

Modeling with mixed-integer nonlinear programs
Summer School on Nonlinear Optimization with Mixed Integer and
Complementarity Constraints

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Modeling with mixed-integer nonlinear programs

- 1 Objective Function and Constraints
- 2 Convexity in Mixed-Integer Nonlinear Optimization
- 3 Basic Nonlinear Modeling Tips
- 4 Modeling with Integer Variables
- 5 Summary and Take-Away Points

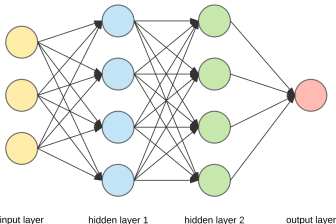
Objective Function and Constraints

Optimization

Art of finding a best solution from collection alternatives under (physical) constraints.

Everyone optimizes: application in ...

- Science: design of experiments
- Engineering: power-grid control and design
- Finance: pricing of options, optimal portfolio
- Medicine: optimal radiation dose design
- Economics: optimal transition to clean energy
- AI/ML: machine learning ... training LLMs



Objective Function and Constraints (Simplified)

Ingredients of Optimization

- **Decision Variables**, x, y : model (free) decisions.
- **Constraints**: model acceptable values ... **general constraints**, $l \leq g(x, y), u$
- **Objective(s)**: model our goals / performance measure.

minimize	$f(x, y)$	objective function
	x, y	
subject to	$g(x, y) \leq 0$	nonlinear constraints
	$y \in \mathbb{Z}^p$	integer decisions

- Variables: $(x, y) \in \mathbb{R}^n \times \mathbb{Z}^p$
- Objective: $f(x, y)$ function $f : \mathbb{R}^n \times \mathbb{Z}^p \rightarrow \mathbb{R}$ smooth
- Constraints: $g(x, y)$ functions $g_i : \mathbb{R}^n \times \mathbb{Z}^p \rightarrow \mathbb{R}$, for $i = 1, \dots, m$ smooth

Objective Function and Constraints

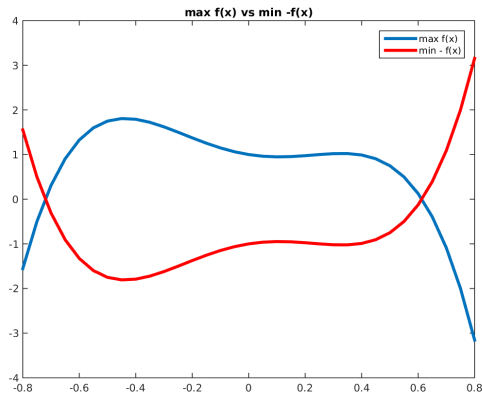
$$\begin{array}{ll}\underset{x,y}{\text{minimize}} & f(x,y) \\ \text{subject to} & g(x,y) \leq 0 \\ & y \in \mathbb{Z}^p\end{array}$$

objective function
nonlinear constraints
integer decisions

To Minimize or To Maximize?

$\max f(x)$ equivalent to $-\min(-f(x))$

... wlog only consider minimization



MINLP Modeling Practices

Modeling plays a fundamental role in MILP see [[Williams, 1999](#)]

... even more important in MINLP

- MINLP combines integer and nonlinear formulations
- Reformulations of nonlinear relationships can be convex
- Interactions of nonlinear functions and binary variables
- Sometimes we can linearize expressions

MINLP Modeling Preference

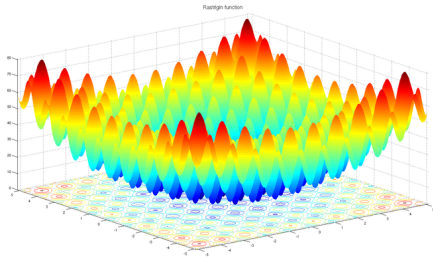
We prefer linear over convex over nonconvex formulations (more later).

