CS498: Algorithmic Engineering

Lecture 7: TSP, MINLP, and Spatial-Branch and Bound.

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Outline

1. Case Study: Travelling Salesman Problem (TSP).
2. Mixed Integer Non Linear Programming (MINLP)
3. Limits of Uniform Linearization and Spatial Branch and Bound
4. Summary and Outlook

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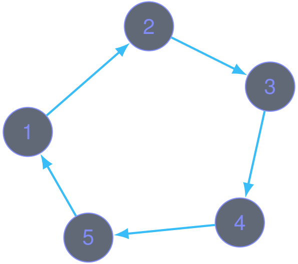
Motivation: The Traveling Salesman Problem (TSP)

The **Traveling Salesman Problem** (TSP) is a classic example that combines binary decisions and ordering.

Setup:

- A set of n cities with pairwise travel costs c_{ij}.
- A salesman must start at one city (say city 1), visit every other city exactly once, and return to the start.
- Goal: minimize total travel cost.



TSP with Arc Variables

Traveling Salesman Problem (TSP):

- n cities, travel costs c_{ij}.
- Binary arc variables $x_{ij} \in \{0, 1\}$:

$$x_{ij} = 1 \;\Leftrightarrow\; \text{tour goes directly from } i \text{ to } j.$$

Degree constraints:

$$\sum_{j \neq i} x_{ij} = 1, \qquad \sum_{j \neq i} x_{ji} = 1 \quad \text{for all } i.$$

These ensure each city has exactly one predecessor and one successor.

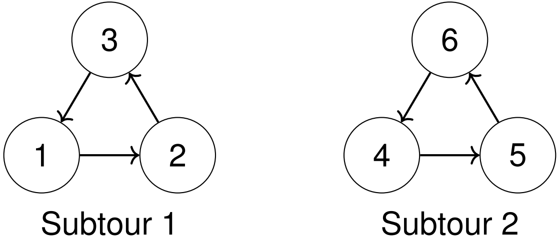
TSP Without Subtour Elimination

The degree constraints ensure:

$$\sum_{j \neq i} x_{ij} = 1, \quad \sum_{j \neq i} x_{ji} = 1$$

for every city i.

But these only make sure every node has one incoming and one outgoing edge, they do **not** guarantee all cities belong to a single tour.



Idea of MTZ (Miller-Tucker-Zemlin): Learn the Visit Order

Goal: forbid subtours by giving each city an *order* in the tour.
Introduce **continuous variables**:

$$u_i \in [1, n] \quad \text{for } i = 1, \ldots, n,$$

where u_i is the position of city i in the tour.

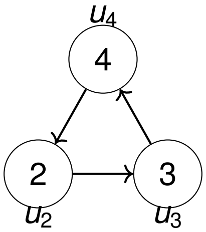
- If the tour goes from i to j ($x_{ij} = 1$), then city j must be visited *later* than city i.

$$x_{ij} = 1 \quad \Rightarrow \quad u_j \geq u_i + 1 \quad \forall i \neq j, i, j \in \{2, ..., n\}.$$

This is exactly a **logical implication** like our earlier patterns.

MTZ Eliminates Subtours (Not Involving City 1)

MTZ enforces a strictly increasing visit order along selected arcs *among cities* $\{2, \ldots, n\}$.



Along the subtour, MTZ requires:

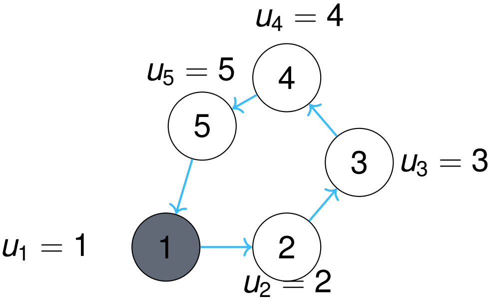
$$u_3 \geq u_2 + 1, \quad u_2 \geq u_4 + 1, \quad u_4 \geq u_3 + 1,$$

which is impossible.

Conclusion: MTZ forbids every cycle that does not include city 1.

