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26 July 2022

Combinatorial Algorithms Used Inside a MIP Solver

Linear and Mixed Integer Programming

- A linear program (LP) is defined as

$$\begin{array}{llll} \min & c^T x & & \\ \text{s.t.} & Ax & \leq & b \\ & x & \in & \mathbb{R}^n \end{array}$$

- A mixed integer program (MIP) is defined as

$$\begin{array}{lllll} \min & c^T x & & & \\ \text{s.t.} & Ax & \leq & b & \\ & x & \in & \mathbb{R}^n & \\ & x_j & \in & \mathbb{Z} & \text{for all } j \in I \end{array}$$

Applications of Mixed Integer Programming

- Accounting
- Advertising
- Agriculture
- Airlines
- ATM provisioning
- Compilers
- Defense
- Electrical power
- Energy
- Finance
- Food service
- Forestry
- Gas distribution
- Government
- Internet applications
- Logistics/supply chain
- Medical
- Mining National research labs
- Online dating
- Portfolio management
- Railways
- Recycling
- Revenue management
- Semiconductor
- Shipping
- Social networking
- Sports betting
- Sports scheduling
- Statistics
- Steel Manufacturing
- Telecommunications
- Transportation
- Utilities
- Workforce scheduling
- ...

$\mathcal{P}$ vs $\mathcal{NP}$

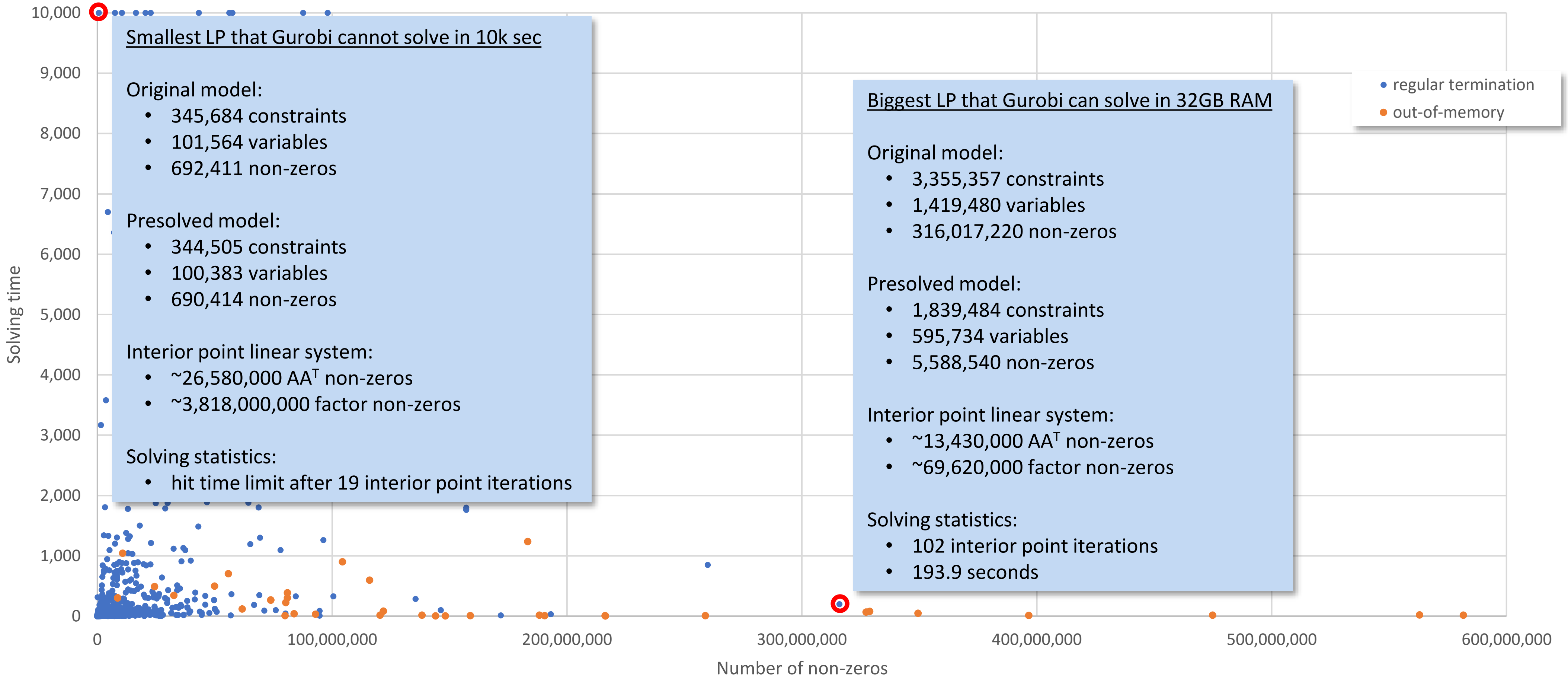
- Problem class $\mathcal{P}$:
  - Problem instance is solvable in worst-case runtime that is polynomial in input size
  - Examples:
    - Sorting
    - Shortest path
    - Maximum weighted matching
    - Linear program
- Problem class $\mathcal{NP}$:
  - Solution for given problem instance can be verified in polynomial time w.r.t. instance size
  - Obviously, $\mathcal{P} \subseteq \mathcal{NP}$
- Problem class $\mathcal{NP}$-complete:
  - $P \in \mathcal{NP}$ is $\mathcal{NP}$-complete if every problem in $\mathcal{NP}$ can be transformed into P using a polynomial transformation
  - Examples:
    - Satisfiability problem (SAT)
    - Knapsack
    - Traveling salesman problem
    - Maximum weighted clique
    - Integer program

$\mathcal{P}$ vs $\mathcal{NP}$ in Practice

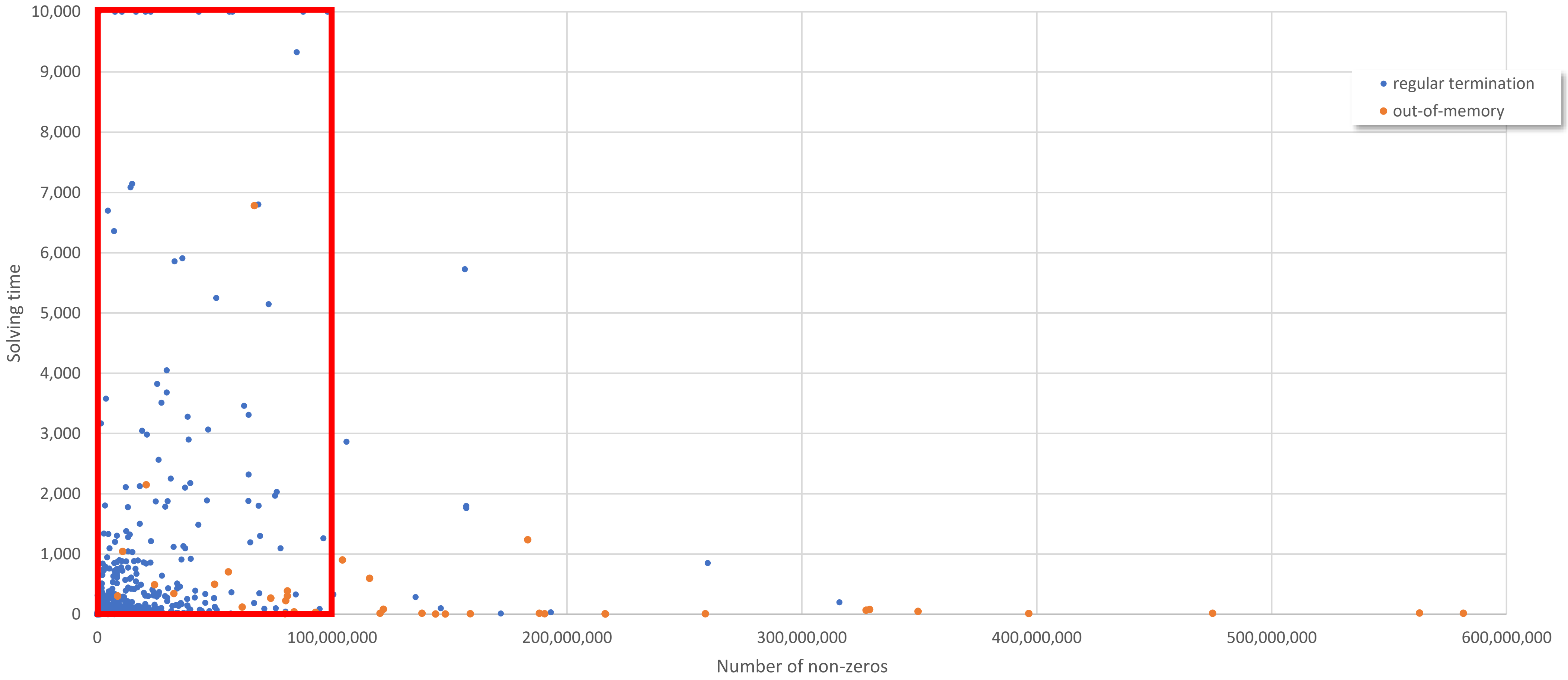
- Theory says:
  - Linear programming is easy
    - Interior point algorithm has polynomial worst-case runtime
  - Integer programming is hard
    - Branch-and-cut has exponential worst-case runtime
      - exponential in number of integer variables
- Let's look at problem sizes and runtime for real-world problem instances
  - LP test set has 2397 instances
  - MIP test set has 7030 instances
  - Gurobi 9.5.0
  - Intel Xeon CPU E3-1240 v3 @ 3.40GHz
  - 4 cores, 8 hyper-threads
  - 32 GB RAM
  - Time limit of 10,000 seconds

