strictly better solution

TSP: 2-opt visualization

Large TSP

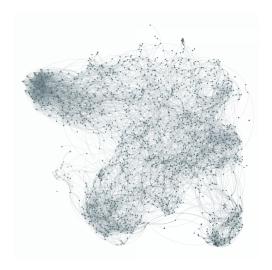


Figure: Heuristics are for large instances

Approximation algorithms

Some heuristics can have theoretical guarantees of their solution quality.

We will study a 2-approximation algorithm for TSP where the cost function satisfies the triangle inequality.

Minimum spanning tree

Definition

A **minimum spanning tree** is a subset of the edges of a connected, edge-weighted undirected graph that connects all vertices, without any cycles, such that total edge weight is minimum

Minimum spanning tree

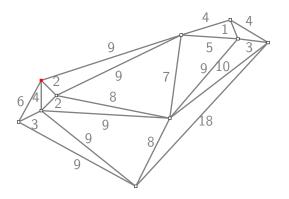


Figure: TSP instance

Minimum spanning tree

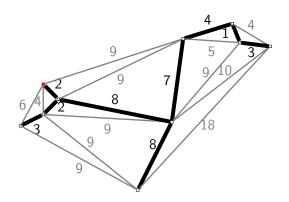


Figure: Minimal spanning tree

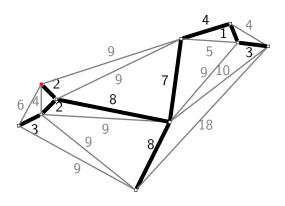


Figure: DFS

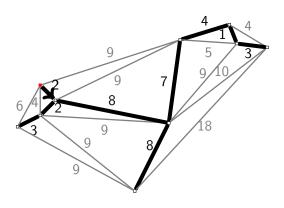


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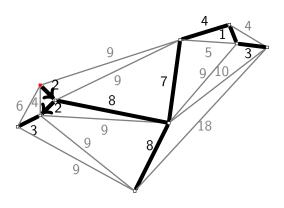


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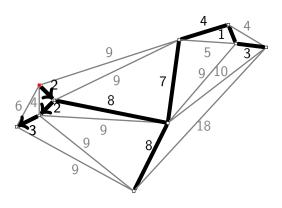


Figure: DFS

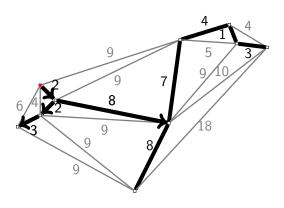


Figure: DFS

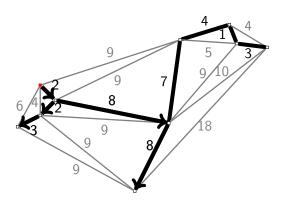


Figure: DFS

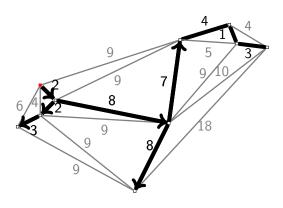


Figure: DFS

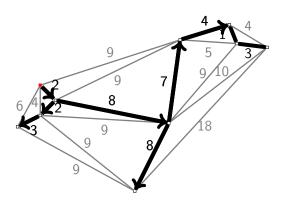


Figure: DFS

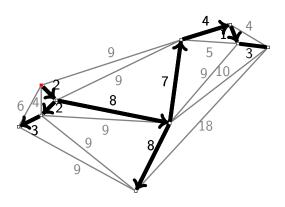


Figure: DFS

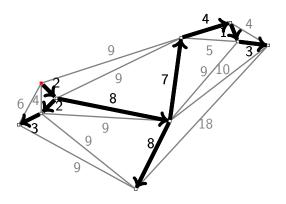


Figure: DFS

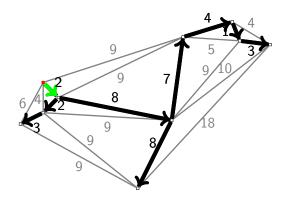


Figure: 2-approximation algorithm

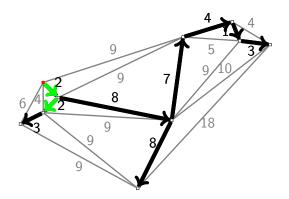


Figure: 2-approximation algorithm

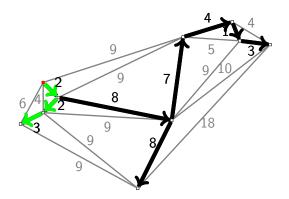


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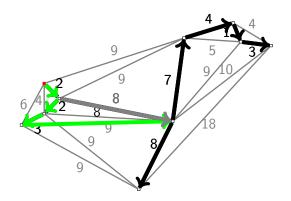