Synonyms: **MINLP** = **MINLP** Mixed-Integer Nonlinear Programming/Optimization

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The Importance of Being Convex

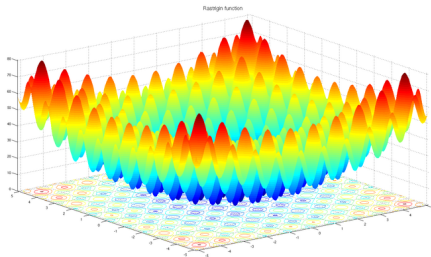


2D Rastrigin Test Function

Not All Solvers Are Equal

Without convexity, many solvers only guarantee **local optimality**

The Importance of Being Convex



2D Rastrigin Test Function

Not All Solvers Are Equal

Without convexity, many solvers only guarantee **local optimality**

Impact of Convexity

- Nonconvex MINLPs are **much harder** to solve ... later in course.
- May not be able to “prove” global optimality ... OK in practice
- Make sure you really need nonconvexity in your MINLP ... reformulate!

Feasible Points, Local, and Global Minima

Consider (compact) mixed-integer nonlinear optimization problem

$$\begin{array}{lll} \underset{x,y}{\text{minimize}} & f(x,y) & \text{objective function} \\ \text{subject to} & g(x,y) \leq 0 & \text{nonlinear constraints} \\ & y \in \mathbb{Z}^p & \text{integers} \end{array}$$

Definition: Feasible Point

A point $(\hat{x}, \hat{y}) \in \mathbb{R}^n \times \mathbb{Z}^p$ is **feasible** if-and-only-if (iff)

$$g(\hat{x}, \hat{y}) \leq 0$$

The **feasible set of MINLP** is denoted by $\mathcal{F} := \{(x, y) \in \mathbb{R}^n \times \mathbb{Z}^p : g(x, y) \leq 0\}$

Feasible Points, Local, and Global Minima

Consider (compact) mixed-integer nonlinear optimization problem

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Definition: Local and Global Minima

① A feasible point $(\hat{x}, \hat{y}) \in \mathbb{R}^n \times \mathbb{Z}^p$ is a **local minimum** iff

$$\exists \text{ neighborhood } \mathcal{N}(\hat{x}, \hat{y}) : f(\hat{x}, \hat{y}) \leq f(x, y), \quad \forall (x, y) \in \mathcal{F} \cap \mathcal{N}(\hat{x}, \hat{y})$$

② A feasible point $(\hat{x}, \hat{y}) \in \mathbb{R}^n \times \mathbb{Z}^p$ is a **global minimum** iff

$$f(\hat{x}, \hat{y}) \leq f(x, y), \quad \forall (x, y) \in \mathcal{F}$$

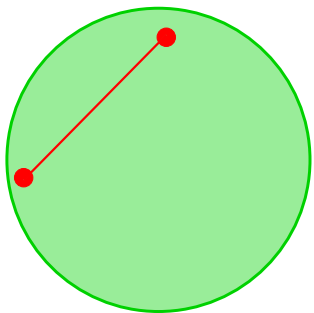
Convexity

Definition (Convex Set)

Set $\mathcal{S} \subset \mathbb{R}^n$ is **convex**, iff

$$x^{(0)}, x^{(1)} \in \mathcal{S} \Rightarrow (1 - \theta)x^{(0)} + \theta x^{(1)} \in \mathcal{S}, \quad \forall \theta \in [0, 1]$$

Set is **convex**, if **for any two points in set, line between points also lies in set.**



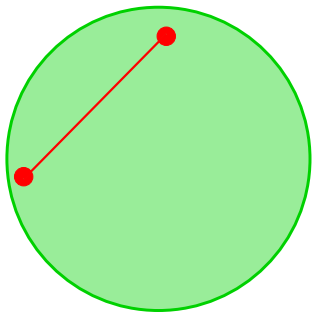
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Nonconvex



Convex

Examples of Convex Sets

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Examples of convex sets

- $\emptyset, \mathbb{R}^n$, single point, line, hyperplane ($a^T x = b$)
- Half-spaces are convex: $a^T x \geq b \Rightarrow$ any linear feasible set is convex
- Given $\hat{x} \in \mathbb{R}^n$, the ball, $\|x - \hat{x}\| \leq r$ is convex
- $\mathcal{S}_i \subset \mathbb{R}^n, i = 1, \dots, m$ convex $\Rightarrow$ intersection $\mathcal{S} = \bigcap_{i=1}^m \mathcal{S}_i$ also convex

Warning: Union of convex sets NOT convex

Example: Coordinate axis $\{x_1 = 0\} \cup \{x_2 = 0\}$ **not** convex

Convex Combination and Convex Hull

Definition (Convex Combination and Convex Hull)

