CS:4980 Topics in Computer Science II

Introduction to Automated Reasoning

Theory Solvers II

Cesare Tinelli

Spring 2024

The University of Iowa

Credits

These slides are based on slides originally developed by **Cesare Tinelli** at the University of Iowa, and by **Clark Barrett**, **Caroline Trippel**, and **Andrew (Haoze) Wu** at Stanford University. Adapted by permission.

Overview

SMT solvers can be used to solve arithmetic problems

Linear Programs (LPs) are a particularly interesting class of arithmetic problems, with stand-alone solvers

Many interesting applications: robotic planning, formal verification, operations research

Some of the slides are contributed by Guy Katz.

Outline

- QF_LRA
- Linear Programming
- The Simplex algorithm

Readings: DP 5.1-5.2

Review: Theory of Real Arithmetics ($\mathcal{T}_{\mathsf{RA}}$)

$\mathcal{T}_{\mathsf{RA}} = \langle \Sigma_{\mathsf{RA}}, \boldsymbol{M}_{\mathsf{RA}} \rangle$

$$\Sigma^S_{\mathsf{RA}} = \{ \mathsf{Real} \} \qquad \Sigma^F_{\mathsf{RA}} = \{ +, -, *, \leq \} \cup \{ q \mid q \text{ is a decimal numeral} \}$$

All $\mathcal{I} \in \boldsymbol{M}_{\mathsf{RA}}$ interpret Real as the set $\mathbb{R}$ of real numbers, and the function symbols in the usual way

Quantifier-free linear real arithmetic (QF_LRA):

1. no quantifiers
2. all occurrences of $*$ have at least one argument that is a decimal numeral

Many SMT solvers (e.g., cvc5, Z3) use a version of the Simplex method as the theory solver for QF_LRA

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Linear Programming

A *linear program (LP)* consists of:

1. An $m \times n$ matrix $\boldsymbol{A}$, the *constraint matrix*
2. An m-dimensional vector $\boldsymbol{b}$
3. An n-dimensional vector $\boldsymbol{c}$, the *objective function*

Let $\boldsymbol{x}$ a vector of n variables

Goal: Find a solution $\boldsymbol{x}$ that maximizes $\boldsymbol{c}^T\boldsymbol{x}$ subject to the linear constraints $\boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{b}$

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Example and Terminology

Maximize $2x_2 - x_1$ subject to:

$$x_1 + x2 \leq 3$$
$$2x_1 - x_2 \leq -5$$

Here:

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad A = \begin{bmatrix} 1 & 1 \\ 2 & -1 \end{bmatrix} \quad b = \begin{bmatrix} 3 \\ -5 \end{bmatrix} \quad c = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$$

Find $\boldsymbol{x}$ that maximizes $\boldsymbol{c}^T\boldsymbol{x}$, subject to $\boldsymbol{Ax} \leq \boldsymbol{b}$

Example and Terminology

Maximize $2x_2 - x_1$ subject to:

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An assignment of $\boldsymbol{x}$ is a *feasible solution* if it satisfies $\boldsymbol{Ax} \leq \boldsymbol{b}$
Otherwise, it is an *infeasible solution*

Is $\langle 0, 0 \rangle$ a feasible solution? ✗
Is $\langle -2, 1 \rangle$ a feasible solution? ✓

For a given assignment of $\boldsymbol{x}$, the value of $\boldsymbol{c}^T\boldsymbol{x}$ is the *objective value*, or *cost*, of $\boldsymbol{x}$

What is the objective value of $\langle -2, 1 \rangle$? 4

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An *optimal solution* is feasible solution with a maximal objective value, over all feasible solutions

If a linear program has no feasible solutions, the linear program is *infeasible*

The linear program is *unbounded* if the objective value of the optimal solution is ∞

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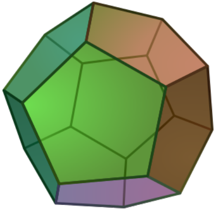
Geometric Interpretation

A *polytope* the generalization of polyhedron from 3-dimensional space to higher dimensions

A polytope P is *convex* if for all $v_1, v_2 \in \mathbb{R}^n \cap P$, $\lambda v_1 + (1 - \lambda) v_2 \in P$ for all $\lambda \in [0, 1]$