Why the One Big Tour Is Still Allowed

City 1 is treated as a special anchor: no MTZ constraints on arcs involving city 1.



The increasing order holds along the tour, and the final arc back to city 1 is allowed because it is *not constrained by MTZ*.

Key point: MTZ eliminates all subtours, while deliberately allowing TSP cycles that pass through city 1.

From Implication to Big-M

Desired logic for each pair $i \neq j, i, j \in \{2, ..., n\}$:

$$x_{ij} = 1 \quad \Rightarrow \quad u_j \geq u_i + 1.$$

Rewrite as an inequality:

$$u_j - u_i - 1 \;\geq\; 0.$$

Now use the same Big-M pattern as before:

When the binary is 1, the inequality is enforced; when it is 0, it can be relaxed.

So we **gate** the inequality with x_{ij}:

$$u_j - u_i - 1 \;\geq\; -M(1 - x_{ij}).$$

- If $x_{ij} = 1$: we get $u_j - u_i - 1 \geq 0 \iff u_j \geq u_i + 1$.
- If $x_{ij} = 0$: $u_j - u_i - 1 \geq -M$, which has to be true if M is large enough.

Choosing M from Variable Bounds

We know $u_i \in [1, n]$ for $i = 1, \ldots, n$.
In the *relaxed* case $x_{ij} = 0$, the constraint is

$$u_j - u_i - 1 \geq -M.$$

Worst case (largest LHS violation) is when u_j is as small and u_i as large as possible:

$$u_j = 1, \quad u_i = n \quad \Rightarrow \quad u_j - u_i - 1 = 1 - n - 1 = -n.$$

To ensure this is always allowed when $x_{ij} = 0$, we need

$$-n \geq -M \quad \Rightarrow \quad M \geq n.$$

Final ILP Formulation: TSP with MTZ

Decision variables

$$x_{ij} \in \{0,1\} \quad (i \neq j) \qquad u_i \in [1,n] \quad (i = 1,\dots,n)$$

Objective: $\min \sum_{i \in V} \sum_{j \in V, j \neq i} c_{ij}\, x_{ij}$.

Degree constraints

$$\sum_{j \neq i} x_{ij} = 1, \qquad \sum_{j \neq i} x_{ji} = 1 \quad \forall i \in V$$

MTZ subtour elimination

$$u_j \;\geq\; u_i + 1 - n(1 - x_{ij}) \quad \forall i \neq j,\; i,j \in \{2,\dots,n\} \qquad u_1 = 1$$

Gurobi: TSP with MTZ Constraints

```
import gurobipy as gp
import numpy as np
n = 1000
V = range(n)              # cities 0,...,n-1
c = np.random.uniform(size=(n, n)) #random costs
m = gp.Model("TSP_MTZ")
x = m.addVars(V, V, vtype=gp.GRB.BINARY, name="x")
u = m.addVars(V, lb=1, ub=n, name="u")

# Objective
m.setObjective(gp.quicksum(c[i,j] * x[i,j] for i in V for j in V if i != j), gp.GRB.MINIMIZE)

# Degree constraints
for i in V:
    m.addConstr(gp.quicksum(x[i,j] for j in V if j != i) == 1)
    m.addConstr(gp.quicksum(x[j,i] for j in V if j != i) == 1)

# MTZ subtour elimination
for i in range(1, n):
    for j in range(1, n):
        if i != j: m.addConstr(u[j] >= u[i] + 1 - n * (1 - x[i,j]))

m.optimize()
```

A Note on Big-M vs Implication

I replaced these lines:

```
# MTZ subtour elimination
for i in range(1, n):
    for j in range(1, n):
        if i != j: m.addConstr(u[j] >= u[i] + 1 - n * (1 - x[i,j]))
```

With:

```
# MTZ subtour elimination
for i in range(1, n):
    for j in range(1, n):
        if i!=j: m.addConstr( (x[i,j]==1) >> (u[j]>=u[i]+1))
```

Same runtime! So why select M?

