CS498: Algorithmic Engineering

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

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Week 04 – 02/10/2026

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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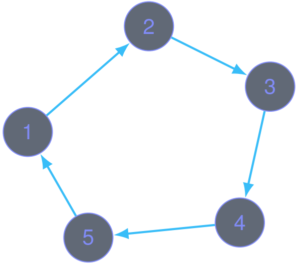

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These ensure each city has exactly one predecessor and one successor.

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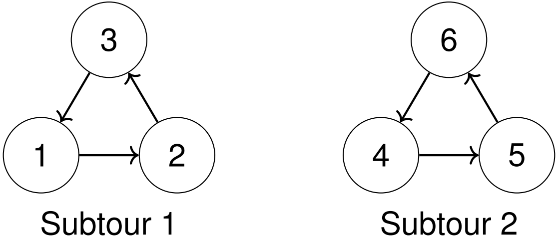

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This is exactly a **logical implication** like our earlier patterns.

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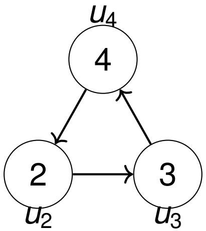

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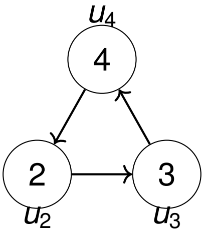

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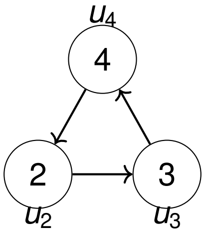

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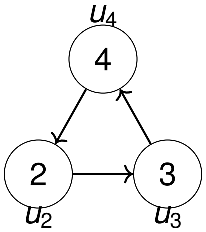

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Conclusion: MTZ forbids every cycle that does not include city 1.

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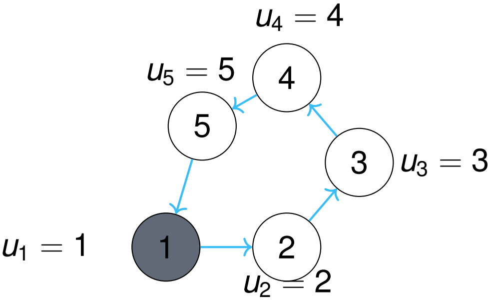

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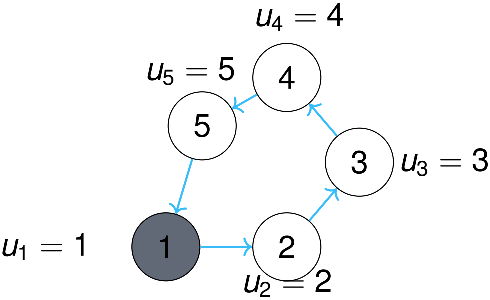

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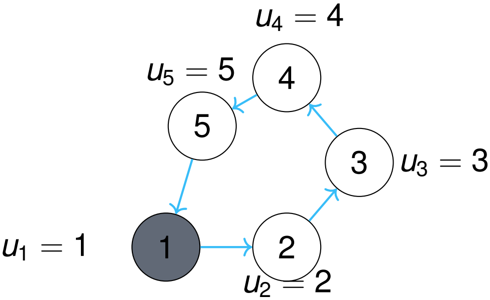

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Key point: MTZ eliminates all subtours, while deliberately allowing TSP cycles that pass through city 1.

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- 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.

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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

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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

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

m.optimize()
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I replaced these lines:

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Same runtime! So why select M?

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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:

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The Reality

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

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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 $M = 10$.

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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**.

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

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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.

Engineering Takeaway: Explicit vs. Implicit

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- Core structural constraints (like TSP subtours, Network Flow).

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“Don’t hide the geometry inside a logical wrapper.”

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

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

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 $x \in [L, U]$.

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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 $\lambda_0, \ldots, \lambda_K$:

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

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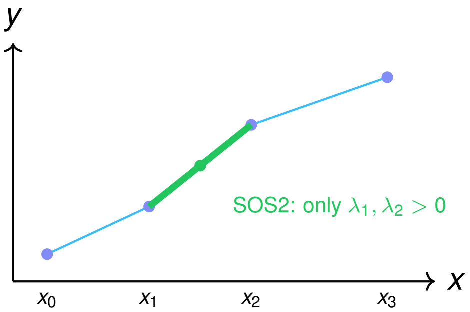
Missing rule: x must lie on *one segment*, not a mixture of far-apart points.
Enter SOS2: at most two adjacent λ_k are nonzero.