In other words, every point on the line segment connecting two points in P is also in P



Note: For an $m \times n$ constraint matrix $\boldsymbol{A}$, the set of points $P = \{ x \mid \boldsymbol{Ax} \leq \boldsymbol{b} \}$ form a *convex polytope* in n-dimensional space

LP goals: find a point in the polytope that maximizes $c^\top x$ for a given c

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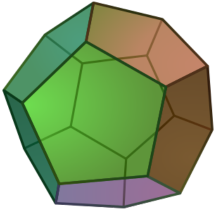

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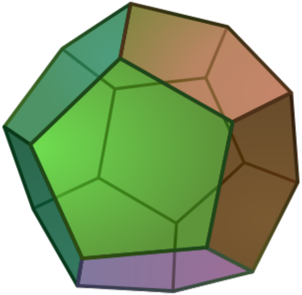

The LP is infeasible iff the polytope is empty

The LP is unbounded iff the polytope is open in the direction of the objective function

The optimal solution for a bounded LP must lie on a vertex of the polytope

Satisfiability as Linear Programming

Our goal: use LP to check the satisfiability of sets of linear $\mathcal{T}_{\text{RA}}$-literals

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A linear $\mathcal{T}_{\mathsf{RA}}$-equality can be written to have the form $\boldsymbol{a}^T\boldsymbol{x} = b$

We rewrite this further as $\boldsymbol{a}^T\boldsymbol{x} \geq b$ and $\boldsymbol{a}^T\boldsymbol{x} \leq b$

And finally to $-\boldsymbol{a}^T\boldsymbol{x} \leq -b$, $\boldsymbol{a}^T\boldsymbol{x} \leq b$

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Step 2: handle inequalities

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A $\mathcal{T}_{\mathrm{RA}}$-literal of the form $\boldsymbol{a}^T\boldsymbol{x} \leq b$ is already in the desired form

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A $\mathcal{T}_{\mathrm{RA}}$-literal of the form $\neg(\boldsymbol{a}^T\boldsymbol{x} \leq b)$ is transformed as follows

$$\neg(\boldsymbol{a}^T\boldsymbol{x} \leq b) \longrightarrow \boldsymbol{a}^T\boldsymbol{x} > b \longrightarrow -\boldsymbol{a}^T\boldsymbol{x} < -b \longrightarrow -\boldsymbol{a}^T\boldsymbol{x} + y \leq -b,\ y > 0$$

where y is a fresh variable used for all negated inequalities

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Example: $\neg(2x_1 - x_2 \leq 3)$ rewrites to $-2x_1 + x_2 + y \leq -3,\ y > 0$

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If there are no negated inequalities, add the inequality $y \leq 1$ where y is a fresh var

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In either case, we have the set of the form $\boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{b} \cup \{\, y > 0 \,\}$

Satisfiability as Linear Programming

Our goal: use LP to check the satisfiability of sets of linear $\mathcal{T}_{\mathsf{RA}}$-literals

Step 3: check the satisfiability of $\boldsymbol{Ax} \leq \boldsymbol{b} \cup \{ y > 0 \}$

Satisfiability as Linear Programming

Our goal: use LP to check the satisfiability of sets of linear $\mathcal{T}_{\mathsf{RA}}$-literals

Step 3: check the satisfiability of $\boldsymbol{Ax} \leq \boldsymbol{b} \cup \{ y > 0 \}$

Encode that as the LP: maximize y subject to $\boldsymbol{Ax} \leq \boldsymbol{b}$

Satisfiability as Linear Programming

Our goal: use LP to check the satisfiability of sets of linear $\mathcal{T}_{\mathsf{RA}}$-literals

Step 3: check the satisfiability of $\boldsymbol{Ax} \le \boldsymbol{b} \cup \{ y > 0 \}$

Encode that as the LP: maximize y subject to $\boldsymbol{Ax} \le \boldsymbol{b}$

The final system is satisfiable iff the optimal value for y is positive

Methods for solving LP problems

- *Simplex* (Dantzig, 1949) Exponential time (probably)
- *Ellipsoid* (Khachian, 1979) Polynomial time
- *Interior-point* (Karmarkar, 1984) Polynomial time