A Note on Big-M vs Implication

I replaced this line:

```
u = m.addVars(V, lb=1, ub=n, name="u")
```

With:

```
u = m.addVars(V, lb=1, ub=2*n, name="u")
```

Runtime went from 48 seconds ($<$ 1 minute) for carefully chosen $M = n$, to more than 10 minutes...

The Mystery: Why was Gurobi 10x Slower?

The Setup:

- **Manual Big-M with correct bounds:** Runs in ~ 1 minutes.
- **Indicator Constraint (‘$\gg$‘) with loose upper bound:** Runs in 10 minutes.

The Assumption: “Gurobi converts ‘$\gg$‘ to Big-M internally with the best M value, so they should be the same.”

The Reality

The assumption is wrong. Gurobi gets **Weak Bounds (The M Value)** and is conservative with how it chooses M.

Automatic M Selection

Scenario: Three resource variables with a budget constraint.

$$x_1, x_2, x_3 \in [0, 100]$$

Global Constraint: The sum cannot exceed 10.

$$x_1 + x_2 + x_3 \leq 10$$

Logical Requirement: If binary $z = 0$, then x_1 must be 0.

$$z = 0 \implies x_1 = 0 \quad (\text{modeled as } x_1 \leq M \cdot z)$$

1. Solver's View (Local) Gurobi looks at the variable object `x[1]`. Declared Upper Bound: 100. "Safe" $M = 100$.

2. Mathematician View (Global) You know $x_2, x_3 \geq 0$. Implied Upper Bound: 10. Tight $M = 10$.

Automatic M Selection

The Relaxation Gap (Suppose we want $x_1 = 5$)

- **Solver's** $M = 100$: $5 \leq 100z \implies z \geq$ **0.05**.
- **Engineer's** $M = 10$: $5 \leq 10z \implies z \geq$ **0.50**.

The solver allows z to be 10x smaller (weaker), creating a massive search tree.

In MTZ TSP. If we set $lb = 1, ub = n$, then using bound propagation gives $M = n$.

One way to check that is to run (before m.optimize()):

```
p = m.presolve()
p.write("presolved.lp") #This is a text file
R966526: 1000 x[967,459] - u[459] + u[967] <= 999 //ub=n
R966526: 2000 x[967,459] - u[459] + u[967] <= 1999 //ub=2n
```

What if we don't set *ub*?

```
u = m.addVars(V, lb=1, name="u")
```

Took longer than 12 hours and did not converge...

Gurobi cannot do bound propagation.

The hard-coded M converged, but after $\approx$ 1 hour (compare to 1 minute with properly set $ub = n$).

Engineering Takeaway: Explicit vs. Implicit

Rule of Thumb

- **Use Indicators ('$\gg$')** for:
  - "One-off" logical conditions (e.g., if factory opens, MinProduction $\geq$ 50).
  - Constraints that do not heavily impact the core combinatorial structure.
- **Use Manual Big-M** for:
- Core structural constraints (like TSP subtours, Network Flow).
- When you can derive a **tight** theoretical bound for M.
- When you need the solver to "see" the geometry for cuts (MIR, Gomory).

"Don't hide the geometry inside a logical wrapper."
"Always set lb and ub to be as tight as possible for your variables."

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Why MINLP?

Many real constraints are not linear:

- Power / energy: cost $\sim x^2$.
- Congestion: latency $\sim (\sum_i x_i)^2$.
- Mixing / quality: averages and ratios.
- Physics / finance: products and quotients everywhere.

Warm-up: Approximate a Curve with Line Segments

We want to model $y \approx f(x)$ on an interval $x \in [L, U]$. Choose breakpoints:

$$(x_0, f_0), (x_1, f_1), \ldots, (x_K, f_K)$$

Then approximate using linear segments between adjacent points.