- For $x^{(1)}, \dots, x^{(m)} \in \mathbb{R}^n$, the point

$$x_\lambda := \sum_{i=1}^m \lambda_i x^{(i)}, \quad \text{with } \sum_{i=1}^m \lambda_i = 1, \lambda_i \geq 0$$

is **convex combination** of $x^{(1)}, \dots, x^{(m)}$

- Convex hull, $\text{conv}(\mathcal{S})$** , of set $\mathcal{S} \subset \mathbb{R}^n$ is set of all convex combinations of all points in $\mathcal{S}$:

$$\left\{ x = \sum_{i=1}^n \lambda_i x^{(i)} \quad \text{with } \sum_{i=1}^m \lambda_i = 1, \lambda_i \geq 0, x^{(i)} \in \mathcal{S} \right\}$$

In $\mathbb{R}^2$, put nails into points, then snap rubber band around nails to get convex hull.

Feasible Set of a Linear or Quadratic Optimization Problem

Theorem (Convexity of Linear Feasible Sets)

Feasible set of a linear optimization problem is convex: $\mathcal{F}_{LP} := \{x \mid Ax = b, x \geq 0\}$

Proof. Let $x^{(0)}, x^{(1)} \in \mathcal{F}_{LP}$ and $\theta \in [0, 1]$

$\Rightarrow (1 - \theta)x^{(0)} + \theta x^{(1)} \geq 0$, because $x^{(0)}, x^{(1)} \geq 0, \theta, 1 - \theta \geq 0$

Now consider linear constraints:

$$A((1 - \theta)x^{(0)} + \theta x^{(1)}) = (1 - \theta)Ax^{(0)} + \theta Ax^{(1)} = (1 - \theta)b + \theta b = b$$

because $x^{(0)}, x^{(1)} \in \mathcal{F}_{LP}$ satisfy $Ax = b$.

Thus, we conclude that $(1 - \theta)x^{(0)} + \theta x^{(1)} \in \mathcal{F}_{LP}$

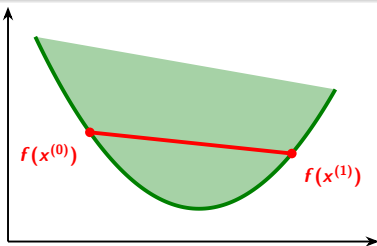


Convex Functions

Definition (Convex Function)

$f(x)$ is a **convex function**, iff its epigraph is convex set:

$$\Leftrightarrow f((1 - \theta)x^{(0)} + \theta x^{(1)}) \leq (1 - \theta)f(x^{(0)}) + \theta f(x^{(1)}), \quad \forall \theta \in [0, 1]$$

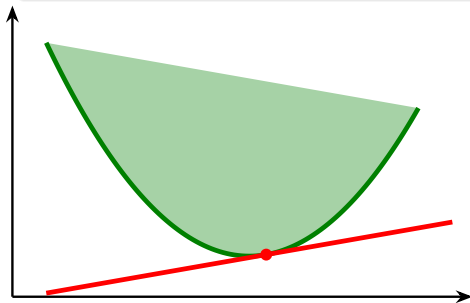


Alternative Definition of Convex Functions

Definition (Convex Differentiable Function)

$f(x)$ differentiable is **convex**, iff any tangent is supporting hyperplane:

$$f(x^{(1)}) \geq f(x^{(0)}) + (x^{(1)} - x^{(0)})^T \nabla f(x^{(0)})$$



$$f(x^{(0)}) + \nabla f(x^{(0)})^T (x - x^{(0)})$$

Examples of Convex Functions

- Linear functions: $a^T x + b$
- $f(x)$ with pos. semi-definite Hessian
- Norms, $\|x\|$
- Convex combinations of convex $f_i(x)$

Convex Programming Problem

Convex Programming Problem **note only continuous variables, x**

$$\begin{array}{ll}\underset{x}{\text{minimize}} & f(x) \\ \text{subject to} & g(x) \leq 0,\end{array}$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ convex functions.

Theorem (Global Solution of Convex Programs)

- *Local solution x^* of convex program is global solution.*
- *The set of global solutions is convex.*

Theorem (First-Order Conditions are Necessary and Sufficient)

KKT conditions are necessary and sufficient for a global minimum of a convex program.

Proofs. Later.