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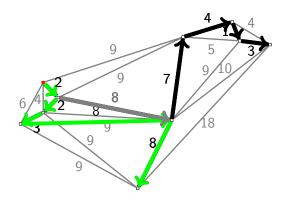


Figure: 2-approximation algorithm

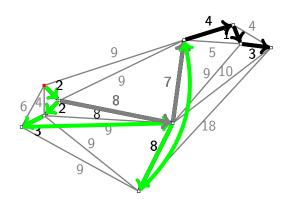


Figure: 2-approximation algorithm

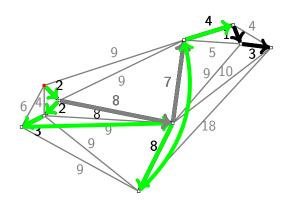


Figure: 2-approximation algorithm

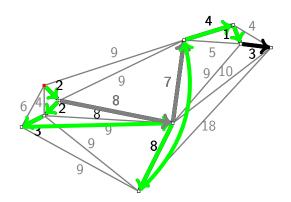


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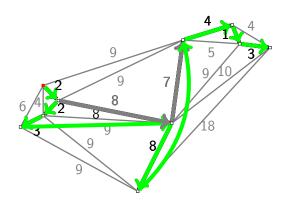


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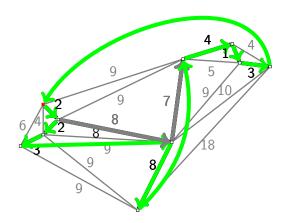


Figure: 2-approximation algorithm

Approximation ratio

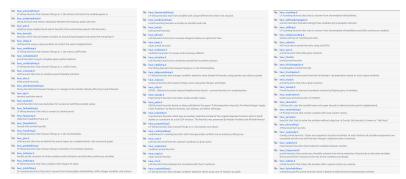
The solution given by this heuristics is at most twice as bad as the optimal solution. Why?

Approximation ratio

The solution given by this heuristics is at most twice as bad as the optimal solution. Why?

Assumption of the triangle inequality. The solution is less than twice the MST. MST is a lower bound.

SCIP heuristics



Modern solvers employ a lot of heuristics.

Meta-Heuristics

Heuristics can often get stuck in local optima.

Meta heuristics are abstractions that work with sets of solutions. Eg: TSP paths instead of cities.

Many accept worsening moves, which tends to work well in avoiding local optima,

Simulated Annealing

Randomly decide to move to a neighboring solution based on its fitness. The probabilities decrease with time. (Show simulated annealing example)

Simulated Annealing

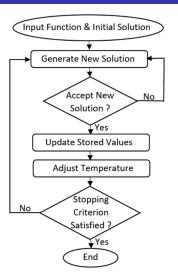


Figure: Simulated Annealing Flowchart

Tabu Search

Initially accept worsening solutions.

Keep a tabu list that forbids recently visited solutions.

Tabu Search

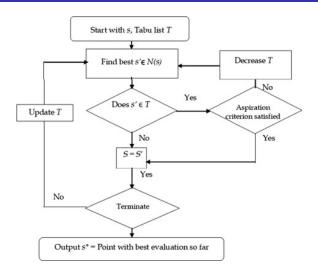


Figure: Tabu Search Flowchart

Genetic Algorithm

Inspired by natural processes, keeps a population of candidate solutions. Iteratively combines them to create new solutions.

Genetic Algorithm

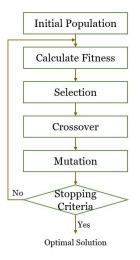


Figure: Genetic Algorithm Flowchart

Genetic Algorithm

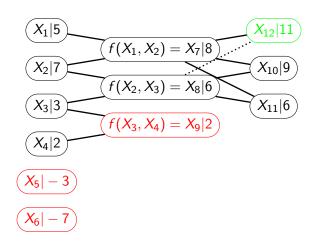


Figure: Illustration of a genetic algorithm

Reformulations

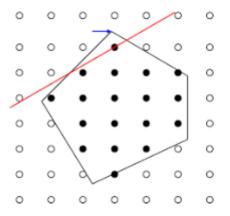


Figure: Integer programs admit infinite formulations

Reformulations

Formulations closer to their linear relaxation are better. Why is that?

Reformulations

Formulations closer to their linear relaxation are better. Why is that?

The provided bound is better, can prune branch and bound tree earlier.

Convex Hull

Definition

Let $X \subseteq \mathbb{R}^n$ be a set. The **convex hull** of X, denoted by conv(X), is the intersection of all convex sets containing X. Equivalently, it is the set of all convex combinations of X.

Perfect Formulation

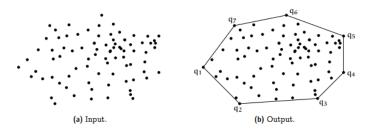


Figure: Linear relaxation equal to convex hull

Perfect Formulation

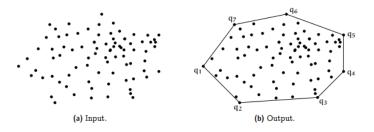


Figure: Linear relaxation equal to convex hull

Which points do we need to check?