Convex Combination Form (Core Pattern)

Introduce weights $\lambda_0, \ldots, \lambda_K$:

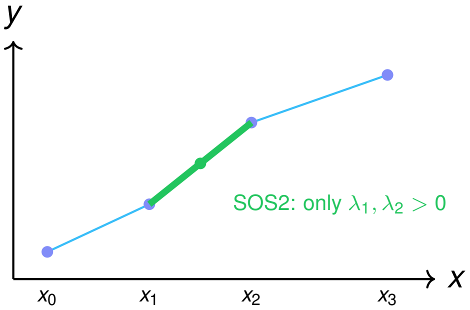
$$\lambda_k \geq 0, \qquad \sum_{k=0}^{K} \lambda_k = 1.$$

Enforce linear constraints:

$$x = \sum_{k=0}^{K} x_k \lambda_k, \qquad y = \sum_{k=0}^{K} f_k \lambda_k.$$

Missing rule: x must lie on *one segment*, not a mixture of far-apart points.
Enter SOS2: at most two adjacent λ_k are nonzero.

A Tiny Picture: PWL Approximation



Gurobi: Piecewise Linear via SOS2

```
import gurobipy as gp
from gurobipy import GRB

# Breakpoints for y ~ x^2 on [0, 4]
xs = [0, 1, 2, 3, 4]
ys = [x*x for x in xs]
m = gp.Model("pwl_square")

lam = m.addVars(len(xs), lb=0.0, name="lam")
x   = m.addVar(lb=0.0, ub=4.0, name="x")
y   = m.addVar(lb=0.0, name="y")

m.addConstr(gp.quicksum(lam[i] for i in range(len(xs))) == 1)
m.addConstr(x == gp.quicksum(xs[i] * lam[i] for i in range(len(xs))))
m.addConstr(y == gp.quicksum(ys[i] * lam[i] for i in range(len(xs))))

# SOS2: only two adjacent lambdas can be nonzero (ordered by xs)
m.addSOS(GRB.SOS_TYPE2, [lam[i] for i in range(len(xs))], xs)

# Example objective: minimize y subject to x >= 2.4 (forces interpolation)
m.addConstr(x >= 2.4)
m.setObjective(y, GRB.MINIMIZE)
m.optimize()
```

From x^2 to $x \cdot y$

Univariate: x^2 is already nonlinear.
Bivariate: $x \cdot y$ is the basic building block of *most* nonlinear models. Why?
Because once you can express products, you get:

- quadratic terms ($x^2 = x \cdot x$),
- interaction terms ($x_i x_j$),
- and much more complex expressions.

Bilinear Constraints as a Universal Modeling Language

Consider:

$$w = \frac{x + z^2}{x - y}.$$

Looks like: rational + quadratic + division $\Rightarrow$ hopeless?
Modeling trick: introduce variables for subexpressions.

Subexpression Variables

Introduce:

$$t = z^2, \qquad u = x + t, \qquad v = x - y.$$

Then:

$$w = \frac{u}{v}.$$

Ratios become bilinear constraints:

$$w = \frac{u}{v} \quad \Longleftrightarrow \quad u = w \cdot v.$$

Final Reformulation (Only Bilinear + Linear)

The original expression is equivalent to:

$$\begin{aligned} t &= z \cdot z, \\ u &= x + t, \\ v &= x - y, \\ u &= w \cdot v. \end{aligned}$$

Grid Linearization for $z \approx xy$ (Idea)

If $x \in [L_x, U_x]$ and $y \in [L_y, U_y]$:

- discretize x into K bins, y into K bins,
- select a cell using binaries,
- interpolate inside the cell (or use a bilinear plane per cell).

Cost: K in 1D becomes K^2 in 2D.
Small ϵ (high resolution) $\Rightarrow$ very large MILP.

Modeling Tradeoff: Accuracy vs Complexity

- PWL accuracy improves as segment length shrinks.
- But: number of variables/constraints grows quickly.

Rule of thumb:

$$\text{Model size} \approx (\text{resolution})^{-d}$$

where d is the number of continuous dimensions you linearize.

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Why Uniform Grids Are Wasteful

Uniform linearization spends the same resolution everywhere.
But the optimum typically lives in a tiny part of the domain:

- most cells/segments are never used,
- we pay the variable/constraint cost anyway.

Question: Can we refine only where it matters?