MINLP Specializations

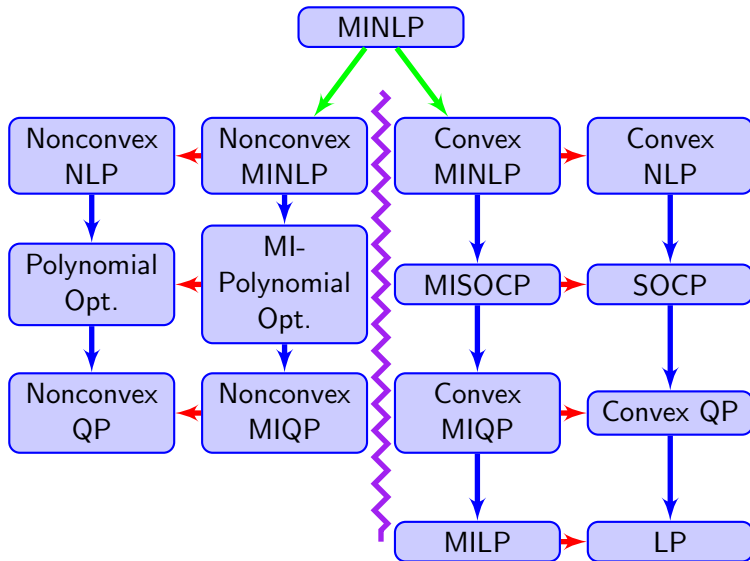
Compact MINLP

$$\underset{x,y}{\text{minimize}} \quad f(x,y) \quad \text{subject to} \quad g(x,y) \leq 0, \quad y \in \mathbb{Z}^p$$

Specializations:

- MISOCP: **Mixed Integer Second Order Cone Program**
 - **Convex**-MINLP with $g_i(x,y) = \|A_i x + b_i\|_2 - p_i^T x + q_i + r_i^T y$
- MIPP: **Mixed Integer Polynomial Program**: $g_i(x)$ polynomial
- MIQP: **Mixed Integer Quadratic Program**
 - May be convex or nonconvex: $g_i(x,y) = x^T Q_i x + p_i^T x + q_i + r_i^T y$
 - Convex MIQP is a special case of MISOCP, if $Q_i \succeq 0$
 - If f is convex quadratic and g is an affine mapping, then there are specialized algorithms for convex-MIQP
- MILP: **Mixed Integer Linear Program**
 - Most efficient solvers: $g_i(x,y) = a_i^T x + b_i^T y - c_i$

MINLO/MINLP Tree



Source: Jeff Linderoth

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Some Useful Nonlinear Variable Transformations

Design of multiproduct batch plant includes nonconvex terms

$$\min \sum_{j \in M} \alpha_j N_j V_j^{\beta_j}; \quad C_i N_j \geq \tau_{ij}; \quad \sum_{i \in N} \frac{\psi_i}{B_i} C_i \leq \gamma$$

where variables are upper case, parameters are Greek letters.

Introduce log-transform variables:

$$v_j = \ln(V_j), \quad n_j = \ln(N_j), \quad b_i = \ln(B_i), \quad c_i = \ln(C_i)$$

Transformed expressions are convex (exercise):

$$\min \sum_{j \in M} \alpha_j e^{n_j + \beta_j v_j}, \quad c_i + n_j \geq \ln(\tau_{ij}), \quad \sum_{i \in N} \psi_i e^{c_i - b_i} \leq \gamma$$

Mini Exercise

Exercise (Convexity of batch-plant transformations)

Consider the transformation used in batch-plant design:

$$\min \sum_{j \in M} \alpha_j e^{n_j + \beta_j v_j}, \quad c_i + n_j \geq \ln(\tau_{ij}), \quad \sum_{i \in N} \psi_i e^{c_i - b_i} \leq \gamma$$

Show that these expressions are convex in the new variables, n_j, v_j, c_i, b_i

Some Useful Rules of Thumb for Modeling

- **Keep it simple!** Reformulate nonlinear (rational) constraint:

$$\frac{3x_1 + 2x_2}{4x_3 - 2x_4} \leq 7 \quad \Leftrightarrow \quad 3x_1 + 2x_2 \leq 7(4x_3 - 2x_4)$$

Rational function in general **nonconvex** ... affine constraint **convex**

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Rational function in general **nonconvex** ... affine constraint **convex**

- **Keep lean!** Prefer small coefficients ...

$$12x_1 + 24x_2 \geq 18 \quad \Leftrightarrow \quad 2x_1 + 4x_2 \geq 3$$

We prefer linear or affine constraints!