Linear Programming

Full test set

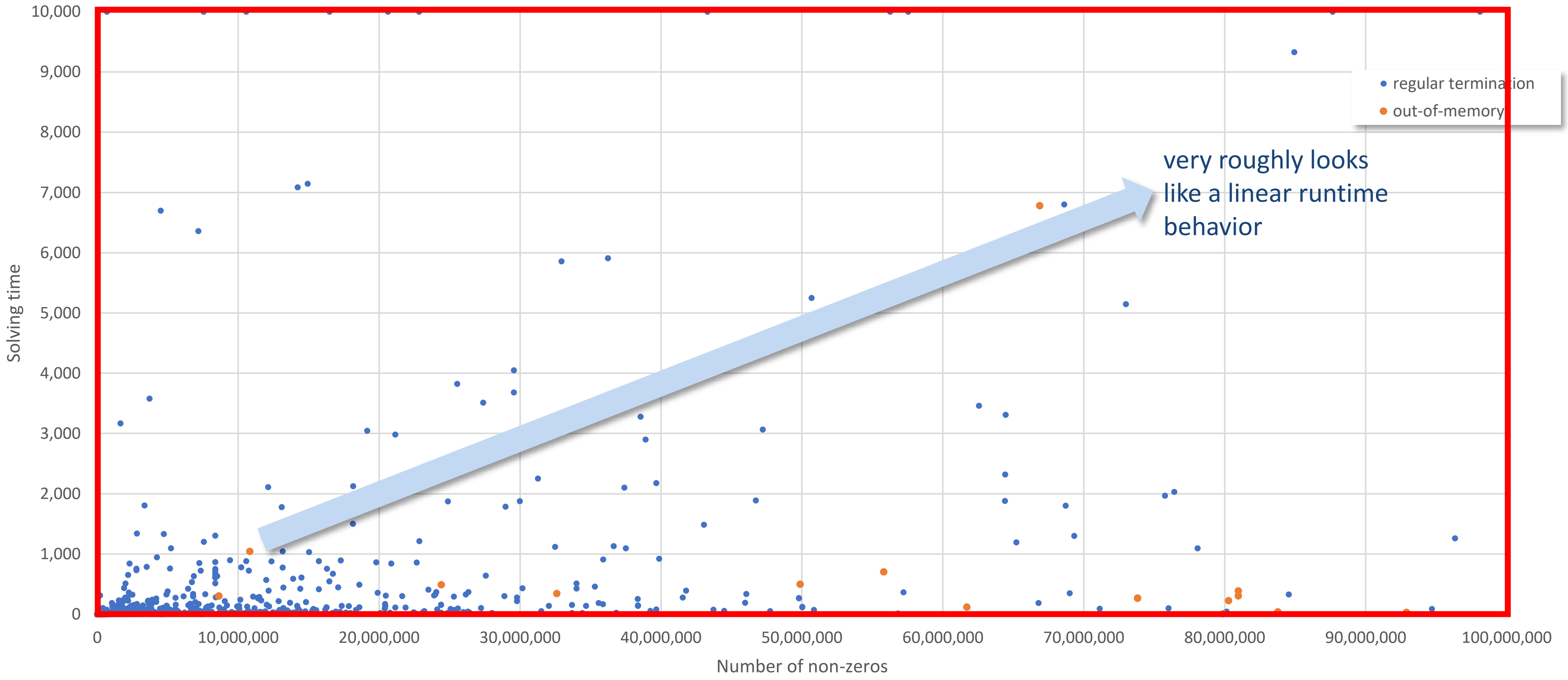


Linear Programming
Full test set



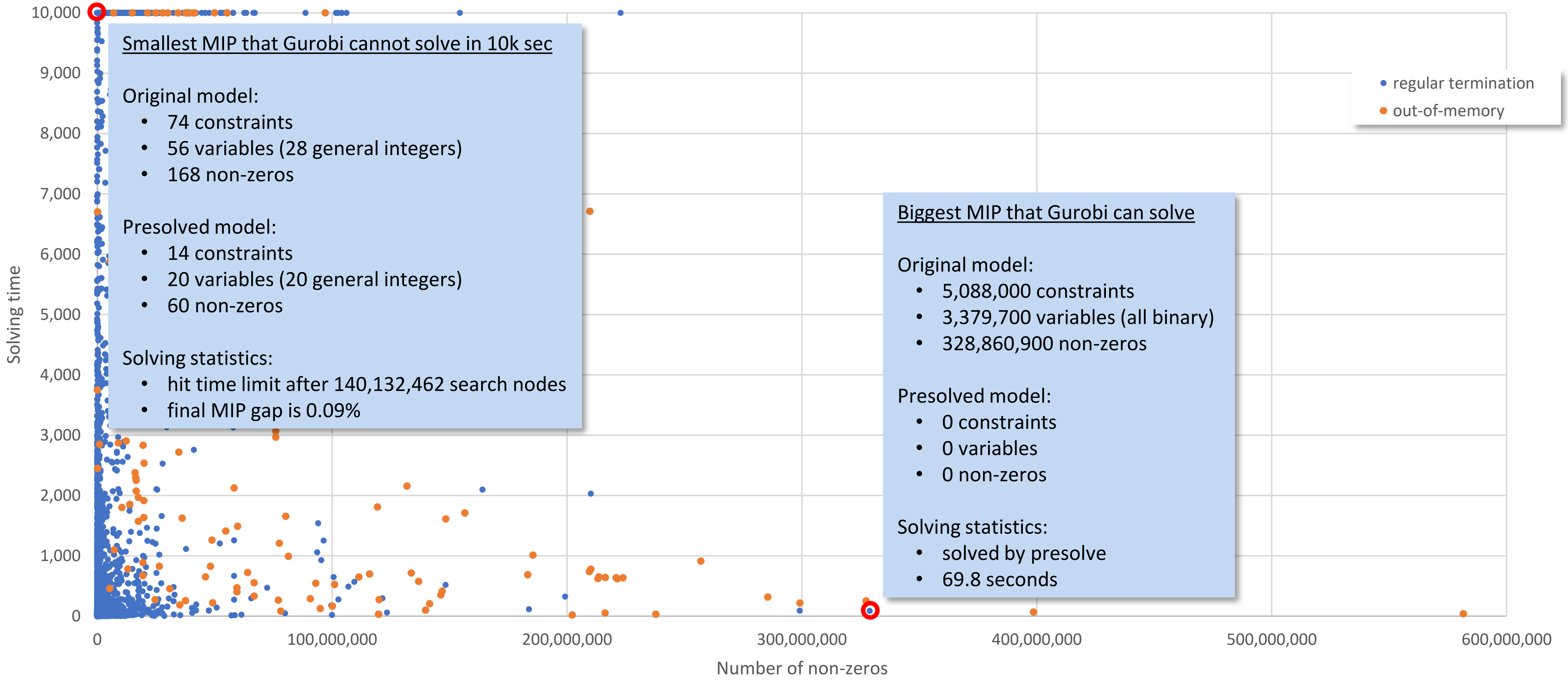
Linear Programming

Models with up to 100 million non-zeros



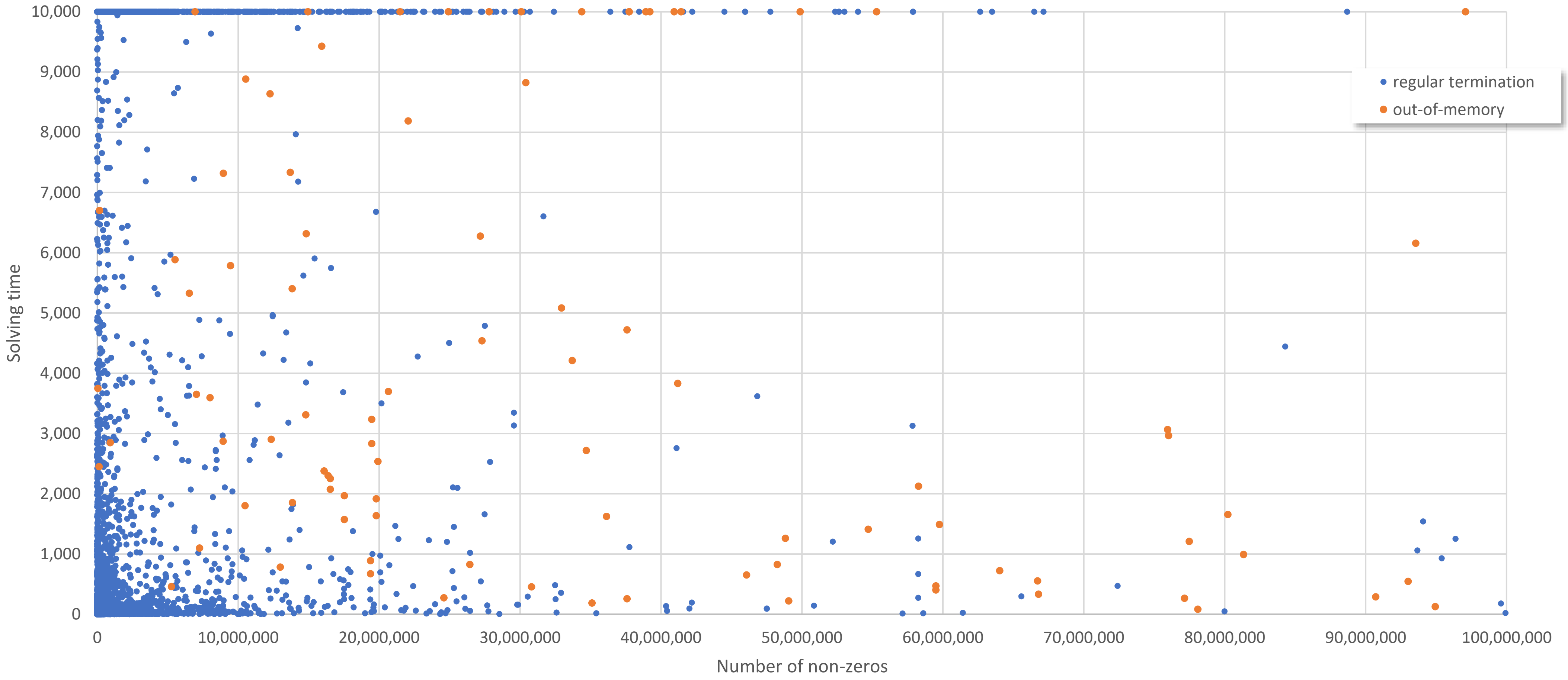
Mixed Integer Programming

Full test set



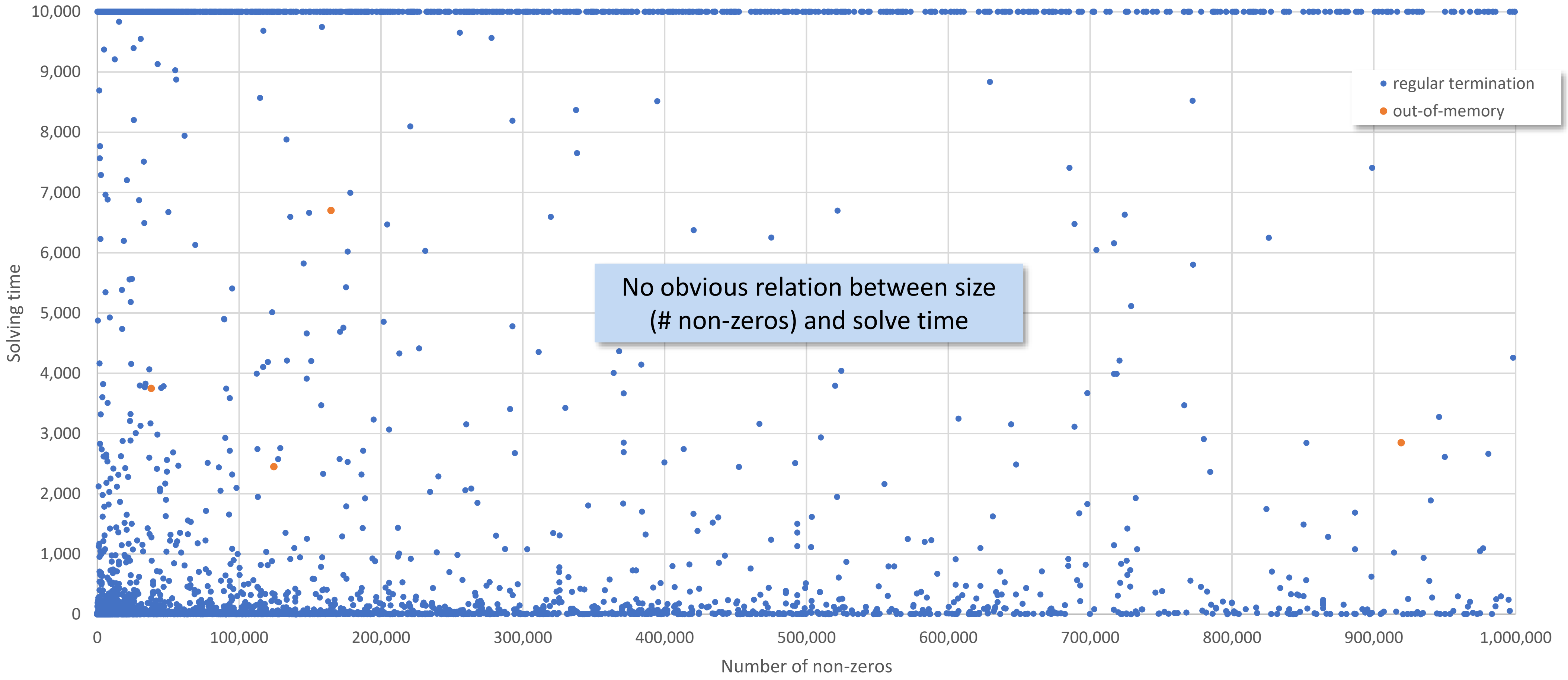
Mixed Integer Programming

Models with up to 100 million non-zeros



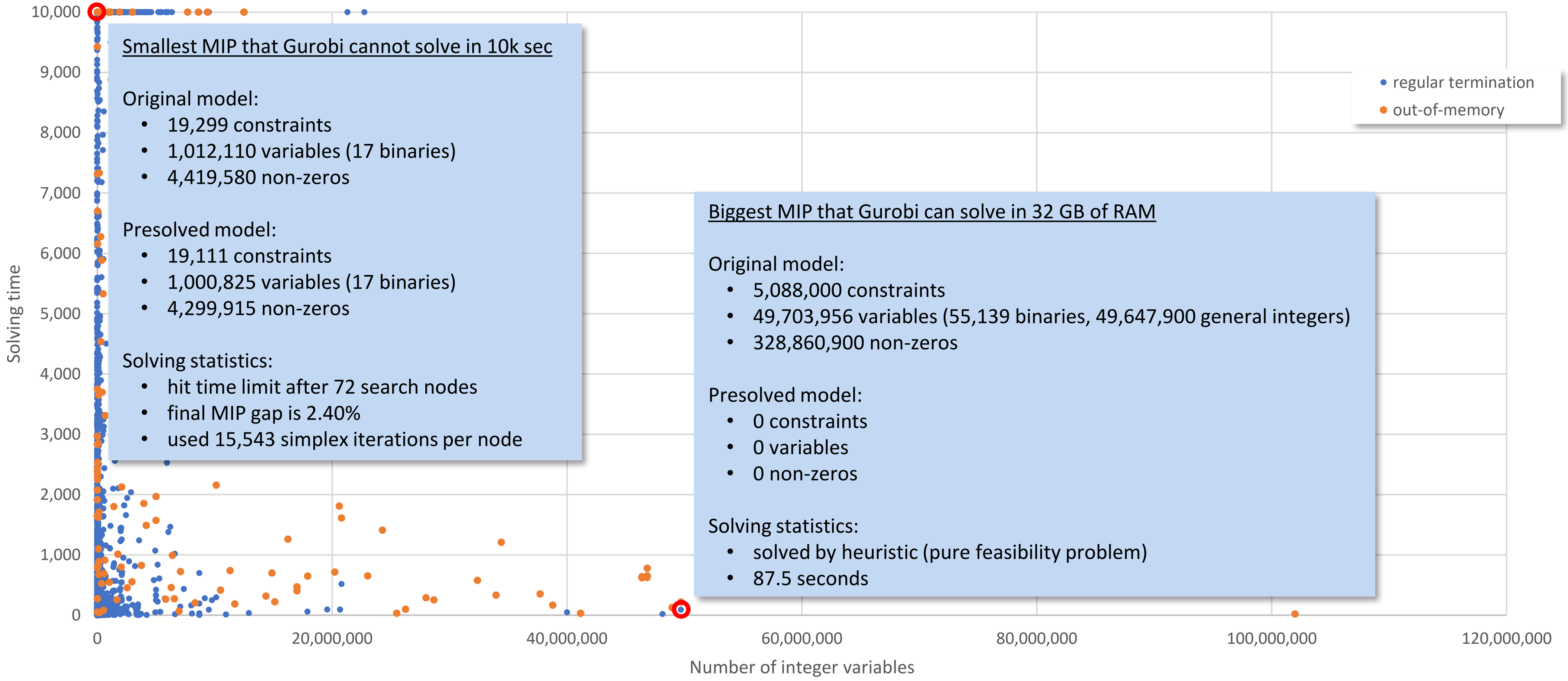
Mixed Integer Programming

Models with up to 1 million non-zeros



Mixed Integer Programming

Full test set



Smallest MIP that Gurobi cannot solve in 10k sec

Original model:

- 19,299 constraints
- 1,012,110 variables (17 binaries)
- 4,419,580 non-zeros

Presolved model:

- 19,111 constraints
- 1,000,825 variables (17 binaries)
- 4,299,915 non-zeros

Solving statistics:

- hit time limit after 72 search nodes
- final MIP gap is 2.40%
- used 15,543 simplex iterations per node

Biggest MIP that Gurobi can solve in 32 GB of RAM

Original model:

- 5,088,000 constraints
- 49,703,956 variables (55,139 binaries, 49,647,900 general integers)
- 328,860,900 non-zeros

Presolved model:

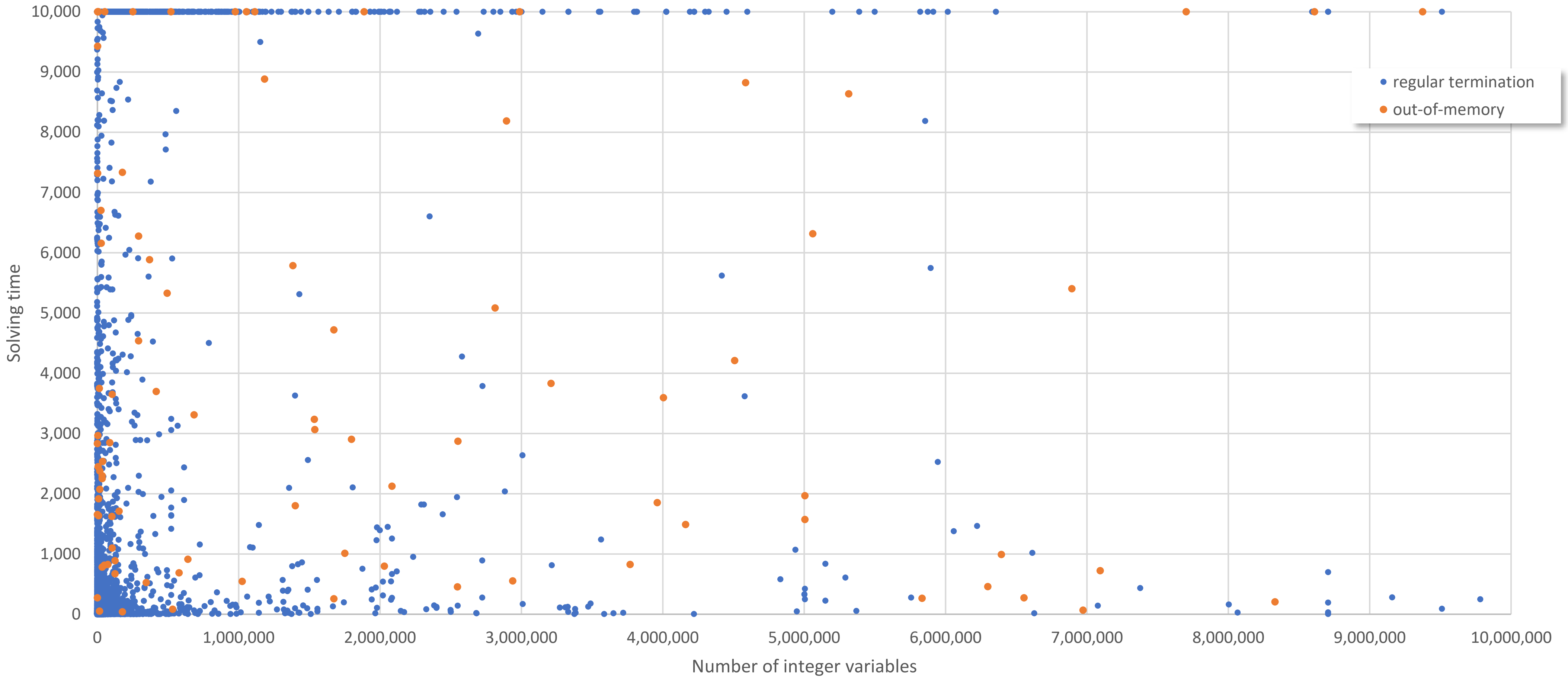
- 0 constraints
- 0 variables
- 0 non-zeros

Solving statistics:

- solved by heuristic (pure feasibility problem)
- 87.5 seconds

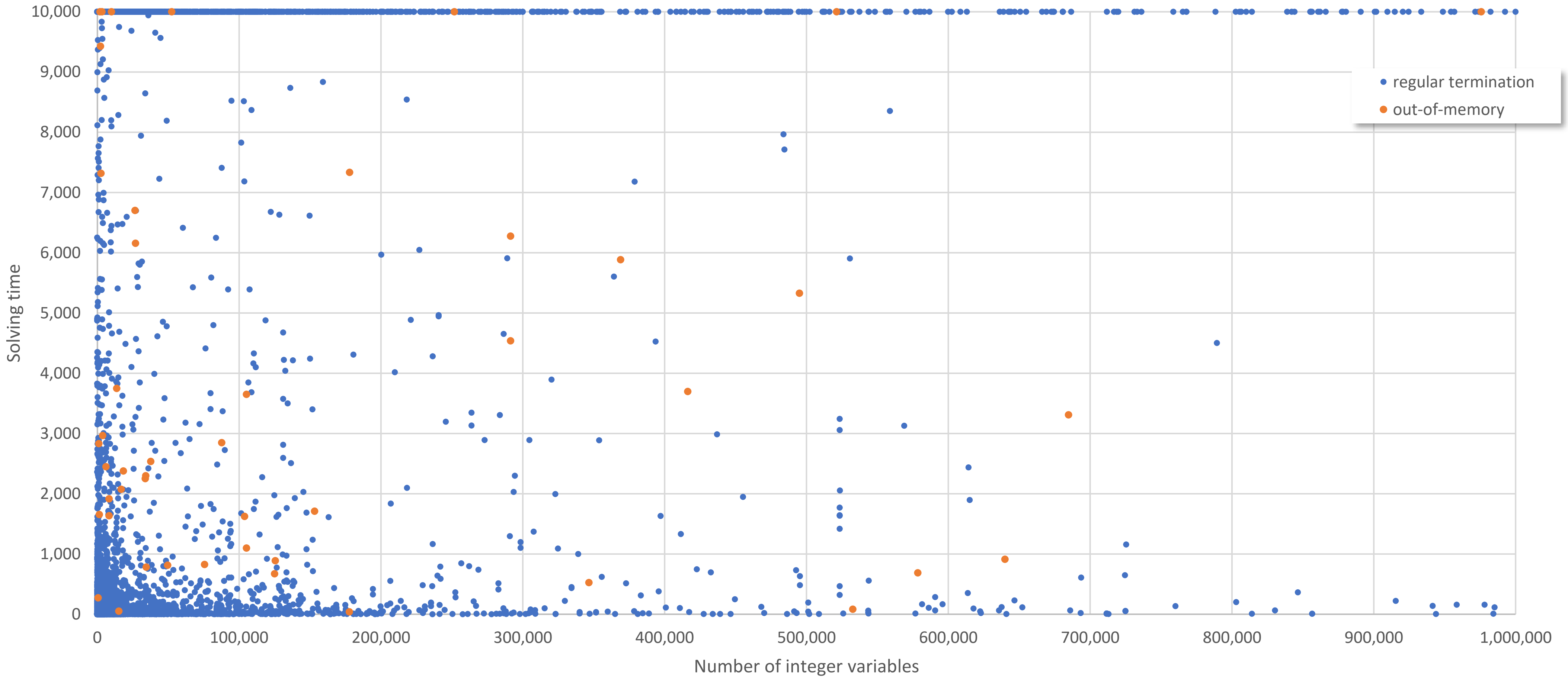
Mixed Integer Programming

Models with up to 10 million integer variables



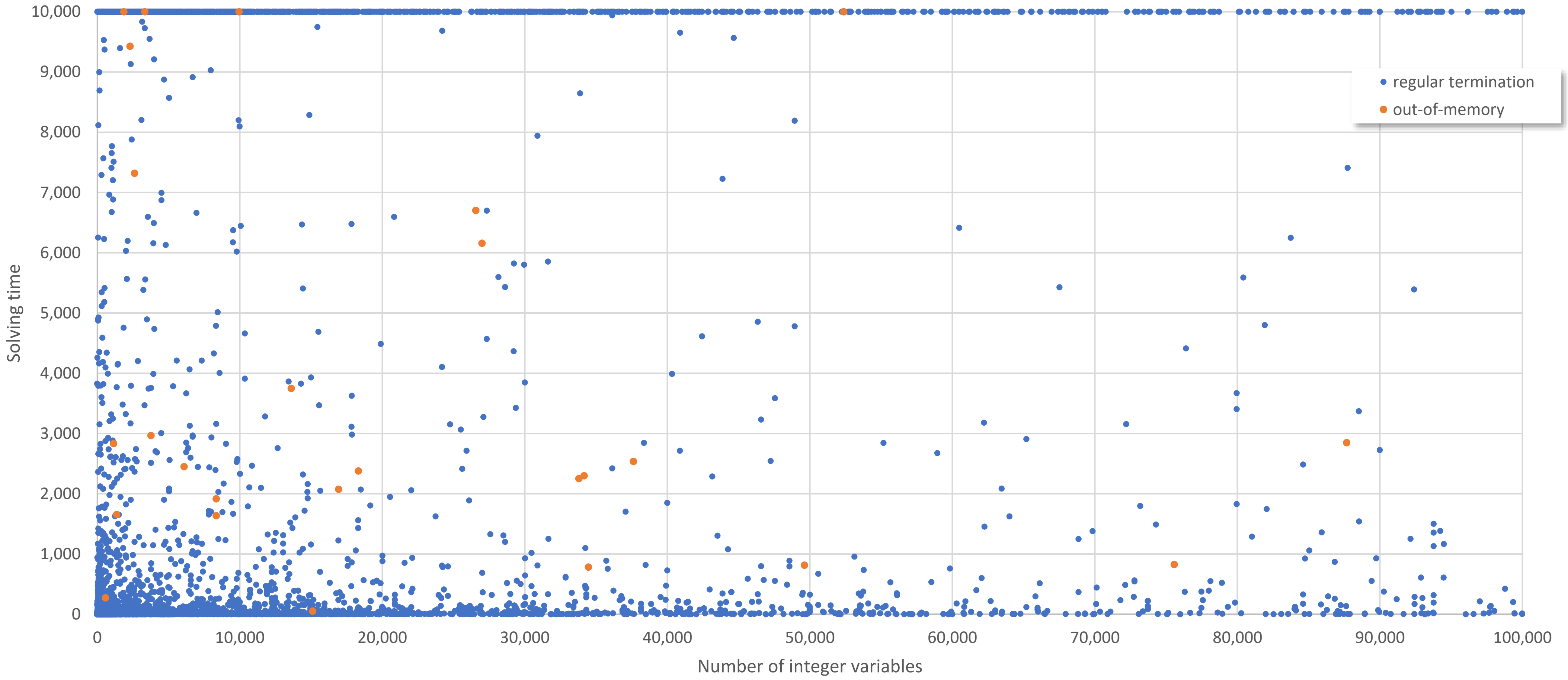
Mixed Integer Programming

Models with up to 1 million integer variables



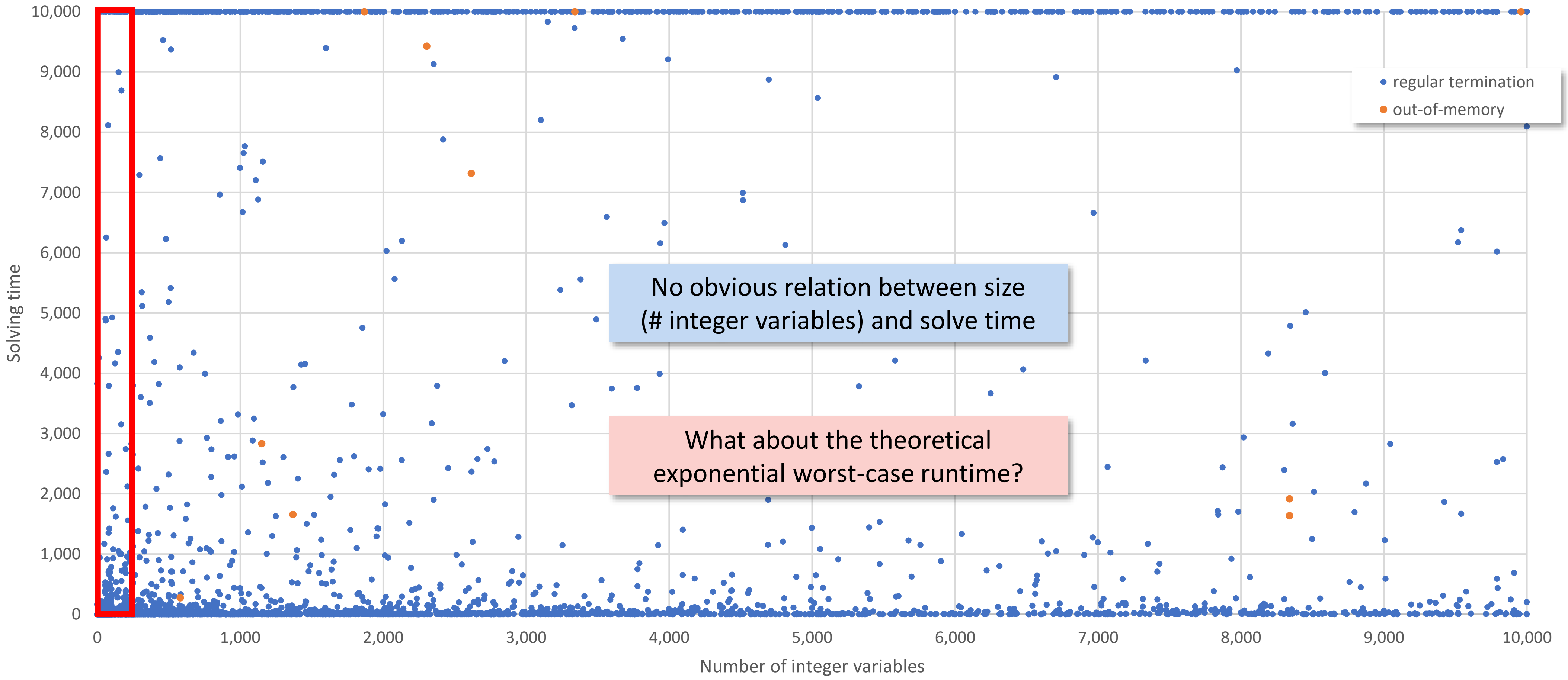
Mixed Integer Programming

Models with up to 100,000 integer variables



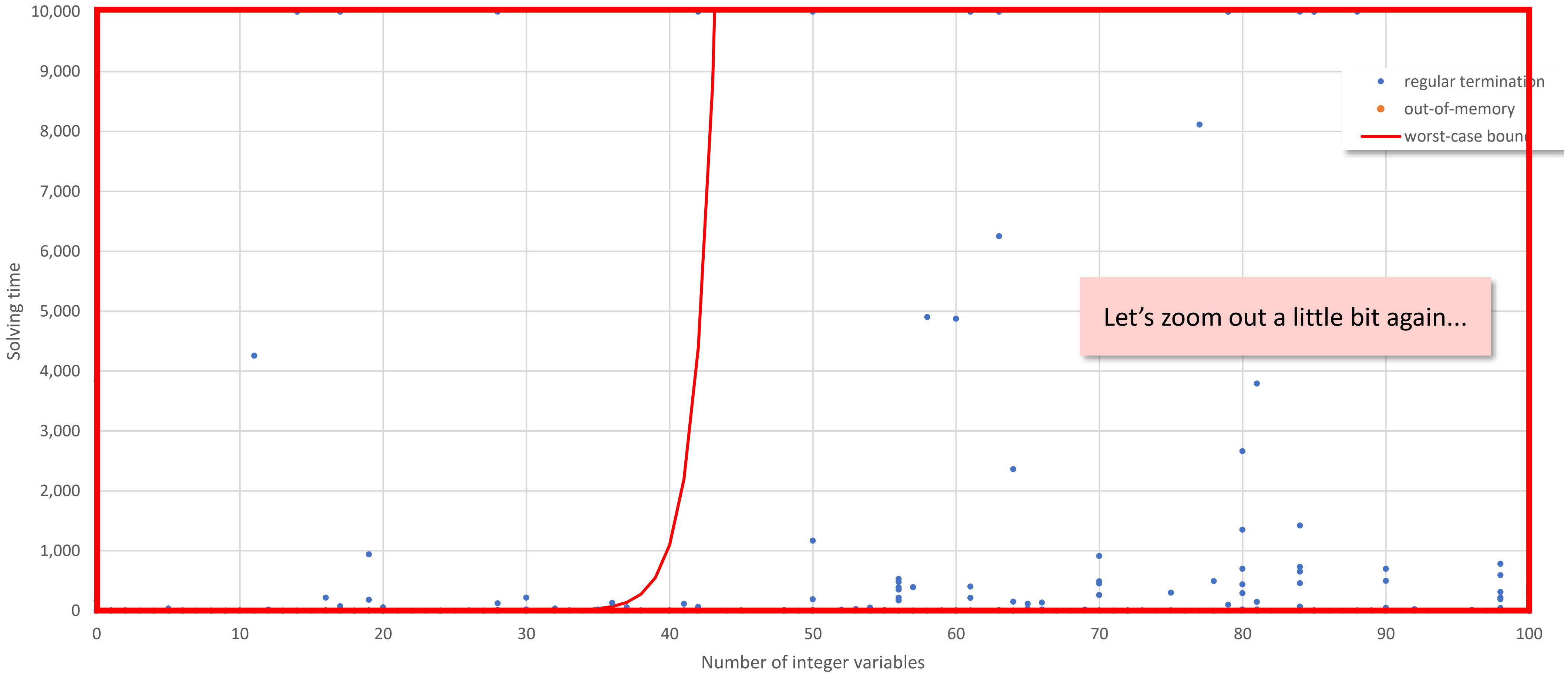
Mixed Integer Programming

Models with up to 10,000 integer variables



MIP is $\mathcal{NP}$-complete: Theory vs Practice

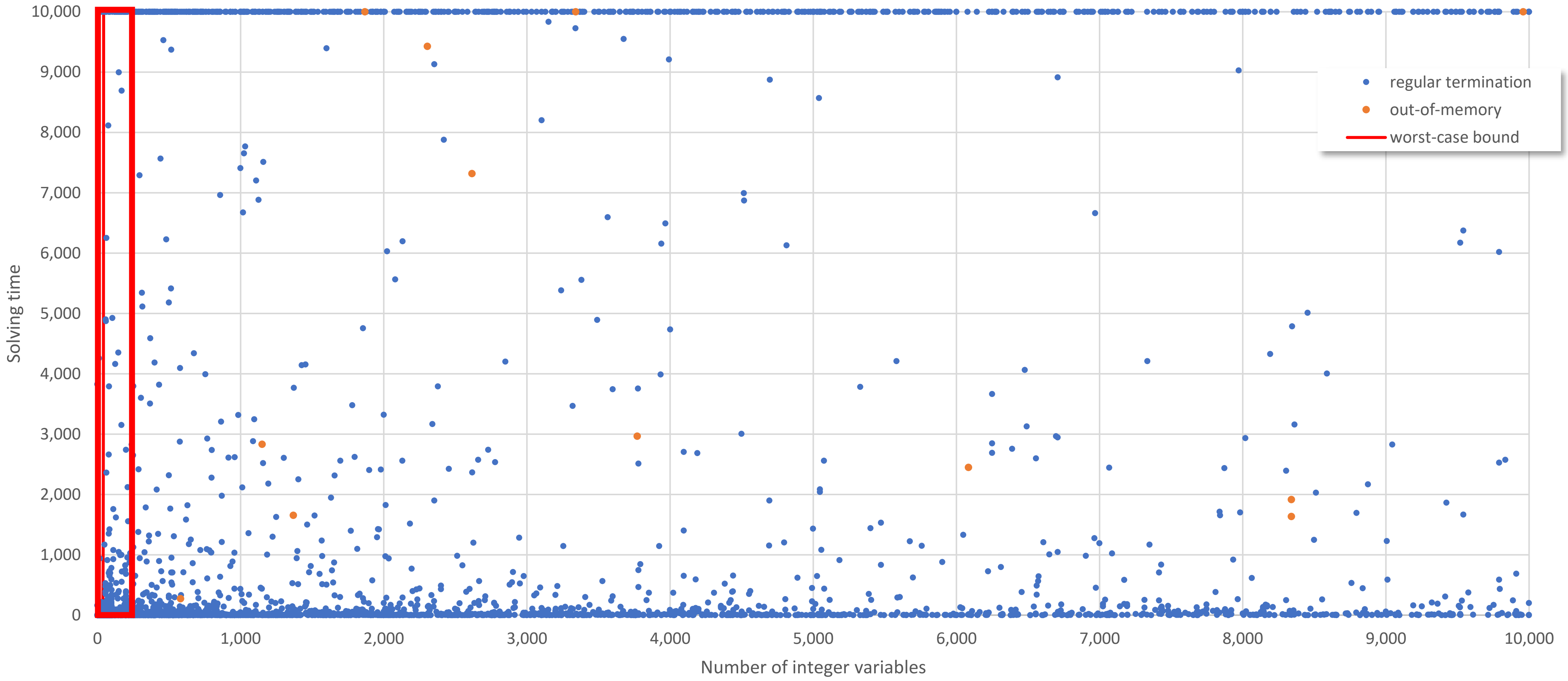
Models with up to 100 integer variables



Worst-case bound for pure binary programs with evaluating 1 billion solutions per second: $2^n/10^9$

MIP is $\mathcal{NP}$-complete: Theory vs Practice

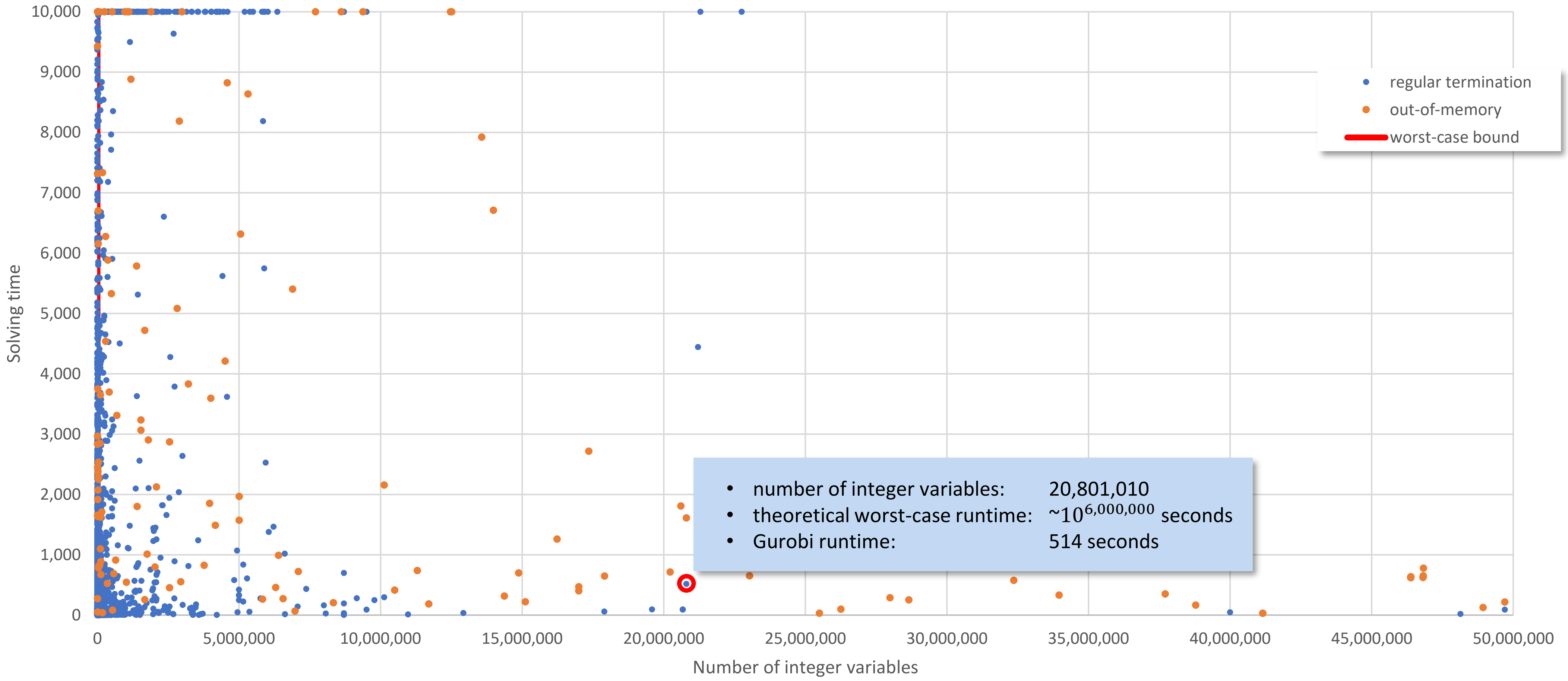
Models with up to 10,000 integer variables



Worst-case bound for pure binary programs with evaluating 1 billion solutions per second: $2^n/10^9$

MIP is $\mathcal{NP}$-complete: Theory vs Practice

Models with up to 50 million integer variables



Worst-case bound for pure binary programs with evaluating 1 billion solutions per second: $2^n/10^9$

Consequences for MIP Solvers

- MIP solvers employ various combinatorial and number theoretic sub-algorithms
- Some of these algorithms have polynomial runtime
  - Does this mean those will always be fast enough?
    - No! Even a quadratic algorithm is too slow in many situations!
    - For example, pair-wise comparison to identify parallel rows in a matrix $A \in \mathbb{R}^{m \times n}$ needs $\mathcal{O}(m^2 n)$ operations
      - Always think about big models!
      - 1 million rows means about 500 billion pairs of rows to check
      - Need an algorithm that is faster in practice, not necessarily in asymptotic behavior
      - Need to include safeguards against quadratic overhead for corner cases

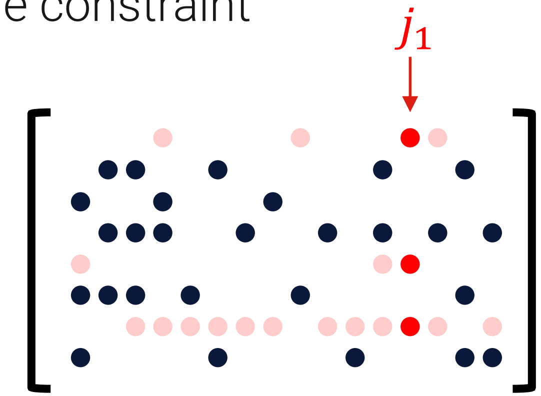
Consequences for MIP Solvers

- MIP solvers employ various combinatorial and number theoretic sub-algorithms
- Some of these algorithms have exponential runtime
  - Does this mean those will never be useful?
    - No! Exponential worst-case runtime does not say anything about practical problem instances!
    - Often, we only need to solve small combinatorial problem instances to optimality
    - In most cases, a heuristic that often finds good solutions is good enough

- The algorithm design should be targeted towards practical problem instances
  - But always think about worst-case behavior to include safeguards in your code!
  - Quadratic loops are not always easy to spot in your code
  - They constitute one of the most frequent “performance bugs” that we need to fix

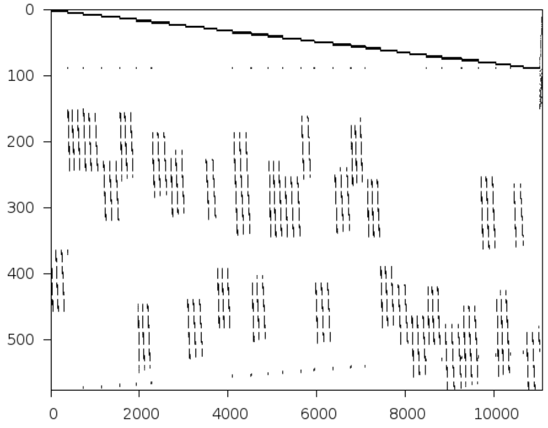
Example: Finding Neighbors in Matrix

- Many algorithms in our code do something with some variable, and then need to update some data for the variable's neighbors
- Definition: in $A \epsilon \mathbb{R}^{m \times n}$ two columns j_1, j_2 are neighbors if $A^T_{\cdot,j_1} A_{\cdot,j_2} \neq 0$
  - Thus, the variables are neighbors if they appear together in at least one constraint
- Algorithm to find neighbors of j_1:
  1. Set $N := \emptyset$
  2. For each non-zero element $a_{i,j_1} \neq 0$ in $A_{\cdot,j_1}$:
     (a) For each non-zero element $a_{i,j_2} \neq 0$ in $A_{i,\cdot}$:
        (i) Set $N := N \cup \{j_2\}$