McCormick Envelopes on The Atomic Constraint: $z = xy$

Suppose:

$$x \in [L_x, U_x], \qquad y \in [L_y, U_y], \qquad z = xy.$$

The set $\{(x, y, z) : z = xy\}$ is nonconvex.
Solvers start with a convex outer approximation: **McCormick envelopes**.

McCormick Envelopes (4 Inequalities)

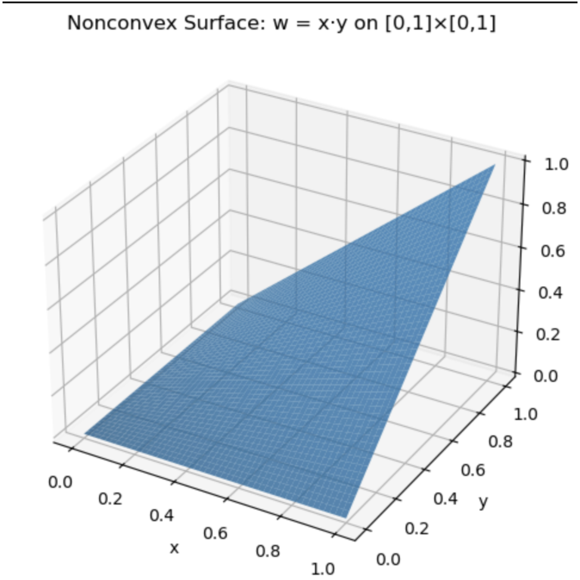
Define $z = xy$ with bounds $x \in [L_x, U_x]$, $y \in [L_y, U_y]$.
The convex hull relaxation over the box is:

$$
\begin{aligned}
z &\geq L_x y + L_y x - L_x L_y, \\
z &\geq U_x y + U_y x - U_x U_y, \\
z &\leq U_x y + L_y x - U_x L_y, \\
z &\leq L_x y + U_y x - L_x U_y.
\end{aligned}
$$

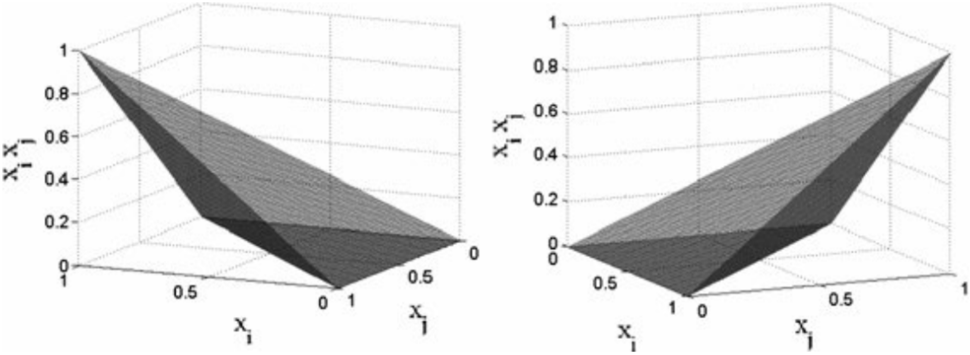
Interpretation:

- These are the tightest possible linear outer bounds on xy over the box.
- Still can be very loose when the box is large.

Geometry

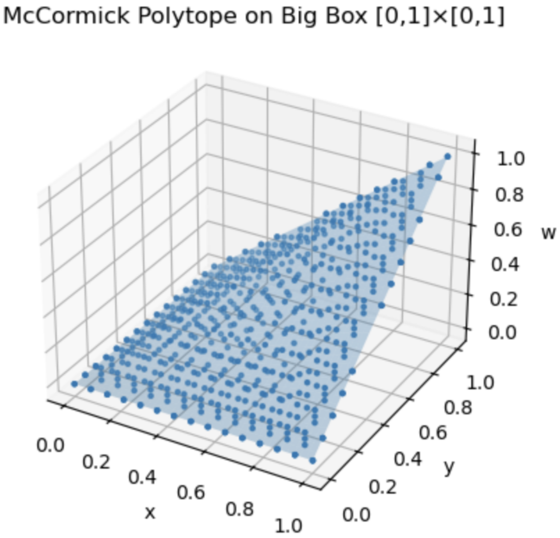

Nonconvex Surface: w = x·y on [0,1]×[0,1]
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
x
0.0
0.2
0.4
0.6
0.8
1.0
y