Although the Simplex method is the oldest and the least efficient in theory
it can be implemented to be quite efficient in practice

It remains the most popular and we focus on it next

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Standard Form

The general form of LP is to maximize objective function subject to a system of inequalities

However, the Simplex method is easier to present
if we make the additional assumption that all variables are non-negative:

$$
\begin{aligned}
\text{maximize} \quad & \sum_{j=1}^{n} c_j x_j \\
\text{s.t.} \quad & \sum_{j=1}^{n} a_{ij} x_j \le b_i \quad \text{for } i = 1, \dots, m \\
& x_j \ge 0 \quad \text{for } j = 1, \dots, n
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We call this the *standard form*

This causes no loss of generality since any LP can be transformed to standard form

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Running example:

$$
\begin{aligned}
\max \quad & 5x_1 + 4x_2 + 3x_3 \\
\text{s.t.} \quad & \begin{cases} 2x_1 + 3x_2 + x_3 \leq 5 \\ 4x_1 + x_2 + 2x_3 \leq 11 \\ 3x_1 + 4x_2 + 2x_3 \leq 8 \\ x_1, x_2, x_3 \geq 0 \end{cases}
\end{aligned}
$$

Slack Variables

Observe the first inequation

$$2x_1 + 3x_2 + x_3 \leq 5$$

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Define a new variable to represent the *slack*:

$$x_4 = 5 - 2x_1 - 3x_2 - x_3, \quad x_4 \geq 0$$

Do this to every each constraint so everything becomes equalities

Define a new variable to represent the objective value: $z = 5x_1 + 4x_2 + 3x_3$

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$$\longrightarrow$$

$$\max \quad z$$
$$\text{s.t.} \quad \begin{cases} x_4 = 5 - 2x_1 - 3x_2 - x_3 \\ x_5 = 11 - 4x_1 - x_2 - 2x_3 \\ x_6 = 8 - 3x_1 - 4x_2 - 2x_3 \\ z = 0 + 5x_1 + 4x_2 + 3x_3 \\ x_1, x_2, x_3, x_4, x_5, x_6 \geq 0 \end{cases}$$

New variables are called *slack variables*

Optimal solution remains optimal for the new problem

Slack Variables

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\text{s.t.} \quad \begin{cases} x_4 = 5 - 2x_1 - 3x_2 - x_3 \\ x_5 = 11 - 4x_1 - x_2 - 2x_3 \\ x_6 = 8 - 3x_1 - 4x_2 - 2x_3 \\ z = 0 + 5x_1 + 4x_2 + 3x_3 \\ x_1, x_2, x_3, x_4, x_5, x_6 \geq 0 \end{cases}
$$

New variables are called *slack variables*

Optimal solution remains optimal for the new problem

The Simplex Strategy

- Start with a feasible solution
  - For our example, assign 0 to all original variables
    - $x_1 \mapsto 0, x_2 \mapsto 0, x_3 \mapsto 0$
  - Assign the introduced vars their computed value
    - $x_4 \mapsto 5, x_5 \mapsto 11, x_6 \mapsto 8, z \mapsto 0$
- Iteratively improve the objective value
  - Go from $\boldsymbol{x}$ to $\boldsymbol{x}'$ only if $z(\boldsymbol{x}) \leq z(\boldsymbol{x}')$

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What can we improve here?

One option: make x_1 larger, leave x_2, x_3 unchanged

- $x_1 = 1 \Rightarrow x_4 = 3, x_5 = 7, x_6 = 1, z = 5$ ✓
- $x_1 = 2 \Rightarrow x_4 = 1, x_5 = 3, x_6 = 2, z = 10$ ✓
- $x_1 = 3 \Rightarrow x_4 = -1, \ldots$ ✗ no longer feasible!