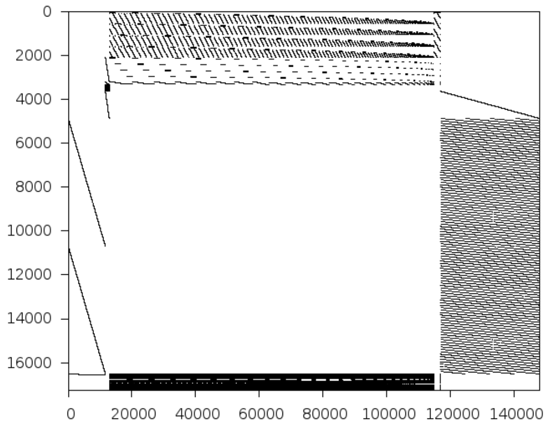


- Now consider a constraint with k non-zero elements
  - If our algorithm touches each of the k variables in the constraint and each time needs to find the neighbors of the current variable, we perform k^2 operations.
  - No problem for $k = 1000$, but very bad for $k = 1{,}000{,}000$

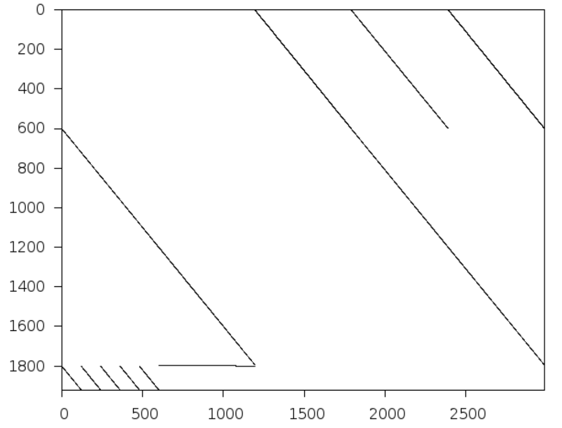
Sparsity Patterns



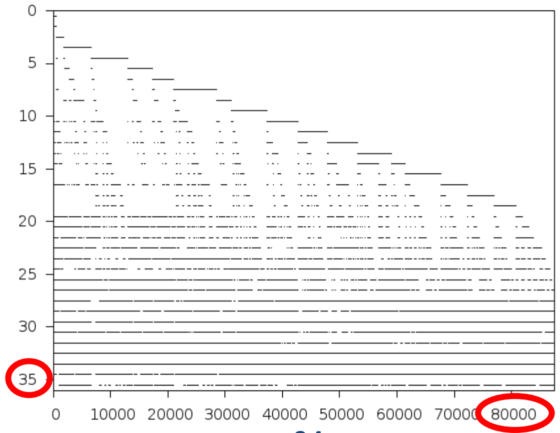
30n20b8



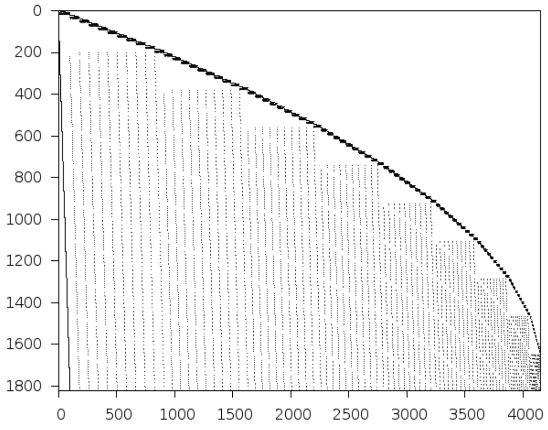
bab2



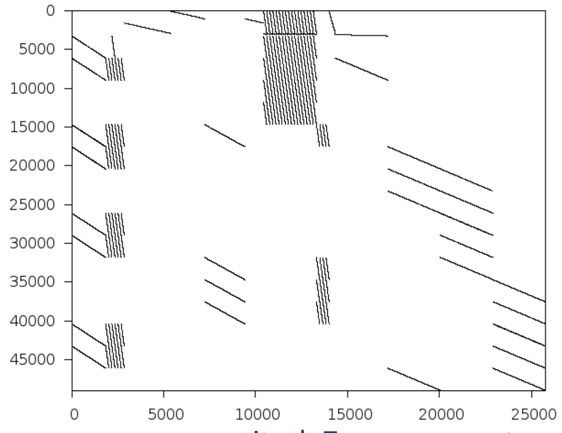
lotsize



nw04



qap10

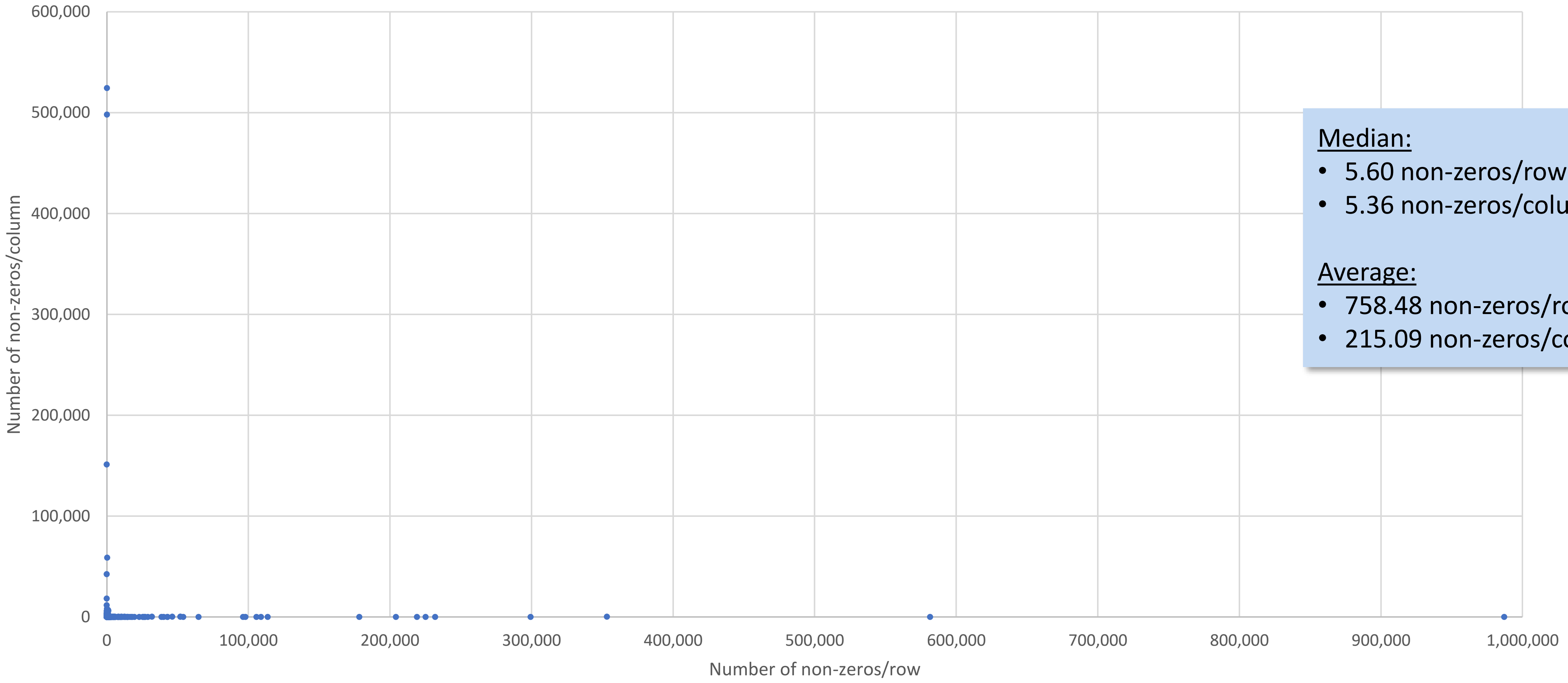


unitcal_7

pictures from miplib.zib.de

Sparsity Statistics

Full MIP test set

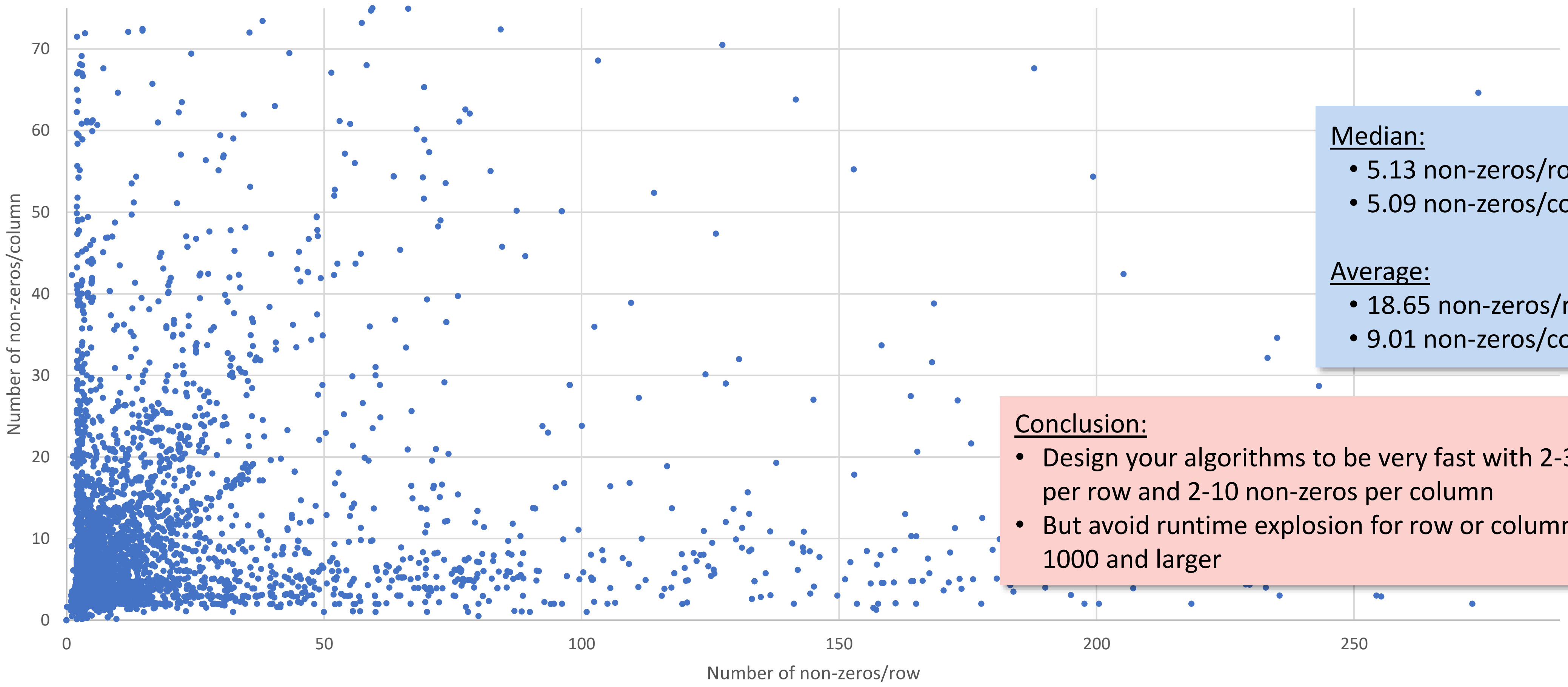


Median:
- 5.60 non-zeros/row
- 5.36 non-zeros/column

Average:
- 758.48 non-zeros/row
- 215.09 non-zeros/column

Sparsity Statistics

MIP test set without 5% of largest nz/row and 5% of largest nz/col ratios



Median:
- 5.13 non-zeros/row
- 5.09 non-zeros/column

Average:
- 18.65 non-zeros/row
- 9.01 non-zeros/column

Conclusion:
- Design your algorithms to be very fast with 2-30 non-zeros per row and 2-10 non-zeros per column
- But avoid runtime explosion for row or column lengths of 1000 and larger

Implementation Considerations

- Algorithms need to be implemented in C
  - Gurobi needs to support ancient and strange platforms like AIX, Solaris, or Windows 32
  - C compiles on every platform
    - Anything else (including C++) can get messy
- Algorithms often need to work on Gurobi's internal data structures
  - If an algorithm is called frequently, we cannot afford translating our data structures into those that the algorithm works on
- Algorithms need to be tuned to the structures and sizes that appear in practical MIP models
- Gurobi provides malloc callbacks that Gurobi should use for its memory management

- Conclusion: need to implement all algorithms ourselves
  - Nice consequence: a lot of fun!