Perfect Formulation

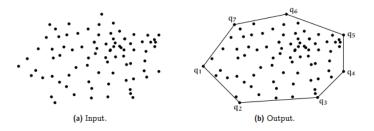


Figure: Linear relaxation equal to convex hull

Which points do we need to check? Why?

Symmetry

The solution space can exhibit a lot of symmetry (equivalent solutions modulo a permutation of the variables, for example). Especially damaging in integer optimization.

Symmetry

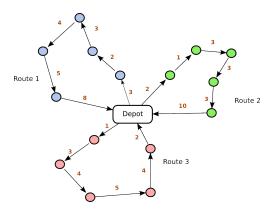


Figure: The vehicle routing problem has a lot of symmetry

Presolving

Presolving: Analyze the problems and reduce the solution space by identifying symmetry, redundant variables, implicit variables, etc.

For example:

- $x \le 1.5, y \ge 0.5, x + y \le 1 \implies x \le 0.5$
- $x \le 1.5, x \in \mathbb{Z} \implies x \le 1$

Presolving

```
presolving (26 rounds: 26 fast, 3 medium, 3 exhaustive):
46 deleted vars, 569 deleted constraints, 0 added constraints, 12680 tightened bounds, 0 add
937 implications, 100 cliques
presolved problem has 2982 variables (120 bin, 0 int, 0 impl, 2862 cont) and 5338 constraints
```

Figure: Example of SCIP presolving

Cutting planes

In theory, every integer program has an equivalent linear programming formulation. Why?

Cutting planes

In theory, every integer program has an equivalent linear programming formulation. Why?

Convex hull, linear relaxation is upper bound, hence optimal solution at vertex.

With binary variables, we can model some logical constraints.

 $\neg \chi$

$$\begin{array}{c|c}
\neg x \\
x \implies y
\end{array}$$

$$\begin{array}{c|c}
\neg x \\
x \Longrightarrow y \\
x \land y
\end{array}
\qquad \begin{array}{c|c}
1 - x \\
x \le y$$

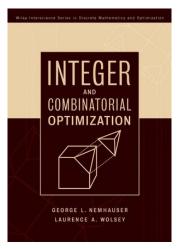
$$\begin{array}{c|ccc}
\neg x & & 1-x \\
x \Longrightarrow y & & x \le y \\
x \land y & & x+y=2 \\
x \lor y & & x+y \ge 1 \\
x \lor y & & x+y=1
\end{array}$$

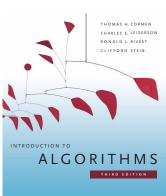
With binary variables, we can model some logical constraints.

$$\begin{array}{c|ccc}
\neg x & & 1-x \\
x \Longrightarrow y & & x \le y \\
x \land y & & x+y=2 \\
x \lor y & & x+y \ge 1 \\
x \lor y & & x+y=1 \\
\exists x & & \sum_{i=1}^{n} x_i \ge 1 \\
\exists !x & & \sum_{i=1}^{n} x_i = 1
\end{array}$$

Table: Formulating logical expressions with integer programming

Bibliography





Suggestions

Light read on integer programming: Link

Discrete Optimization with Professor Pascal Van Hentenryck, on Coursera: Link

Exercises

Decomposition Methods

Sometimes difficult problems have a structure that can be explored.

Big linear programs tend to only use a small subset of columns in the optimal solution.

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Column generation idea:

• Start with a small subset of columns. Optimize the resulting problem.

Big linear programs tend to only use a small subset of columns in the optimal solution.

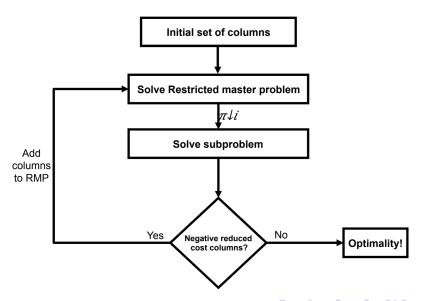
Column generation idea:

- Start with a small subset of columns. Optimize the resulting problem.
- Use dual values of the optimal solution to generate new columns

Big linear programs tend to only use a small subset of columns in the optimal solution.

Column generation idea:

- Start with a small subset of columns. Optimize the resulting problem.
- Use dual values of the optimal solution to generate new columns
- If no columns can improve the solution, it is optimal



Master Problem

With the available solutions, pick the ones that optimize the objective.

Subproblem

Out of all available columns, pick one that improves the solution of the restricted master problem. How?