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Moral of the story:

- Can't increase x_1 too much
- Increase it as much as possible, without compromising feasibility

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Select the tightest bound, $x_1 \le \frac{5}{2}$

- New assignment: $x_1 \mapsto \frac{5}{2}, x_2 \mapsto x_3 \mapsto x_4 \mapsto 0, x_5 \mapsto 1, x_6 \mapsto \frac{1}{2}, z \mapsto \frac{25}{2}$
- This indeed improves the value of z

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Currently,

$x_1 \mapsto \frac{5}{2}, x_2 \mapsto x_3 \mapsto x_4 \mapsto 0, x_5 \mapsto 1, x_6 \mapsto \frac{1}{2}, z \mapsto \frac{25}{2}$

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For the first iteration we had:

- A feasible solution ✓
- An equation system, where
  - variables with positive value are expressed in terms of variables with 0 value

Does the current equation system satisfy this property? No

Need to update the equations

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Isolate x_1, eliminate from right-hand-side

$$x_4 = 5 - 2x_1 - 3x_2 - x_3 \longrightarrow x_1 = \frac{5}{2} - \frac{3}{2}x_2 - \frac{1}{2}x_3 - \frac{1}{2}x_4$$

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Option 1: decrease x_2 or x_4
but we can't since $x_2, x_4 \geq 0$

Option 2: increase x_3
By how much?

x_3's bounds: $x_3 \leq 5, x_3 \leq \infty, x_3 \leq 1$

So we increase x_3 to 1

- New assignment: $x_1 \mapsto 2, x_2 \mapsto 0, x_3 \mapsto 1, x_4 \mapsto 0, x_5 \mapsto 0, x_6 \mapsto 0$
- This gives $z = 13$, which is again an improvement

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$$\begin{cases} x_1 = \frac{5}{2} - \frac{3}{2}x_2 - \frac{1}{2}x_3 - \frac{1}{2}x_4 \\ x_5 = 1 + 5x_2 + 2x_4 \\ x_6 = \frac{1}{2} + \frac{1}{2}x_2 - \frac{1}{2}x_3 + \frac{3}{2}x_4 \\ z = \frac{25}{2} - \frac{7}{2}x_2 + \frac{1}{2}x_3 - \frac{5}{2}x_4 \end{cases}$$

x_3's bounds: $x_3 \leq 5, x_3 \leq \infty, x_3 \leq 1$

So we increase x_3 to 1

- New assignment: $x_1 \mapsto 2, x_2 \mapsto 0, x_3 \mapsto 1, x_4 \mapsto 0, x_5 \mapsto 0, x_6 \mapsto 0$
- This gives $z = 13$, which is again an improvement

The Simplex Strategy

$$x_1 \mapsto \tfrac{5}{2}, x_2 \mapsto 0, x_3 \mapsto 0, x_4 \mapsto 0$$

How can we improve z further?

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The Simplex Strategy

Analogously to before, we switch x_6 and x_3, and eliminate x_3 from the right-hand sides

$$\begin{cases} x_1 = \frac{5}{2} - \frac{3}{2}x_2 - \frac{1}{2}x_3 - \frac{1}{2}x_4 \\ x_5 = 1 + 5x_2 \qquad\qquad + 2x_4 \\ x_6 = \frac{1}{2} + \frac{1}{2}x_2 - \frac{1}{2}x_3 + \frac{3}{2}x_4 \\ z = \frac{25}{2} - \frac{7}{2}x_2 + \frac{1}{2}x_3 - \frac{5}{2}x_4 \end{cases} \longrightarrow \begin{cases} x_1 = 2 - 2x_2 - 2x_4 + x_6 \\ x_5 = 1 + 5x_2 + 2x_4 \\ x_3 = 1 + x_2 + 3x_4 - 2x_6 \\ z = 13 - 3x_2 - x_4 - x_6 \end{cases}$$

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Can we improve z again?