Combinatorial Algorithms

Median algorithm
Depth first search
Shortest path
Min cut / max flow
Minimum vertex separator
Max clique
Dynamic programming
Graph automorphism
Union find

GUROBI OPTIMIZATION

Median Algorithm

Single constraint linear program

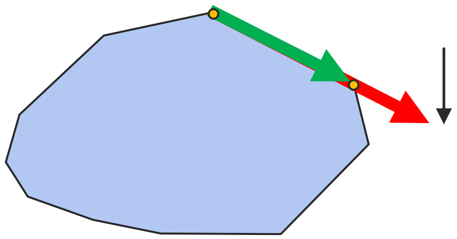
- Consider a single constraint linear program with bounds on the variables:

$$\begin{array}{llll} \max & c^T x & & \\ \text{s.t.} & a^T x & \leq & b \\ & x_j & \in & [0, u_j] \quad \text{for all } j \end{array}$$

- This can be solved by sorting the elements: $\frac{c_1}{a_1} \geq \frac{c_2}{a_2} \geq \cdots \geq \frac{c_n}{a_n}$
  - Then, the solution is
    $x_1 = u_1, \ldots, x_{k-1} = u_{k-1}, x_k = \frac{1}{a_k}\left(b - \sum_{j=1}^{k-1} a_j u_j\right), x_{k+1} = \cdots = x_n = 0$
- But sorting is too slow: $\mathcal{O}(n \cdot \log(n))$
- Median algorithm can find critical element x_k in $\mathcal{O}(n)$ steps

Median Algorithm

Dual simplex ratio test with bound flipping



- Dual pricing selects infeasible basic variable x_i to leave the basis
- Ratio test then selects non-basic variable x_j to enter the basis
  - Geometrically: follow ray in dual space until first dual constraint is hit
  - Finding first dual constraint that is hit means to find smallest value in list of "ratios"
- But instead of letting x_j enter the basis we may flip x_j to its opposite bound
  - Only possible if this flip in the primal space keeps x_i infeasible
  - If flip is valid, we can continue following this ray until next dual constraint is hit
- Thus, we have:
  - The infeasibility of x_i is our budget
  - For each ratio test candidate x_j we calculate how much of budget a bound flip costs
  - Simple algorithm would be to sort by ratio, then flip candidates until budget is exhausted and let the critical element enter the basis
  - Replace sorting by median algorithm to get linear runtime
- Performance impact on dual simplex algorithm:
  - 8.0% slower overall with sorting instead of median
  - 16.6% slower on models that take at least 10 seconds to solve

Median Algorithm

Domain propagation

- Basic domain propagation for single constraint

$$
\begin{aligned}
a_0 x_0 \quad + \quad a^T x \quad &\leq \quad b \\
x_j \quad &\in \quad [l_j, u_j] \quad \text{for all } j
\end{aligned}
$$

  - Relax constraint for other variables

$$a_0 x_0 + \min\{a^T x | x \in [l, u]\} \quad \leq \quad b$$

  - Yields bound for x_0
    - If $a_0 > 0$: $x_0 \leq b'$
    - If $a_0 < 0$: $x_0 \geq b'$
    - With $b' = \frac{1}{a_0}(b - \min\{a^T x | x \in [l, u]\}) = \frac{1}{a_0}\left(b - \sum_{a_j > 0} a_j l_j - \sum_{a_j < 0} a_j u_j\right)$

- Can we get stronger propagation by considering more than one constraint?

Median Algorithm

Domain propagation

- Domain propagation using two constraints
  - Pick two constraints of the MIP

$$\begin{array}{rcrcll} a_0 x_0 & + & a^T x & \leq & b & \\ & & \bar{a}^T x & \leq & \bar{b} & \\ & & x_j & \in & [l_j, u_j] & \text{for all } j \end{array}$$

  that have some overlap (i.e., $a^T \bar{a} \neq 0$)

  - Relax constraint for other variables

$$a_0 x_0 + \min\{a^T x \,|\, \bar{a}^T x \leq \bar{b}, x \in [l, u]\} \quad \leq \quad b$$

  - Yields bound for x_0
    - If $a_0 > 0$: $x_0 \leq b'$
    - If $a_0 < 0$: $x_0 \geq b'$
    - With $b' = \frac{1}{a_0}\left(b - \min\{a^T x \,|\, \bar{a}^T x \leq \bar{b}, x \in [l, u]\}\right)$
  - Inner problem $\min\{a^T x \,|\, \bar{a}^T x \leq \bar{b}, x \in [l, u]\}$ is a single constraint LP with bounds

Median Algorithm

Writing search tree nodes to disk

- If search tree grows too large, store uninteresting nodes to disk
    - Uninteresting: nodes with large dual bound
- Pick number of nodes we want to store to disk
- Nodes are not fully sorted, but stored in a heap
- Use median algorithm to find dual bound threshold in node heap
- Move all nodes with larger dual bound to disk, keep others in heap

Depth First Search
Disconnected components

- Consider a MIP with disconnected components

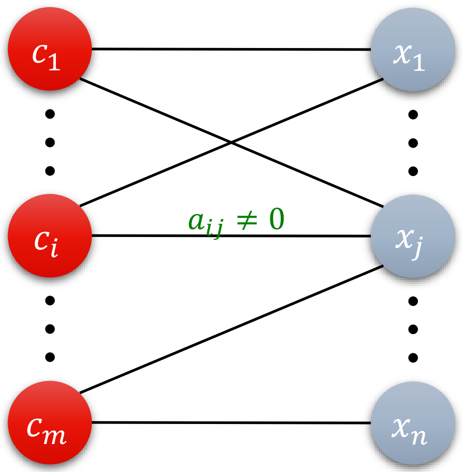
$$
\begin{array}{lccccccl}
\min & c^T x & + & \bar{c}^T \bar{x} & & & \\
\text{s.t.} & Ax & & & \leq & b & \\
& & & \bar{A}\bar{x} & \leq & \bar{b} & \\
& x & & & \in & \mathbb{R}^n & \\
& & & \bar{x} & \in & \mathbb{R}^{\bar{n}} & \\
& x_j & , & \bar{x}_{\bar{j}} & \in & \mathbb{Z} & \text{for all } j \in I, \bar{j} \in \bar{I}
\end{array}
$$

- Solving this as a single MIP with branch-and-cut has worst-case runtime $\mathcal{O}\left(2^{n+\bar{n}}\right)$
- Solving the two MIPs separately has worst-case runtime $\mathcal{O}\left(2^n + 2^{\bar{n}}\right)$
- Significant speed-up also occurs in practice

Depth First Search

Disconnected components

- How to find disconnected components in matrix A?
- Consider bipartite graph

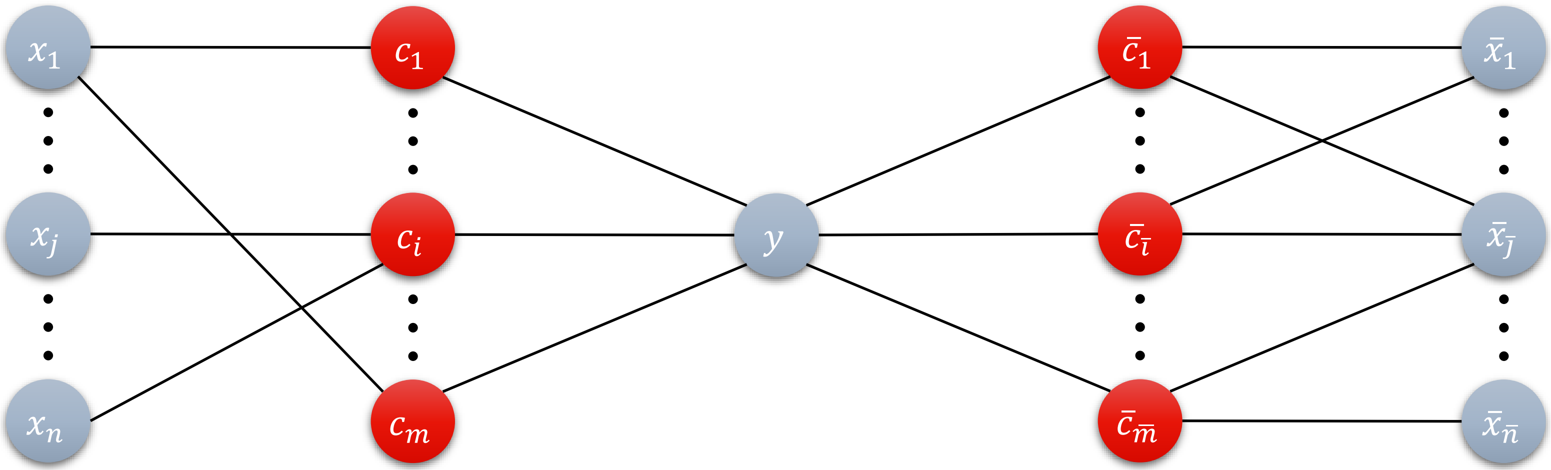


- Depth first search in this graph finds disconnected components of A
- Data structure: store A twice
  - In row-wise sparse compressed form
  - In column-wise sparse compressed form

Depth First Search

Biconnected components

- Assume the bipartite matrix graph has an articulation point



- If this articulation point is a binary variable $y \in \{0,1\}$:
  - Solve smaller component as MIP for $y = 0$ and $y = 1$: optimal solutions $\bar{x}^0$ and $\bar{x}^1$
  - Aggregate variables: $\bar{x}_j \coloneqq \bar{x}^0 + (\bar{x}^1 - \bar{x}^0)y$
- Find articulation points: Tarjan's Algorithm for strongly connected components
  - Need to use non-recursive version of Tarjan (recursion depth may exceed stack size)

Shortest Path

Invalid cycle cuts

- With linear and SOS1 constraints you can model so-called indicator constraints

$$z = 0 \rightarrow x_i = x_j \quad \text{or} \quad z = 0 \rightarrow x_i \neq x_j$$

  for binary variables z, x_i and x_j

- Such constraints appear in some practical applications
- For example, MIPLIB model 'toll-like' is about the balanced subgraph problem
  - Appears in bioinformatics: finding monotone subsystems in gene regulatory networks
  - See http://miplib.zib.de/instance_details_toll-like.html and references

Shortest Path

Invalid cycle cuts

- Consider a set of indicator constraints

$$\begin{aligned} z_k = 0 \rightarrow x_{i_k} = x_{j_k} \text{ for } k \in E \\ z_k = 0 \rightarrow x_{i_k} \neq x_{j_k} \text{ for } k \in U \end{aligned}$$

- Then, for an inequality indicator

$$z_{s,t} = 0 \rightarrow x_s \neq x_t$$

and a path of constraints

$$\begin{array}{cccccc} z_{s,k_1} & = & 0 & \rightarrow & x_s & \doteqdot & x_{k_1} \\ z_{k_1,k_2} & = & 0 & \rightarrow & x_{k_1} & \doteqdot & x_{k_2} \\ & & & \dots & & & \\ z_{k_n,t} & = & 0 & \rightarrow & x_{k_n} & \doteqdot & x_t \end{array}$$

$$\doteqdot \in \{=, \neq\}$$

with an even number of inequality indicators, we can see that

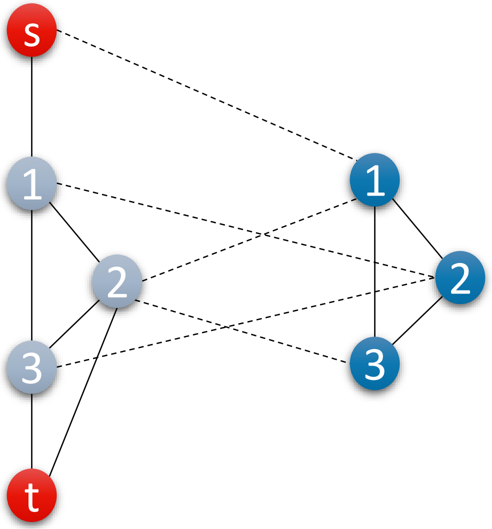
$$z_{s,t} + z_{s,k_1} + z_{k_1,k_2} + \cdots + z_{k_n,t} \geq 1$$

is valid.

Shortest Path

Invalid cycle cuts

- Cut separation algorithm for $z_{s,t} + z_{s,k_1} + z_{k_1,k_2} + \cdots + z_{k_n,t} \geq 1$
  - Start with $z_{s,t}$ with fractional LP solution $z^*_{s,t} \notin \{0,1\}$
  - Search for shortest path $s \rightarrow k_1 \rightarrow \cdots \rightarrow k_n \rightarrow t$
    - Lengths given by the LP values $z^*_{i,j}$
    - Only consider paths with even number of inequality indicators
- Trick for even number of inequality indicators
  - Two copies of graph: G_1 and G_2
  - Equality indicators connect vertices within each copy
  - Inequality indicators connect vertices between copies
  - Nodes s and t only exist in G_1
- Use Dijkstra's algorithm to find shortest path



Shortest Path

Invalid cycle cuts

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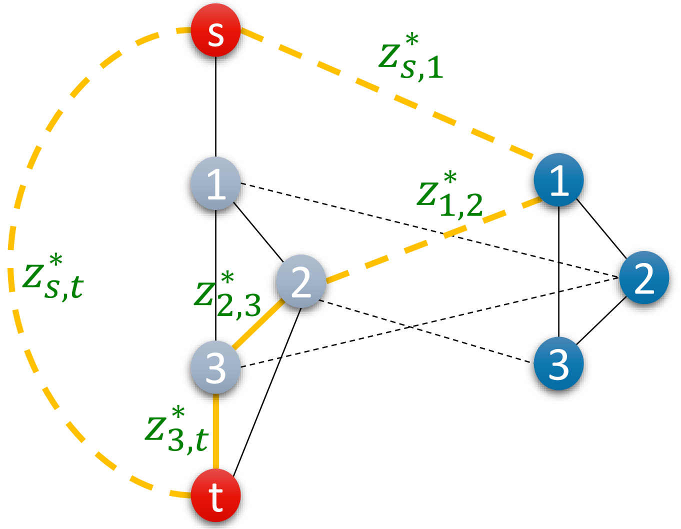
  - Nodes s and t only exist in G_1
- Use Dijkstra's algorithm to find shortest path



$$z_{s,t} + z_{s,1} + z_{1,2} + z_{2,3} + z_{3,t} \geq 1$$

Shortest Path

Mod-2 and mod-k cuts

- Very similar construction possible to separate mod-2 and mod-k cuts
  - Caprara and Fischetti (1996): {0,½}-Chvátal-Gomory cuts
  - Caprara, Fischetti and Letchford (2000): On the separation of maximally violated mod-k cuts
  - Andreello, Caprara and Fischetti (2007): Embedding {0,½}-Cuts in a Branch-and-Cut Framework: A Computational Study
- But Gurobi uses different approach for these cuts
  - Gaussian LU factorization in mod-k space
  - Koster, Zymolka and Kutschka (2009): Algorithms to Separate {0,½}-Chvátal-Gomory Cuts