Ensure convexity & efficient solves

See also [[Levy, 2022](#)]

Keep Constraints Simple: Help Your Solvers!

Solve nonlinear optimizations problems ...

$$\min_x f(x) \quad \text{s.t. } g(x) = 0, A^T x = b, x \geq 0$$

... iteratively (e.g. Newton's method) ... iterates $x^{(k)}, k = 1, 2, \dots$

Not all constraints are equal

Constraint satisfaction by constraint type at iterates $x^{(k)}, k = 1, 2, \dots$:

- Simple bounds hold (almost) exactly: $x^{(k)} \geq 0, \forall k$
- Linear constraints hold accurately: $\|A^T x - b\| \leq \kappa$, for $\kappa > 0$ unit round-off
- Nonlinear constraints hold in limit: $\lim_{k \rightarrow \infty} g(x^{(k)}) = 0$ only

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Exercise (Mini-Exercise)

How would you safeguard $\log(x_2^3 + 1) + 2x_1 \leq 0$ against IEEE exceptions?

The Good, The Bad, and The Ugly ... Constraint

The Ugly Constraint:

$$\log(x_2^3 + 1) + 2x_1 \leq 0$$

... log undefined for negative arguments, e.g. $x_2 < -1$

The Good, The Bad, and The Ugly ... Constraint

The Ugly Constraint:

$$\log(x_2^3 + 1) + 2x_1 \leq 0$$

... $\log$ undefined for negative arguments, e.g. $x_2 < -1$

The Bad Reformulation:

$$\log(x_2^3 + 1) + 2x_1 \leq 0, \quad x_2^3 + 1 \geq 0$$

... $x_2^3 + 1 \geq 0$... may not hold for all iterates

The Good, The Bad, and The Ugly ... Constraint

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The Bad Reformulation:

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... $x_2^3 + 1 \geq 0$... may not hold for all iterates

The Good Formulation:

$$\log(s) + 2x_1 \leq 0, \quad s = x_2^3 + 1, \quad s \geq 0$$

... solvers ensure $s \geq 0$ for all iterates

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Modeling with Integer Variables

Linderoth “Fundamental Theorem of Integer Variables”

97.238% of MINLPs have integer variables for two purposes only:

- 1 Binary variables to make a “multiple choice” selection
- 2 Binary indicator variables that turn on/off continuous variables and/or constraints.

1 Multiple Choice Selection

$$d \in \{D_1, D_2, \dots, D_k\}$$

where D_i are discrete parameters (e.g. pipe diameters)

2 Indicator Variables

if $y_i = 1$ then $g_i(x) \leq 0$, otherwise $g_i(x) \leq \infty$ not enforced

Modeling Multiple Choice Selection

Discrete Choices

Model $d \in \{D_1, D_2, \dots, D_k\}$, where D_i discrete parameters as special ordered set (SOS) [Beale and Tomlin, 1970]

$$d = \sum_{i=1}^k y_i D_i, \quad 1 = \sum_{i=1}^k y_i, \quad y_i \in \{0, 1\}$$

- Similarly linearize univariate functions $f(y)$, $y \in \mathbb{Z}$
- Generalizes to higher dimensions, [Beale and Forrest, 1976]
- Solvers detect SOS structure and use special branching rules

Multiple Choice Selection as Linearization Trick

Consider modeling pipe diameter in a water network $d \in \{D_1, D_2, \dots, D_k\}$ with

$$d_{ijl} = \sum_{l=1}^k y_{ijl} D_l, \quad 1 = \sum_{l=1}^k y_{ijl}, \quad y_{ijl} \in \{0, 1\}$$

Pressure drop along arc (i, j) in water networks (Weymouth equation)

$$h_i - h_j = 10^{-3} D_{ij} \frac{|q_{ij}|^{4.33} q_{ij}}{d_{ij}^2}$$

where D_{ij} distance between nodes i, j

- h_i, h_j head/height (pressure) at nodes i, j
- q_{ij} flow on arc (i, j)
- d_{ij} diameter of arc (i, j)

Exercise (Water Network Model)

Can you linearize the expression $1/d_{ij}^2$ using the SOS1?