- No, because $x_2, x_4, x_6 \geq 0$ and
- all appear with negative signs in the objective function

So we are done, and the optimal value of z is 13

The optimal solution is then $x_1 \mapsto 2, x_2 \mapsto 0, x_3 \mapsto 1$

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The Simplex Algorithm

$$\text{maximize} \quad \sum_{j=1}^{n} c_j x_j$$

$$\text{s.t.} \quad \sum_{j=1}^{n} a_{ij} x_j \leq b_i \quad \text{for } i = 1, \ldots, m$$

$$x_j \geq 0 \quad \text{for } j = 1, \ldots, n$$

1. Introduce slack variables $x_{n+1}, \ldots, x_{n+m}$
2. Set $x_{n+i} = b_i - \sum_{j=1}^{n} a_{ij} x_j$ for $i = 1, \ldots, m$
3. Start with initial, feasible solution ($x_1 \mapsto 0, \ldots, x_n \mapsto 0$ in our example)
4. If some addends in the current objective function have positive coefficients, update the feasible solution to improve the objective value; otherwise, stop
5. Update the equations to maintain the invariant that all right-hand side vars have value 0
6. Go to step 4

Updating the Equations: Pivoting

As we progress towards the optimal solution, equations are updated

This computational process of constructing the new equation system is called *pivoting*

$$\begin{cases} x_4 = 5 - 2x_1 - 3x_2 - x_3 \\ x_5 = 11 - 4x_1 - x_2 - 2x_3 \\ x_6 = 8 - 3x_1 - 4x_2 - 2x_3 \\ z = 5x_1 + 4x_2 + 3x_3 \end{cases}$$

Invariants:

- Number of equations (m) never changes
- Variables are either on the left-hand side or the right-hand side, never both
  - Left-hand side variables are called *basic*
  - Right-hand side variables are called *non-basic*
- Non-basic variables always pressed against their bounds (always 0)
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The set of basic variables is the *basis*

In the pivoting step:

- A non-basic variable enters the basis (the *entering* variable)
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How is the entering variable chosen? To increase the value of z

One strategy (*Dantzig's rule*) picks the variable with the largest coefficient

How is the leaving variable chosen? To maintain feasibility

Select the basic variable corresponding to the tightest upper-bound

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Tableau and Implementation

We have presented the equation system as a *dictionary*

A more popular version uses a matrix, or a *tableau*:

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3	4	2	1	0	1	0	8
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The pivoting process can be understood as a series of matrix operations

See [Guoqing Hu] for a description and example

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Some Challenges

Possible problems of the procedure that we described so far:

- **Initialization**: how to obtain an initial feasible solution?
- **Termination**: can we generate an infinite sequence of dictionaries, without reaching an optimal z?

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Challenges: initialization

$$\begin{aligned} \text{maximize} \quad & \sum_{j=1}^{n} c_j x_j \\ \text{s.t.} \quad & \sum_{j=1}^{n} a_{ij} x_j \le b_i \quad \text{for } i = 1, \dots, m \\ & x_j \ge 0 \quad \text{for } j = 1, \dots, n \end{aligned}$$

Easy when all b_i's are non-negative (set all x_j to 0)

What can we do for negative b_i's?

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Solution: switch to an auxiliary problem with a known feasible solution

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For the auxiliary problem, a feasible solution is easy to find:

set $x_1, \ldots, x_n$ to 0, and make x_0 sufficiently large

Original problem is feasible iff the optimal solution for the auxiliary problem has $x_0 \mapsto 0$

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Initialization: example

$$
\text{maximize} \quad x_1 + 2x_2 \qquad \text{s.t.} \quad \begin{cases} 2x_1 - 3x_2 \le -2 \\ 4x_1 - x_2 \le -4 \\ x_1, x_2 \ge 0 \end{cases}
\quad \longrightarrow \quad
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The dictionary of the auxiliary problem:

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\begin{aligned} x_3 &= -2 - 2x_1 + 3x_2 + x_0 \\ x_4 &= -4 - 4x_1 + x_2 + x_0 \\ z &= -x_0 \end{aligned}
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Initial feasible solution: $x_0 \mapsto 4, x_1 \mapsto 0, x_2 \mapsto 0$

Any issues? Variables on the right-hand side need to be 0

Solution: perform a pivot step to move x_0 into the basis

$$
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Initialization: example

$$\text{maximize} \quad x_1 + 2x_2 \qquad \text{s.t.} \begin{cases} 2x_1 - 3x_2 & \leq -2 \\ 4x_1 - x_2 & \leq -4 \\ x_1, x_2 & \geq 0 \end{cases}$$

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Initial feasible solution: $x_0 \mapsto 4, x_1 \mapsto 0, x_2 \mapsto 0$

Any issues? Variables on the right-hand side need to be 0

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Challenges: Termination

Recall the goal of every iteration is to increase the objective function z

In each pivoting step, we swap a non-basic variable with a basic variable:

- The non-basic (entering) variable has a positive coefficient in the objective function
- If no such variable exists, the objective function is optimal and we can stop
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An iteration will never make z worse

So when might we not converge to the optimal z?