A Tiny Picture: PWL Approximation



Gurobi: Piecewise Linear via SOS2

```python
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.

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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:

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

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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:

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

Subexpression Variables

Introduce:

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

Then:

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

Ratios become bilinear constraints:

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

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).

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.

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- 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.

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Question: Can we refine only where it matters?

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

Suppose:

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

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

The set $\{(x, y, z) : z = xy\}$ is nonconvex.

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:

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

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.

McCormick Envelopes (4 Inequalities)

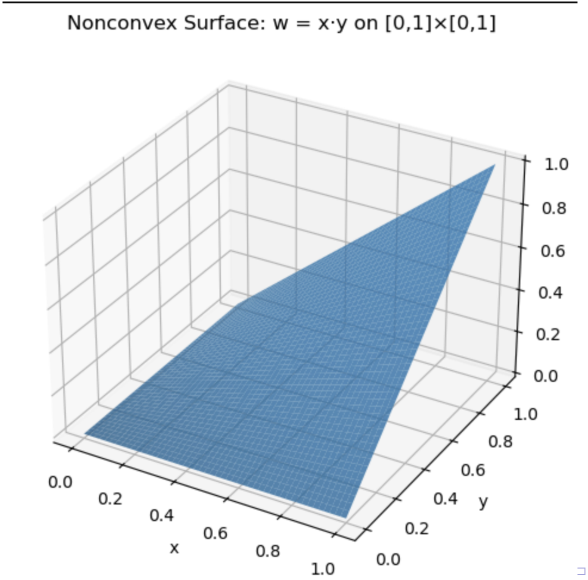
Define $z = xy$ with bounds $x \in [L_x, U_x]$, $y \in [L_y, U_y]$.
The convex hull relaxation over the box is:

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

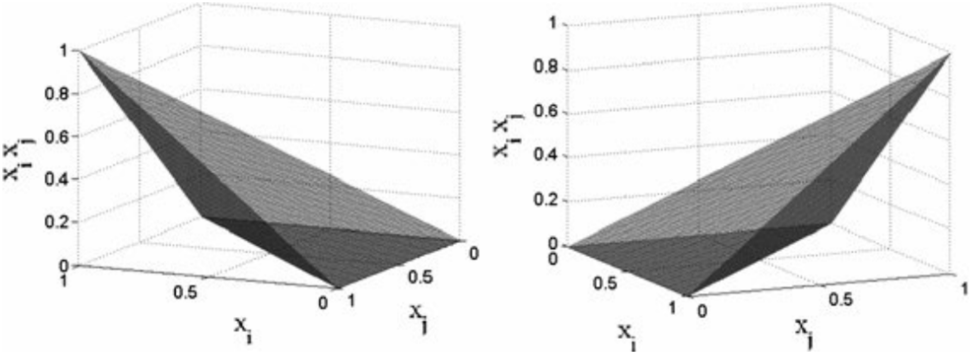
Interpretation:

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

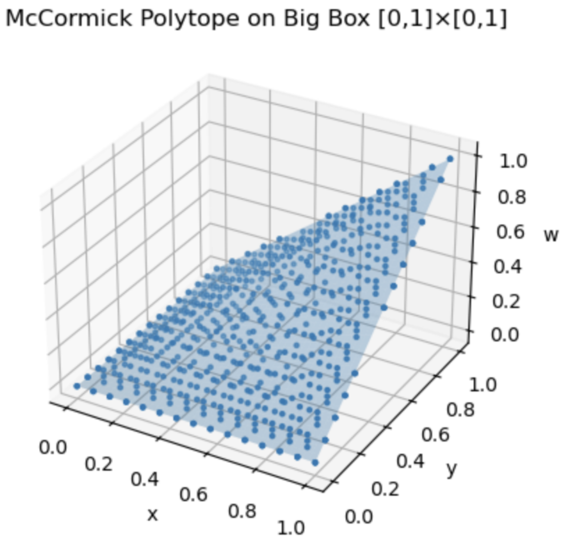
Geometry


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

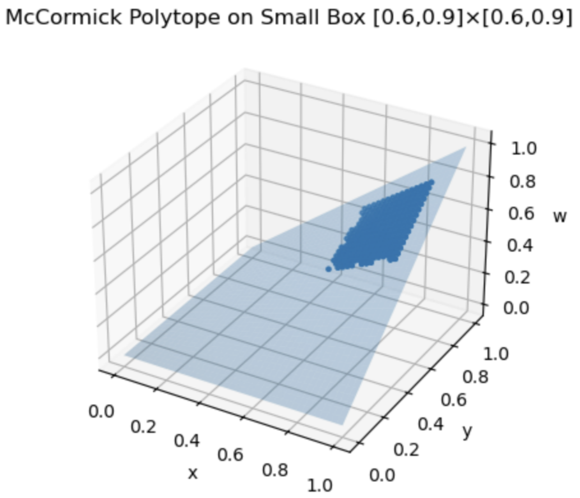
Geometry



Geometry


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

Geometry


McCormick Polytope on Small Box [0.6,0.9]×[0.6,0.9]
1.0
0.8
0.6
0.4
0.2
0.0
w
x
0.0
0.2
0.4
0.6
0.8
1.0
y
0.0
0.2
0.4
0.6
0.8
1.0

Spatial B&B: Adaptive Refinement of Bounds

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

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

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At each node:

- shrink variable bounds,

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At each node:

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- rebuild McCormick envelopes on the smaller box for bi-linear terms,

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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.

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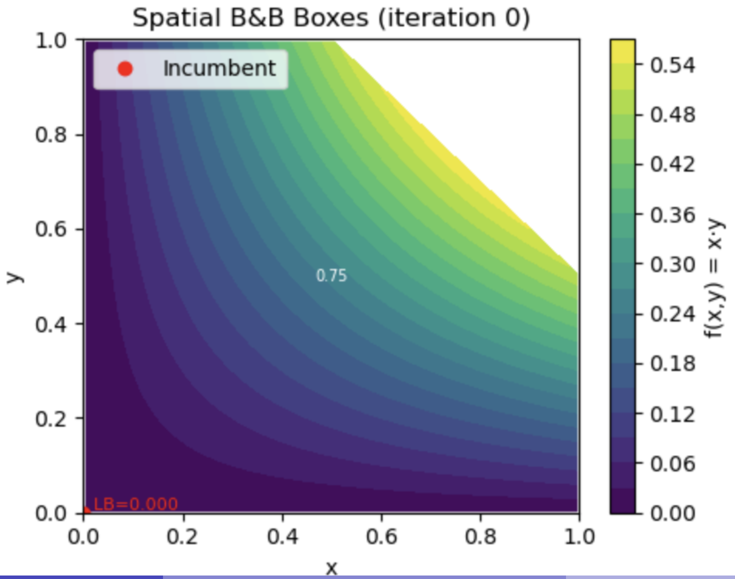