Geometry



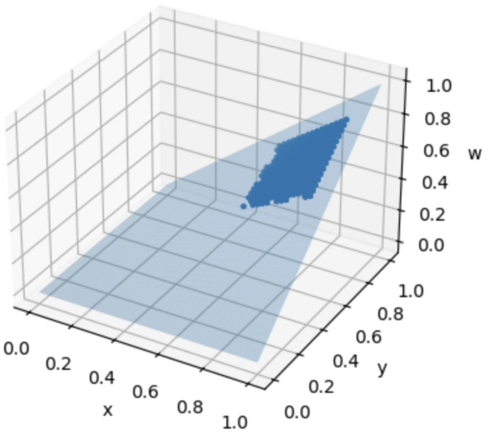
1
0.8
0.6
0.4
0.2
0
1
0.5
0
0
0.5
1
$x_i x_j$
x_i
x_j
1
0.8
0.6
0.4
0.2
0
0
0.5
1
0
0.5
1
$x_i x_j$
x_i
x_j

Geometry


McCormick Polytope on Big Box [0,1]×[0,1]
1.0
0.8
0.6
0.4
0.2
0.0
w
0.0
0.2
0.4
0.6
0.8
1.0
x
0.0
0.2
0.4
0.6
0.8
1.0
y

Geometry

McCormick Polytope on Small Box [0.6,0.9]×[0.6,0.9]



Spatial B&B: Adaptive Refinement of Bounds

If McCormick is loose over a big box, tighten it by splitting the box:

$$x \in [L_x, U_x] \Rightarrow [L_x, \frac{L_x + U_x}{2}] \cup [\frac{L_x + U_x}{2}, U_x].$$

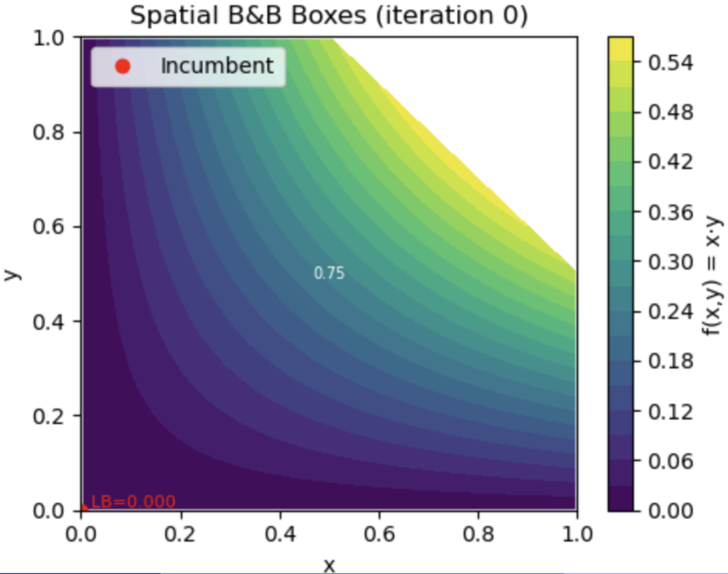
At each node:

- shrink variable bounds,
- rebuild McCormick envelopes on the smaller box for bi-linear terms,
- solve the resulting relaxation to get a bound,
- prune if bound is bad, or continue branching.

This is **branch-and-bound on continuous domains**. What Gurobi implements.