Multiple Choice Selection as Linearization Trick

SOS-1 model of pipe diameters

$$d_{ij} = \sum_{l=1}^k y_{ijl} D_l, \quad 1 = \sum_{l=1}^k y_{ijl}, \quad y_{ijl} \in \{0, 1\}$$

Define function $f(d_{ij}) = 1/(d_{ij}^2)$

Multiple Choice Selection as Linearization Trick

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Define function $f(d_{ij}) = 1/(d_{ij}^2)$

Pre-compute constants $1/(D_l^2), l = 1, \dots, k$... then

Multiple Choice Selection as Linearization Trick

SOS-1 model of pipe diameters

$$d_{ij} = \sum_{l=1}^k y_{ijl} D_l, \quad 1 = \sum_{l=1}^k y_{ijl}, \quad y_{ijl} \in \{0, 1\}$$

Define function $f(d_{ij}) = 1/(d_{ij}^2)$

Pre-compute constants $1/(D_l^2), l = 1, \dots, k \dots$ then

$$f(d_{ij}) = \frac{1}{d_{ij}^2} = \frac{1}{\left(\sum_{l=1}^k y_{ijl} D_l\right)^2} = \sum_{l=1}^k y_{ijl} \frac{1}{D_l^2}$$

... because exactly one y_{ijl} is equal one (“one-hot-encoding”)

Pressure drop along arc (i, j) in water networks (Weymouth equation)

$$h_i - h_j = 10^{-3} D_{ij} \frac{|q_{ij}|^{4.33} q_{ij}}{d_{ij}^2} = 10^{-3} D_{ij} |q_{ij}|^{4.33} q_{ij} \left(\sum_{l=1}^k y_{ijl} D_l^{-2} \right)$$

Calculus of Logical Modeling: Indicator Variables

Recall ...

Indicator Variable

$y_i \in \{0, 1\}$ to force a constraint to hold

$$y_i = 1 \Rightarrow g_i(x) \leq 0$$

can be modeled as

$$y_i \in \{0, 1\} \quad \text{and} \quad g_i(x) \leq M(1 - y_i)$$

where $M > 0$ is known upper bound on $g_i(x)$ for $x \in \mathcal{X}$

Never Multiply a Constraint by Binary Variable

Bad formulation: $y_i g_i(x) \leq 0$... violates constraint qualification

Calculus of Logical Modeling: Lookout Variables

The inverse of an indicator is a lookout

Lookout Variable

$y_i \in \{0, 1\}$ is forced if a constraint holds

$$a_i^T x + b_i \leq 0 \quad \Rightarrow \quad y_i = 1$$

can be modeled as

$$y_i \in \{0, 1\} \quad \text{and} \quad a_i^T x + b_i \geq (m - \epsilon)y_i$$

$m > 0$ lower bound on $a_i^T x + b_i$ for $x \in \mathcal{X}$, and $\epsilon > 0$ is tolerance tol (e.g. 10^{-4})

Both indicator and lookout variables have weak relaxations

Base Case of Induction to “Linderoth Theorem”

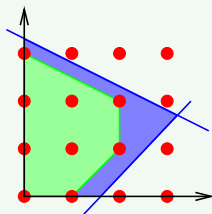
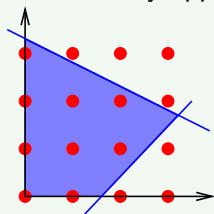
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Building on Years of MIP Expertise

- Mixed Integer **Linear** Programmers carefully study simple problem structures ... for “good” formulations of problems
- Goal: closely approximate convex hull of feasible points



... solve LP relaxation

Advanced Modeling: Summary and Take-Away Points

- Defined optimization problem & its ingredients:
 - ① Objective ... goal that we optimize
 - ② Variables ... decision variables
 - ③ Constraints ... restrictions on choices
- Convexity is **great divide** in optimization
 - ① Efficient and robust solvers for convex problems
 - ② Nonconvex problem much harder
- Nonlinear constraints are powerful modeling paradigm ...
... “with great power comes great responsibility” [Uncle Ben in Spiderman]
- Linear constraints are easier than nonlinear
- SOS-1 variables to model multiple choices (discrete)
- Indicator and Lookout variables
- **Never multiply a nonlinear function by a binary**



Beale, E. and Tomlin, J. (1970).

Special facilities in a general mathematical programming system for non-convex problems using ordered sets of variables.

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