Shortest Path

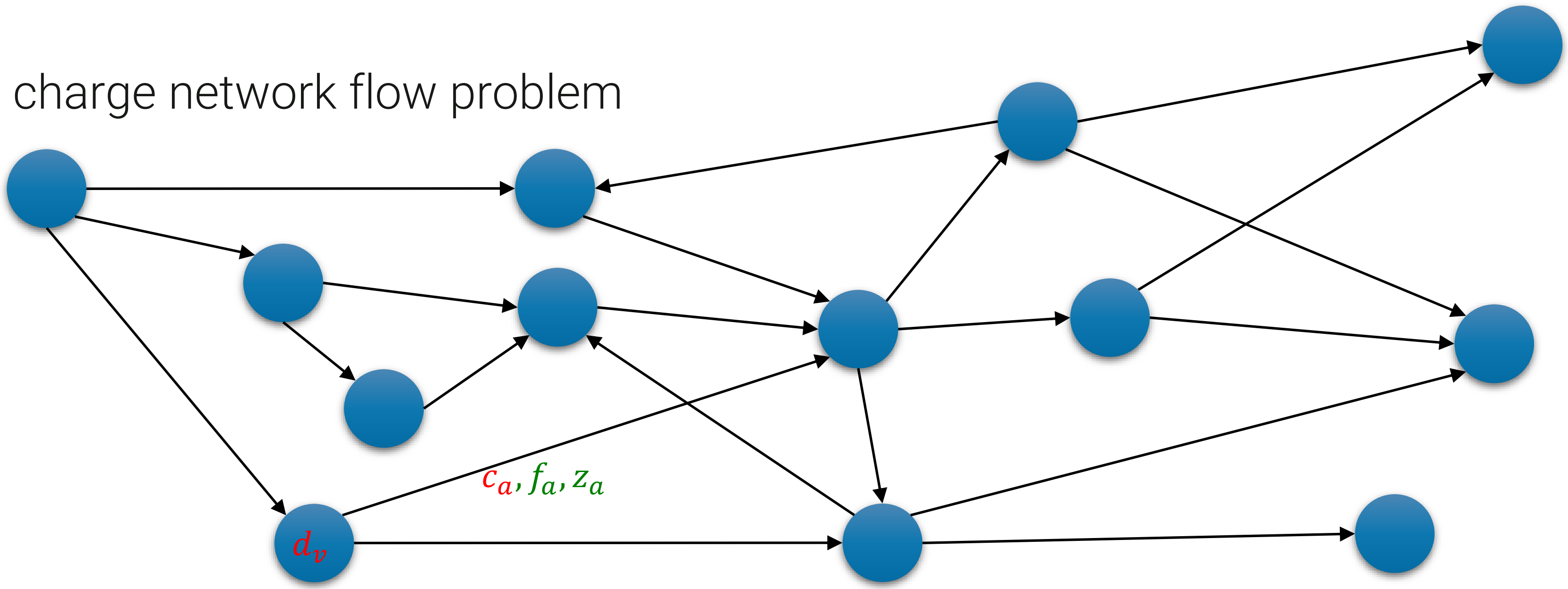
Other applications in MIP

- Network heuristic
  - Find negative cost cycles to improve solution for problems with network structure
- Network simplex algorithm
  - Find negative cost cycles to detect negative reduced costs for pricing selection

Min-Cut / Max-Flow

Network cut separation

- Fixed charge network flow problem

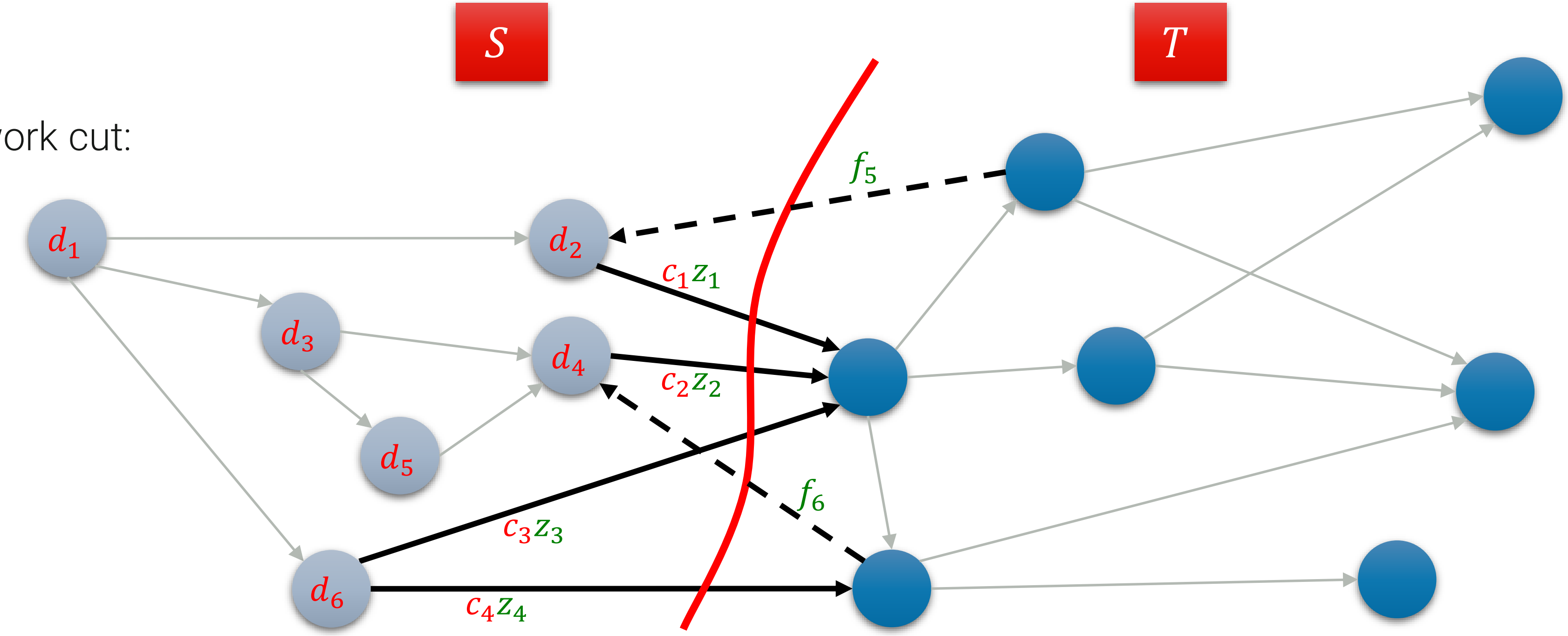


- Flow conservation constraints: $\sum_{a \in \delta^+(v)} f_a - \sum_{a \in \delta^-(v)} f_a = d_v$
- Arc capacity constraints: $f_a - c_a z_a \leq 0$
- Flow variables: $f_a \geq 0$
- Arc selection variables: $z_a \in \{0,1\}$

Min-Cut / Max-Flow

Network cut separation

- Network cut:



- Capacity on network cut must be large enough to transport demand from S to T plus the flow that goes from T back to S:

$$\sum_{a \in \delta^+(S)} c_a z_a - \sum_{a \in \delta^-(S)} f_a \geq \sum_{v \in S} d_v$$

- Dividing by any of the c_a and applying mixed integer rounding yields cut-set inequalities

Min-Cut / Max-Flow

Network cut separation

- Heuristic to separate network cuts
  - Assign arc weights to be $w_a := s_a^* - |\pi_a^*|$
    - LP slack value s_a^* for capacity constraint on arc a
    - Dual solution value π_a^* for capacity constraint on arc a
  - Search for minimum weighted cut in resulting graph
  - Note that weights can be negative!
    - Minimum cut problem with negative weights is $\mathcal{NP}$-hard
- Use heuristic for minimum cut problem
  - Try all single node sets $S = \{v\}$
  - Additionally, contract nodes in non-increasing order of weights w_a until only 5 super nodes are left; then enumerate all cuts
    - Bienstock, Chopra, Günlük, Tsai (1998): Minimum cost capacity installation for multicommodity network flows
    - Günlük (1999): A branch and cut algorithm for capacitated network design problems
    - Achterberg and Raack (2010): The MCF-Separator – Detecting and Exploiting Multi-Commodity Flow Structures in MIPs

Minimum Vertex Separator

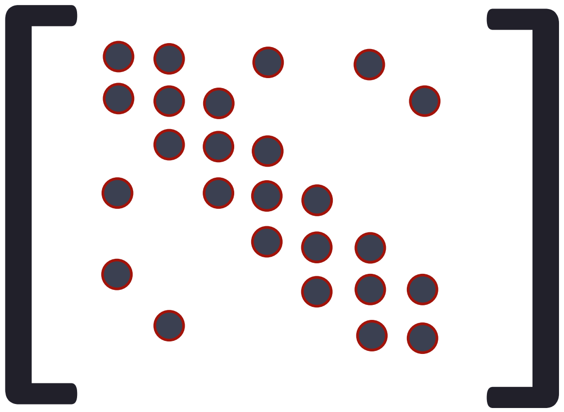
Nested-dissection fill-reducing ordering for interior point LP solver

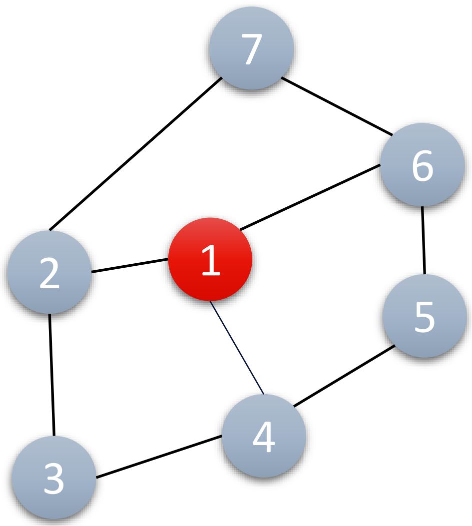
- Runtime for interior point LP solver is dominated by cost of computing a sparse Cholesky factorization on AA^T
- Cost depends heavily on *elimination order* (ordering of rows of A)
  - Some orderings can lead to catastrophic fill-in
- Problem of finding optimal fill-reducing ordering is $\mathcal{NP}$-complete
  - Yannakakis (1981): Computing the Minimum Fill-In is NP-Complete

Minimum Vertex Separator

Nested-dissection fill-reducing ordering for interior point LP solver

- Adjacency graph in sparse Cholesky factorization
  - Simple correspondence between symmetric sparse matrix (structure) and adjacency graph

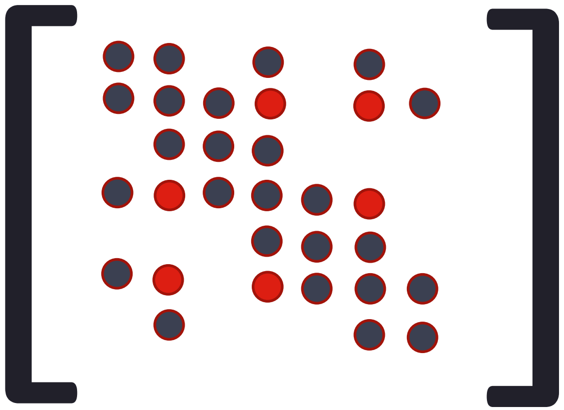


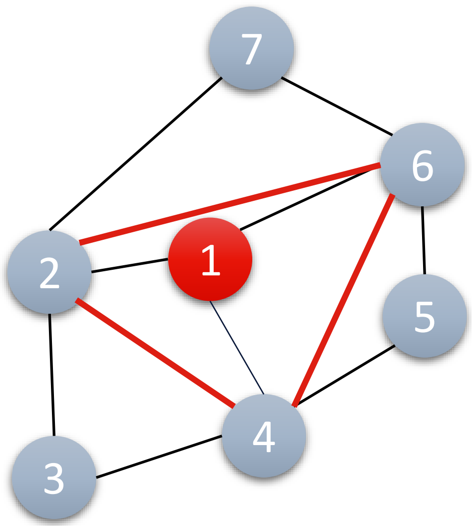


Minimum Vertex Separator

Nested-dissection fill-reducing ordering for interior point LP solver

- Adjacency graph in sparse Cholesky factorization
  - Simple correspondence between symmetric sparse matrix (structure) and adjacency graph
- Gaussian elimination produces cliques



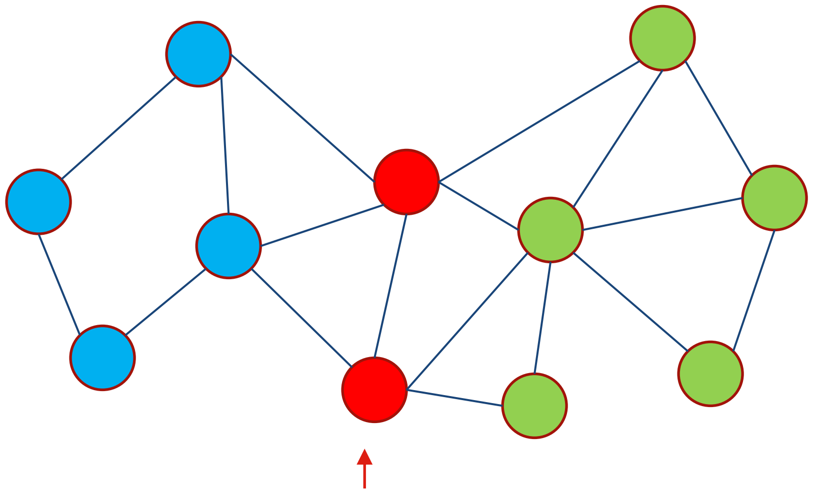


Minimum Vertex Separator

Nested-dissection fill-reducing ordering for interior point LP solver

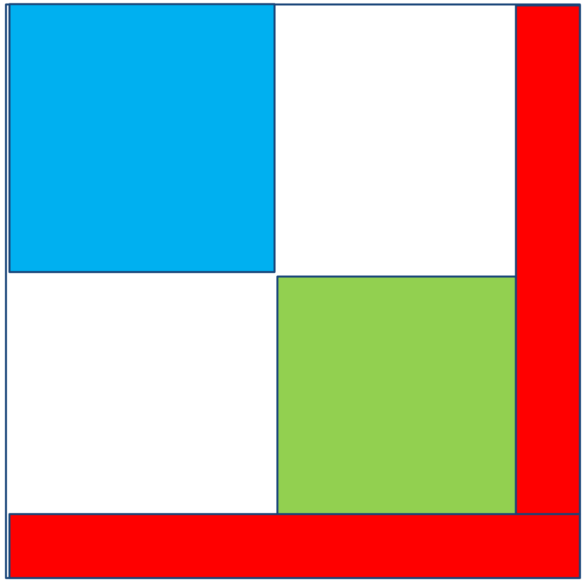
- Nested dissection ordering heuristic
  - Divide and conquer
  - Vertex separators disconnect the problem