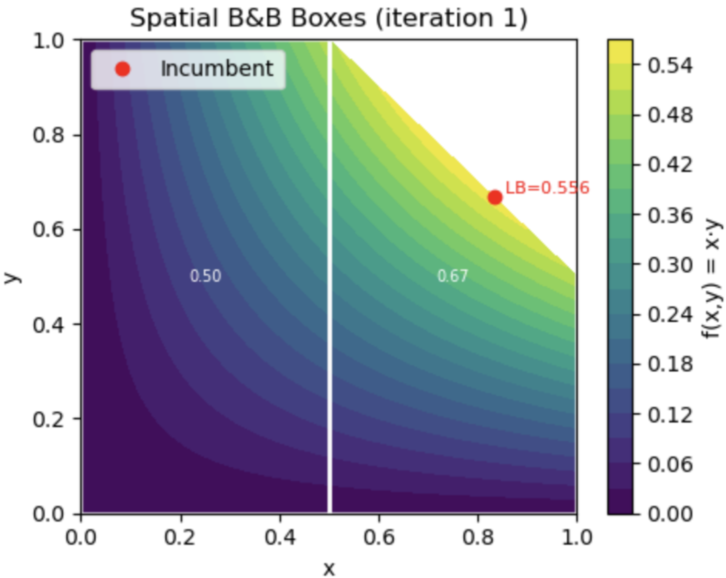
Example: $\max xy$ s.t $x + y \leq 1.5, 0 \leq x, y \leq 1$.

Geometry

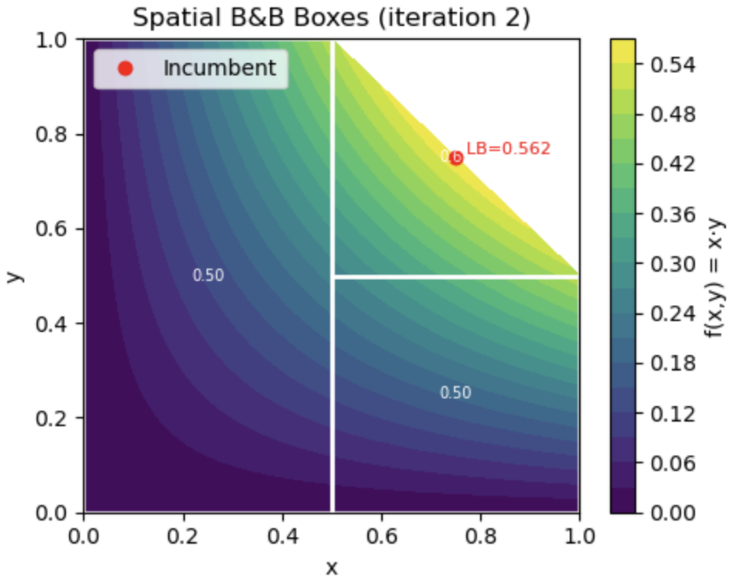


Spatial B&B Boxes (iteration 0)
Incumbent
0.75
LB=0.000
1.0
0.8
0.6
0.4
0.2
0.0
y
0.0
0.2
0.4
0.6
0.8
1.0
x
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry

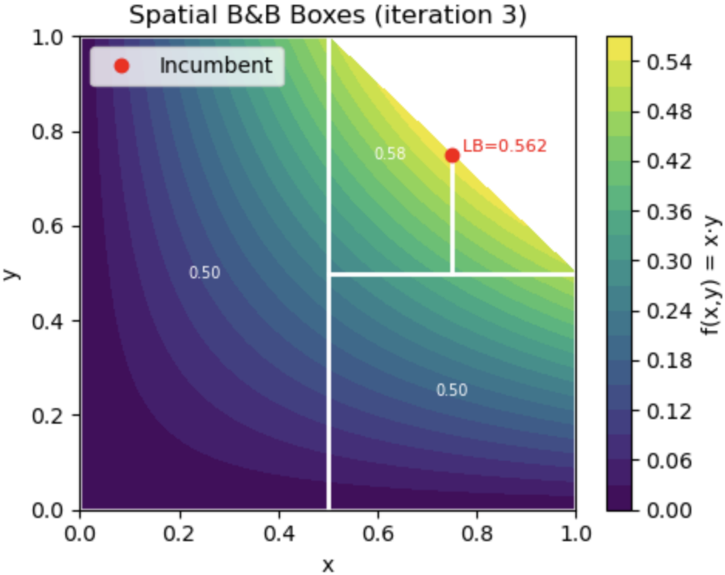

Spatial B&B Boxes (iteration 1)
Incumbent
LB=0.556
0.50
0.67
1.0
0.8
0.6
0.4
0.2
0.0
y
0.0
0.2
0.4
0.6
0.8
1.0
x
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry