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The simplex method fails to terminate iff it cycles, i.e., it generates the same dictionary infinitely often.

Proof sketch:

1. There are only finitely many bases;
2. each bases uniquely defines the dictionary;
3. therefore, there are only finitely many values of z to try

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Degenerate Pivots

Example: Current feasible solution: $x_1 \mapsto 0, x_2 \mapsto 0, x_3 \mapsto 0, x_4 \mapsto 0$

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\begin{aligned}
x_1 &= -2x_2 + 3x_3 \\
z &= 5x_2 - x_3 + 4x_4
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Dantzig's rule: pick x_2 as the entering variable

Leaving variable is x_1, but the highest x_2 can be is 0

So the value of z does not change after switching x_1 and x_2

A pivot is *degenerate* if it does not change the objective value

Cycling can only occur in the presence of a degenerate pivot

Note: Degenerate pivots are empirically rare

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There are variable selection strategies that guarantee termination

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Example: $z = -5x_1 - 3x_2 + 4x_3 + 40x_4$

The entering variable is: x_3

Leaving variable: still the one imposing the tightest constraint, but break tie by picking the smaller subscript

Pivoting Strategies

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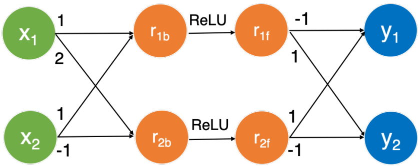
Complexity: the common strategies all have worse-case exponential time

Possible improvements

- More sophisticated pivoting strategy
- Use rational-number instead of floating-point representation
  (to handle numerical instability and avoid solutions unsoundness)
- Handle general Linear Programs
  (variables can have non-zero lower bounds and/or finite upper bounds)
- Extract irreducible infeasible subset in case of infeasibility
  (theory explanations)
- …

Application: Neural Network Verification



Property to verify: $\forall x_1 . x_2 . (x_1 \in [-2, 1] \wedge x_2 \in [-2, 2] \Rightarrow y_1 < y_2)$

1. Encoding of the neural network α_n (linear + Rectified Linear Units):

$$r_{1b} = x_1 + x_2 \quad r_{2b} = 2x_1 - x_2 \qquad (r_{1b} \leq 0 \wedge r_{1f} = 0) \vee (r_{1b} \geq 0 \wedge r_{1f} = r_{1b})$$

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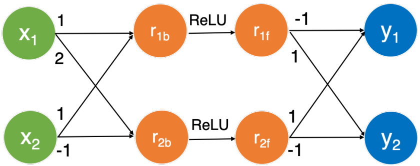

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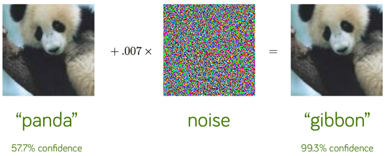
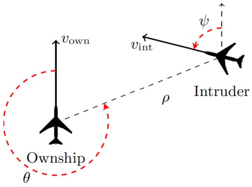
Practical properties

Robustness: $\forall x'.\ \|\mathbf{x} - x'\| < \epsilon \Rightarrow \|N(\mathbf{x}) - N(x')\| < \delta$



There is no adversarial input within ϵ distance

Reachability: $\forall x.\ x \in [x_l, x_u] \Rightarrow y \in [y_l, y_u]$



Whenever intruder is near and to the right advise strong left

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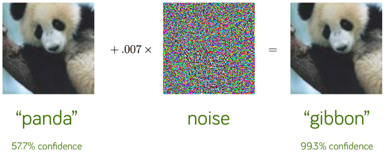

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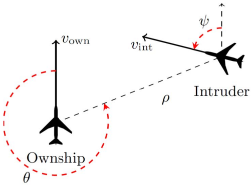

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