Adjacency graph



Vertex separator

Sparse matrix



Max Clique

Clique merging in presolve

- Very common constraints in MIP are set packing constraints

$$x_1 + \cdots + x_k \leq 1$$

  for binary variables x_j

- Multiple set packing constraints can be merged, for example:

$$\begin{array}{ccccccc} x_1 & + & x_2 & & & \leq & 1 \\ x_1 & & & + & x_3 & \leq & 1 \\ & & x_2 & + & x_3 & \leq & 1 \end{array}$$

  can be equivalently represented by

$$x_1 + x_2 + x_3 \leq 1$$

- The latter has a much stronger LP relaxation than the former
  - For example, $x_1 = x_2 = x_3 = 0.5$ is feasible for the former, but not for the latter

Max Clique

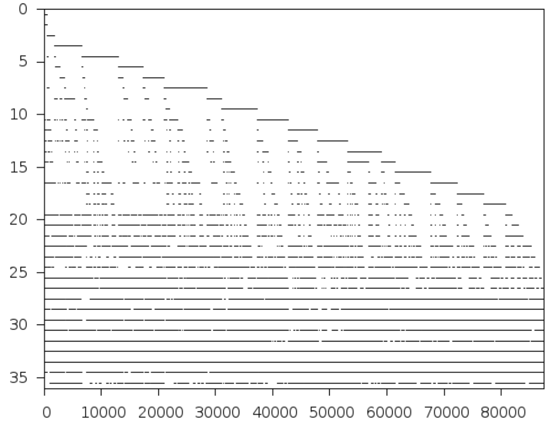
Clique merging in presolve

- Consider stable set relaxation of a MIP
  - Graph $G = (V, E)$ with nodes V being the (complemented) binary variables of the problem and edges $E = \{(i,j) | x_i, x_j \text{ share a set packing constraint}\}$
- For each set packing constraint $S \subseteq V$ find large clique $C \supseteq S$
  - Ideally, find maximum clique
  - Max clique is $\mathcal{NP}$-complete
  - Use heuristic to find large clique
- Replace $\sum_{j \in S} x_j \leq 1$ by $\sum_{j \in C} x_j \leq 1$
- Discard all set packing constraints with $S' \subseteq C$

Max Clique

Clique merging in presolve

- Many heuristics for max clique available
  - E.g., Robson (2001): Finding a maximum independent set in time $\mathcal{O}(2^{n/4})$
- But: problem is not given as $G = (V, E)$
  - Instead, problem is given as $G = (V, \mathcal{C})$ with $\mathcal{C}$ being a set of cliques
    - Edges E implicitly given as all edges defined by cliques $\mathcal{C}$
  - Consider set partitioning instances like nw04
    - Constraints with 50,000 variables imply >1 billion edges!
    - Cannot afford to create $G = (V, E)$ explicitly



nw04

picture from miplib.zib.de

Max Clique

Clique merging in presolve

- Gurobi heuristic is a greedy clique growing heuristic to obtain a maximum clique
  - Start by adding all variables of initial clique S to C
    - Main operation: filter out nodes that are not neighbors of the recently added node v
      - Mark all cliques in which v appears
      - Check for remaining candidates if they appear in one of the marked cliques
        - If not, remove candidate from list
    - Speed-up for main operation:
      - Consider nodes of starting clique in batches of size 32
      - Use bit logic for clique membership check
  - Then, add one or more of the remaining candidates to C
    - Add largest set of candidates that appear in a common clique
    - Safeguard: only process first 10 candidates to count clique cover number
      - Otherwise, too expensive for model with 4 million set packing constraints but only 6800 variables

Max Clique

Clique merging in presolve

- Main operation of Gurobi heuristic traverses columns of matrix
  - Find neighbors by processing the rows of the matrix
  - On average, this touches $\bar{l}_c + \bar{l}_c \cdot \bar{l}_r$ non-zero matrix entries
    - $\bar{l}_c$ and $\bar{l}_r$ being the average number of non-zeros in columns and rows
  - If all set packing constraints are of size 2, this means to touch $3\bar{l}_c$ non-zeros
- Separate clique merging algorithm specialized for short cliques
  - Considers only set packing constraints of size up to 100
  - Explicitly forms $G = (V, E)$, only storing one direction for each edge
  - Reduces memory access for size 2 cliques from $3\bar{l}_c$ to $\bar{l}_c$
    - Typically, translates into a runtime improvement of almost 3x

- See Achterberg, Bixby, Gu, Rothberg and Weninger (2019): Presolve Reductions in Mixed Integer Programming

Max Clique

Clique cuts

- Clique cut separation very similar to clique merging
- Differences:
  - Start with subset of clique
    - Only variables with $x_j^* > 0$
  - Weighted max clique
    - Maximize sum of LP solution values
    - Initially, only consider variables with $x_j^* > 0$
    - Final step is to grow clique further using variables with $x_j^* = 0$

Dynamic Programming

Knapsack coefficient strengthening

- Given a knapsack constraint

$$a_0x_0 + a_1x_1 + \cdots + a_nx_n \leq b$$

  with $a_j > 0$ and binary variables x_j
- Use dynamic programming to calculate

$$\alpha^0 := \max\left\{\left\{\textstyle\sum_{j=1}^{n} a_jx_j \,\middle|\, x \in \{0,1\}^n\right\} \cap [0,b]\right\}$$
$$\alpha^1 := \max\left\{\left\{\textstyle\sum_{j=1}^{n} a_jx_j \,\middle|\, x \in \{0,1\}^n\right\} \cap [0,b-a_0]\right\}$$

  for the activity of the other variables $j = 1, \dots, n$, given $x_0 = 0$ or $x_0 = 1$
- Lifting:
  - If $d^1 := b - a_0 - \alpha^1 > 0$: set $a_0 := a_0 + d^1$
  - If $d^0 := b - \alpha^0 > 0$: set b $:= b - d^0$ and $a_0 := \max\{a_0 - d^0, 0\}$

Dynamic Programming

Knapsack coefficient strengthening

- Example:

$$3x_0 + 4x_1 + 7x_2 + 8x_3 \leq 20$$

- Use dynamic programming to calculate

$$\alpha^0 := \max\left\{\{4x_1 + 7x_2 + 8x_3 | x \in \{0,1\}^n\} \cap [0,20]\right\} = 19$$
$$\alpha^1 := \max\left\{\{\{4x_1 + 7x_2 + 8x_3 | x \in \{0,1\}^n\} \cap [0,17]\}\right\} = 15$$

- Lifting:
  - If $d^1 := b - a_0 - \alpha^1 = 2 > 0$: set $a_0 := a_0 + d^1 = 5$
  - If $d^0 := b - \alpha^0 = 1 > 0$: set b $:= b - d^0 = 19$ and $a_0 := \max\{a_0 - d^0, 0\} = 4$
- Result:

$$4x_0 + 4x_1 + 7x_2 + 8x_3 \leq 19$$

Dynamic Programming

Knapsack coefficient strengthening

- Apply coefficient strengthening
  - on all knapsack constraints in an inner presolve loop
  - on all cutting planes generated during the search
- Thus, this is a very heavily used algorithm!
- Dynamic programming to calculate lifting values is $\mathcal{O}(2^n)$
  - Apply only for knapsacks of length up to 10
  - Otherwise, use more complicated algorithm that
    - deals with a number of special cases,
    - calculates at most 64 different values inside the dynamic program, and
    - aborts if the required number of values exceeds 64

Dynamic Programming

Knapsack cover cut separation

- Given a knapsack constraint

$$a_1 x_1 + \cdots + a_n x_n \leq b$$

  with $a_j > 0$ and binary variables x_j
- A subset $C \subseteq N := \{1, \dots, n\}$ is called a *cover* if $\sum_{j \in C} a_j > b$
- Resulting cover cut: $\sum_{j \in C} x_j \leq |C| - 1$

- Separation:
  - Set $C^0 := \{j | x_j^* = 0\}$, $C^1 := \{j | x_j^* = 1\}$, $C^f := N \backslash C^0 \backslash C^1$
  - Find greedy minimum cover C for $\sum_{j \in C^f} a_j x_j \leq b - \sum_{j \in C^1} a_j$
  - Safeguard: only proceed if $|C| \cdot n \leq 10^9$
  - Up-lift variables in $C^f \backslash \mathrm{C}$ to make cut stronger
  - Down-lift variables in C^1 to make cut valid for N
  - Up-lift variables in C^0 to make cut stronger

Graph Automorphism

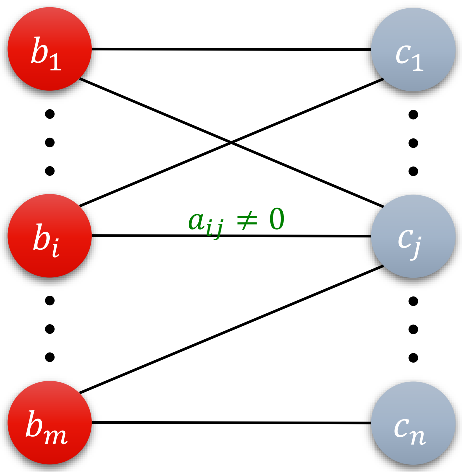
Symmetry detection

- A bijection $f: \mathbb{R}^n \to \mathbb{R}^n$ is called a *symmetry* for a given MIP if
  - it maps the feasible solution space X of the MIP to itself: $f(X) = X$, and
  - it preserves objective values: $c^T f(x) = c^T x$ for all $x \in X$
- This definition based on feasible solution space X is not practical, as deciding whether $X = \emptyset$ is $\mathcal{NP}$-complete
- In practice: consider permutations that leave constraints and objective invariant
  - A permutation $\pi: N \to N$ of column indices is a *formulation symmetry* if there exists a permutation $\sigma: M \to M$ of row indices such that
    - $\pi(I) = I$ (i.e., π preserves integer variables),
    - $\pi(c) = c$,
    - $\sigma(b) = b$, and
    - $A_{\sigma(i),\pi(j)} = A_{i,j}$ for all $i \in M$, $j \in N$

Graph Automorphism

Symmetry detection

- Detecting formulation symmetries for MIP can be reduced to detecting graph automorphisms



  - Bipartite graph with nodes for constraints and variables, edges for non-zero coefficients
  - Constraint nodes are colored with right hand side values b_i
  - Variable nodes are colored with objective values c_j (and integrality property)
  - Edges are colored with matrix coefficients
- Graph automorphism that respects colors is formulation symmetry of MIP

Graph Automorphism

Symmetry detection

- Complexity status of graph automorphism problem is still unknown
  - No polynomial algorithm known
  - Not proven to be $\mathcal{NP}$-hard
  - See Read and Corneil (1977): The graph isomorphism disease
- Efficient algorithms in practice exist
  - nauty
  - saucy
  - bliss
- Gurobi implements a variant of these algorithms
- See also Pfetsch and Rehn (2019): A computational comparison of symmetry handling methods for mixed integer programs

Graph Automorphism

Symmetry detection in Gurobi

- Maintain two sets of partitions for constraints and variables
  - $\overline{\Sigma}$ and $\overline{\Pi}$ to group constraints and variables that could potentially be in same orbit
  - $\underline{\Sigma}$ and $\underline{\Pi}$ to group constraints and variables that are definitely in the same orbit
- Initially, $\overline{\Sigma}$ and $\overline{\Pi}$ are defined by node colors, $\underline{\Sigma}$ and $\underline{\Pi}$ are all singletons
- Recursively refine $\overline{\Sigma}$ and $\overline{\Pi}$ using hash values
  - calculated from hash values of neighbor nodes
- If fix point is reached, branch on a non-singleton part of $\overline{\Sigma}$ or $\overline{\Pi}$
  - Failed branch refines partitions and thus hash values
  - Leaf branching node corresponds to valid symmetry generator and updates $\underline{\Sigma}$ and $\underline{\Pi}$
- Perform branching with backtracking until
  - $\overline{\Sigma} = \underline{\Sigma}$ and $\overline{\Pi} = \underline{\Pi}$ (generators to produce all symmetries have been found), or
  - a work limit has been hit (generators produce a subset of the symmetries)

Graph Automorphism

Symmetry detection in Gurobi

- Important tricks to get good performance in practice
  - Sparse updates of data structures
    - Only touch those constraints and variables in refinement that have changed
    - When splitting a partition class, assign new label to smaller part
  - Special treatment of singleton partition classes
    - Remove them from graph after hash update, as their hashes won't change anymore
  - Use very good hash function to avoid hash collisions
  - Initially, check whether old symmetry generators are still valid
    - If we search for symmetry again after some problem changes
  - Check work limits regularly to avoid bad corner cases

- Why care?
  - Exploiting symmetry yields ~20% performance improvement overall
  - ~2x speed-up on affected models
  - See Achterberg and Wunderling (2013): Mixed Integer Programming: Analyzing 12 Years of Progress

Union Find

Symmetry aggregations

- Consider a symmetry generator $g: N \rightarrow N$ that is
  - non-overlapping
    - No x_j appears in the same constraint as $x_{g(j)}$
  - or that does not affect integer variables
    - For all $j \in I$ we have $g(j) = j$
- Then we can aggregate all variables according to the generator:

$$x_j \coloneqq x_{g(j)}$$

- Each symmetry generator extends sets of equivalent variables
- This can be efficiently recorded with a union find data structure

Other Interesting Algorithms

Sorting

Euclidean algorithm

Hashing

Random number generation

... not covered today

GUROBI
OPTIMIZATION