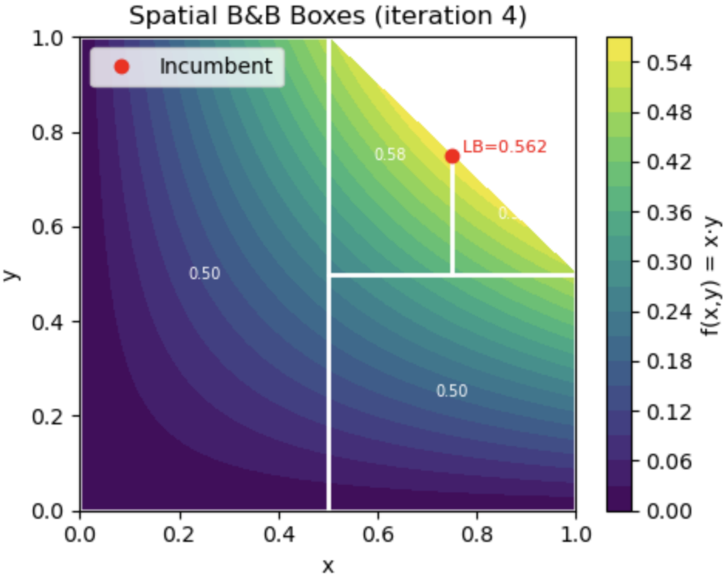
Spatial B&B Boxes (iteration 2)
Incumbent
LB=0.562
0.50
0.50
y
x
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry



Spatial B&B Boxes (iteration 3)
Incumbent
0.58
LB=0.562
0.50
0.50
1.0
0.8
0.6
0.4
0.2
0.0
y
0.0
0.2
0.4
0.6
0.8
1.0
x
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry



Spatial B&B Boxes (iteration 4)
Incumbent
LB=0.562
0.58
0.50
0.50
y
x
f(x,y) = x·y
0.0
0.2
0.4
0.6
0.8
1.0
0.00
0.06
0.12
0.18
0.24
0.30
0.36
0.42
0.48
0.54

Practical MINLP in Gurobi

Since version 9.0, Gurobi automates Spatial B&B. You do not need to implement McCormick envelopes manually.

The “NonConvex” Parameter

By default, Gurobi assumes quadratic constraints are **convex** (PSD). If you add $z = x \cdot y$ or $y = \sin(x)$, it will throw an error. You must explicitly enable the global solver.

Engineering Note: Just like Big-M, Spatial B&B relies heavily on **variable bounds** (L_x, U_x) to build tight envelopes. Always bound your continuous variables in MINLP!

Practical MINLP in Gurobi

```
m = gp.Model("bilinear_example")
x = m.addVar(lb=0, ub=10, name="x")  # Bounds are CRITICAL for envelopes!
y = m.addVar(lb=0, ub=10, name="y")
z = m.addVar(name="z")

# 1. Add the bilinear constraint directly
#    Gurobi detects this is non-convex
m.addConstr(z == x * y)

# 2. REQUIRED: Enable non-convex handling
#    0 = error if non-convex (default)
#    2 = translate to McCormick & use Spatial B&B
m.setParam("NonConvex", 2)

m.optimize()
```

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Summary of Lecture 7

- TSP and its formulation using Big-M.
- Piecewise linearization (PWL) is the simplest bridge from nonlinear to MILP.
- SOS2 = solver-native structure for tight PWL modeling.
- Bilinear terms $x \cdot y$ are the main “modeling atom” of MINLP.
- Many complicated expressions (including ratios) reduce to bilinear equalities via auxiliary variables.
- Uniform approximation is powerful but can explode in size. Deal with it using spatial branch-and-bound and McCormick envelopes.