At each node:

- 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.

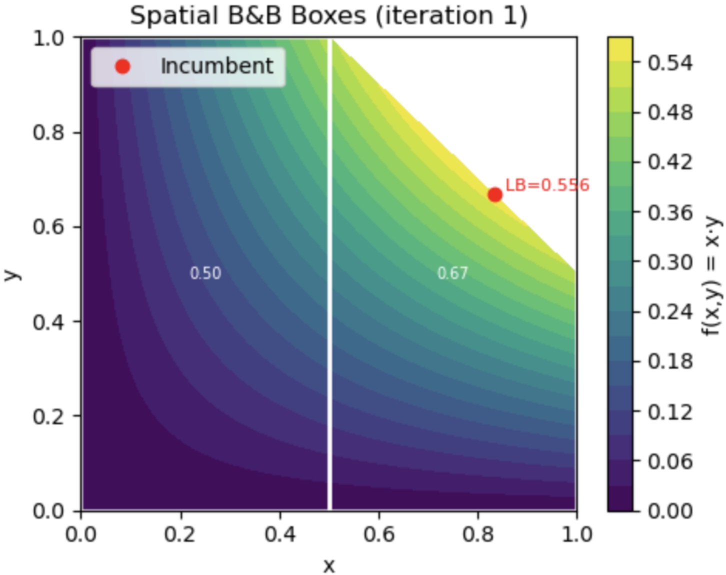
This is **branch-and-bound on continuous domains.** What Gurobi implements.

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

Geometry

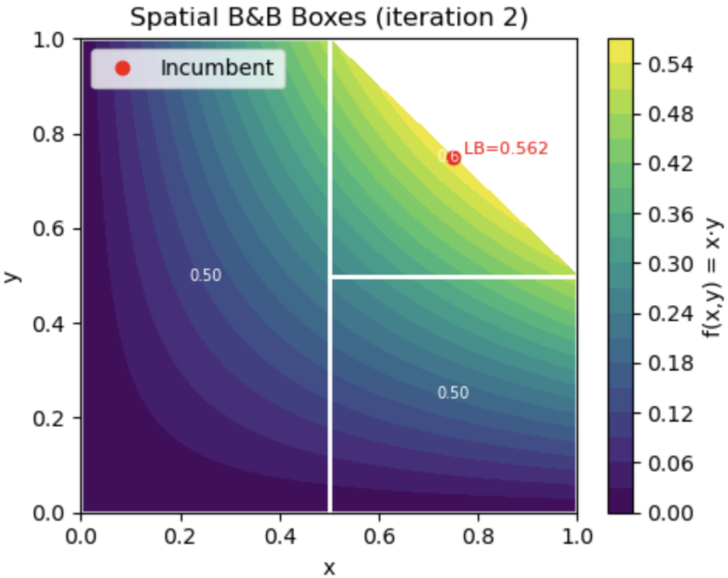

Spatial B&B Boxes (iteration 0)
Incumbent
0.75
LB=0.000
1.0
0.8
0.6
0.4
0.2
0.0
y
0.0
0.2
0.4
0.6
0.8
1.0
x
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry



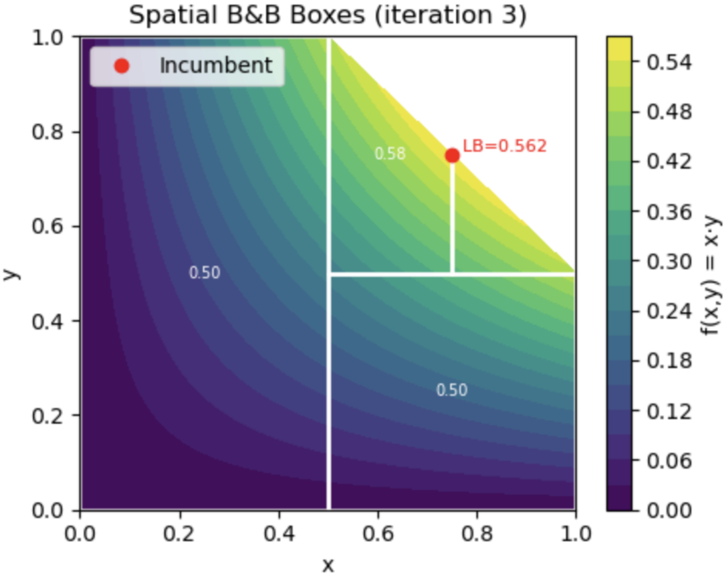
Spatial B&B Boxes (iteration 1)
Incumbent
LB=0.556
0.50
0.67
1.0
0.8
0.6
0.4
0.2
0.0
y
0.0
0.2
0.4
0.6
0.8
1.0
x
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry



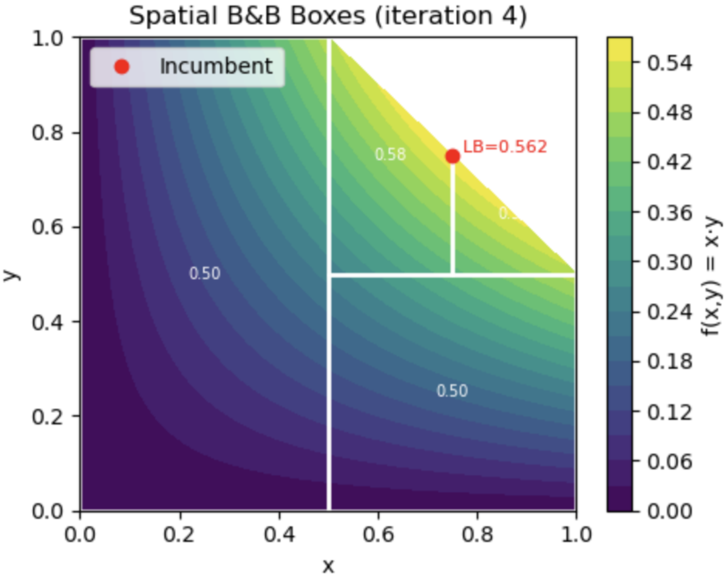
Spatial B&B Boxes (iteration 2)
Incumbent
LB=0.562
0.50
0.50
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
x
y
0.54
0.48
0.42
0.36
0.30
0.24
0.18
0.12
0.06
0.00
f(x,y) = x·y

Geometry



Spatial B&B Boxes (iteration 3)
Incumbent
LB=0.562
0.58
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
x
y
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.

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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.

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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

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.