Reduced Cost

Get the change in the objective by increasing a variable by a small amount, i.e., the first derivative from a certain point on the polyhedron that constrains the problem.

Reduced Cost

Get the change in the objective by increasing a variable by a small amount, i.e., the first derivative from a certain point on the polyhedron that constrains the problem. The **reduced cost** can be computed in the following manner:

$$c - A^{\mathsf{T}} y$$

Cutting Stock Revisited

$$\begin{aligned} & \min & & \sum_{j=1}^{M} y_{j} \\ & \text{s.t.} & & \sum_{j=1}^{M} x_{ij} = d_{i}, & & & i \in [n] \\ & & & \sum_{i=1}^{n} l_{i} x_{ij} \leq L, & & & j \in [m] \\ & & & x_{ij} \leq d_{i} y_{j}, & & & i \in [n], j \in [m] \\ & & & x_{ij} \in \mathbb{Z}^{+}, & & & i \in [n], j \in [m] \\ & & & y_{j} \in \{0, 1\}, & & & j \in [m] \end{aligned}$$

How do solutions look like?

Master problem

Pricing Problem

Pricing Problem

This is precisely the knapsack problem!

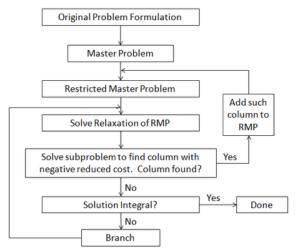
Column generation Tips

- The pricing problem should be easy.
- Solve the pricing problem heuristically. How many times does it need to be solved to optimality?
- Add multiple columns per iteration
- Remove columns from the RMP that have been inactive for many iterations

PySCIPOpt

Branch-and-Price

Column generation embedded in a Branch-and-bound tree. Branch on fractional variables.



Dantzig-Wolfe Decomposition

When can we use column generation? Is there a systematic way to do it?

When does this work?

(Weak) Minkowsi-Weyl Theorem

Theorem

Let $P \subseteq \mathbb{R}^n$ be a bounded polyhedron. Then there is a finite set Q such that P = conv(Q)

(The actual theorem is an equivalence and with possibly unbounded polyhedron)

DW-decomposition master problem

DW-decomposition pricing problem

What if instead of easy subproblems linked by a few constraints, we have a difficult problem that becomes easy if we fix a few variables?

What if instead of easy subproblems linked by a few constraints, we have a difficult problem that becomes easy if we fix a few variables? For example, a MIP with integer variables fixed.

$$\min_{x,y} \quad c^{\mathsf{T}}x + d^{\mathsf{T}}y \\
\text{s.t.} \quad Ax + By \ge b \\
y \in Y \\
x \ge 0$$

Fix y to \overline{y} .

$$\min_{x,y} \quad c^{\mathsf{T}}x + d^{\mathsf{T}}\overline{y}$$
s.t.
$$Ax + B\overline{y} \ge b$$

$$x \ge 0$$

Algorithm Idea

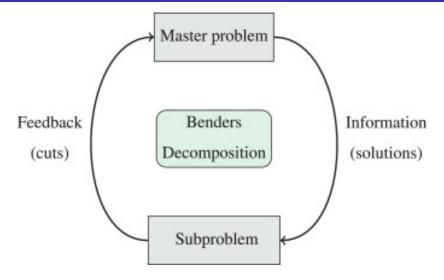


Figure: Benders' Decomposition Idea

The previous problem has the following dual:

$$\min_{u} \quad (b - B\overline{y})^{\mathsf{T}}u + d^{\mathsf{T}}\overline{y}$$
s.t.
$$A^{\mathsf{T}}u \le c$$

$$u \ge 0$$

The original problem is equivalent to:

$$\min_{y \in Y} [d^\intercal y + \max_{u \geq 0} \{(b - By)^\intercal u \mid A^\intercal u \leq c\}]$$

Outer Problem

Optimize the problem for a fixed y.

Inner Problem

Use the solution from the outer problem to choose better *y*s in the outer problem.

Duality revisited

Proposition

Let P be an LP and D the corresponding dual. We have the following:

- lacktriangledown D is infeasible \Longrightarrow P is unbounded
- 2 D is unbounded \implies P is infeasible
- **3** D has an optimal solution $y^* \implies P$ has an optimal solution x^* and $b^{\mathsf{T}}y \le c^{\mathsf{T}}x^*$

Optimality cuts

If the inner problem is feasible, we can derive bounds for the outer problem.

$$z \ge (b - By)^{\mathsf{T}}\overline{u} + d^{\mathsf{T}}y$$

Feasibility cuts

If the inner problem is unbounded, we know the fixed y cannot be chosen.

$$(b - By)^{\mathsf{T}}\overline{u} \leq 0$$

Suggestions

Light read on column-generation: Link

More in-depth explanation of column-generation/Dantzig-Wolfe: Link

Exercises