An Exact Branch and Bound Algorithm

with

Symmetry Breaking

for the

Maximum Balanced Induced Biclique Problem

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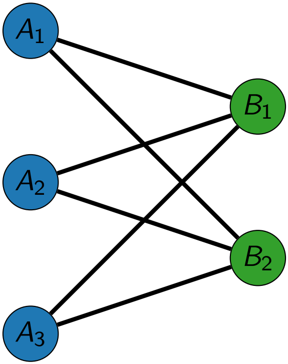
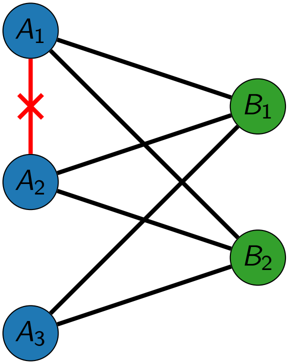
Maximum Balanced Induced Bicliques

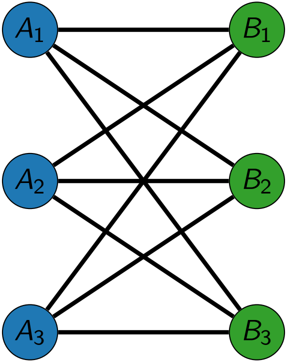
Bicliques



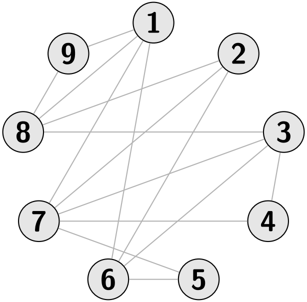
Induced Bicliques



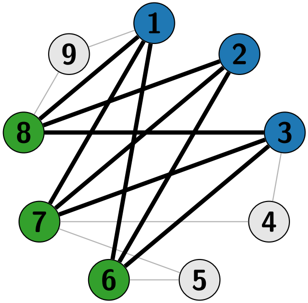
Balanced Bicliques



The Maximum Balanced Induced Biclique Problem



The Maximum Balanced Induced Biclique Problem



Existing Results

Complexity

- NP-hard, even in a bipartite graph (Garey and Johnson).

Other Biclique Variants

- Maximum vertex non-induced biclique:
  - Trivially useless.
- Maximum vertex biclique in a bipartite graph:
  - Easy (König's theorem and bipartite matching).
  - Corollary: maximum clique for a union of two cliques is easy.
- Maximum vertex induced biclique in an arbitrary graph:
  - NP-hard
  - Applications in data mining.
- Maximum edge induced biclique in a bipartite graph:
  - NP-hard
  - Applications in data mining.

Applications

?

Why Care?

- Interesting algorithmic properties:
  - Non-hereditary, but still reasonably well-behaved.
  - We have a good bound.
  - One simple symmetry.

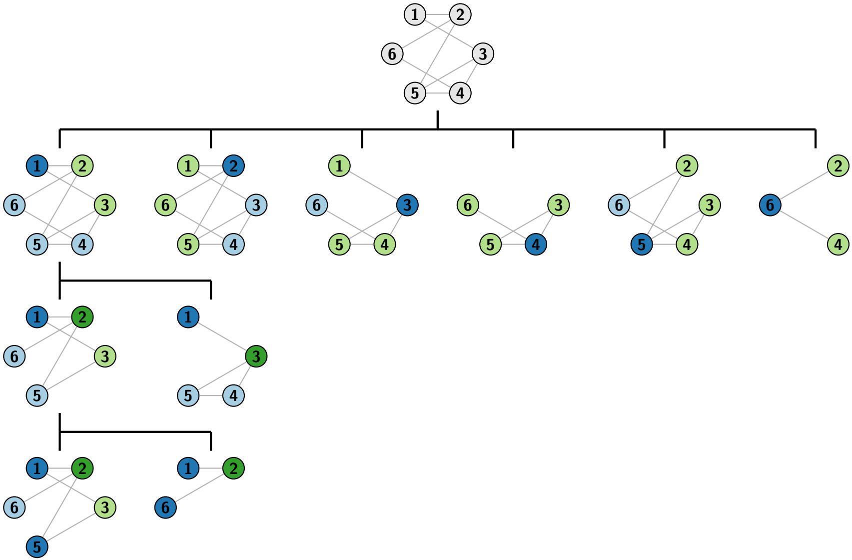
Our Algorithm

Inspiration

- Maximum clique algorithms by Tomita et al.
- Bitset encodings by San Segundo et al.
    - A speedup of between two and twenty for maximum clique.

Branch...

- Recursively grow two compatible independent sets, A and B.
- Have two candidate sets, P_a and P_b.
- Recursively expand:
  - Pick a vertex v from P_a, add it to A.
  - So we must remove adjacent vertices from P_a, and non-adjacent vertices from P_b.
  - Now recurse, swapping the roles of A and B.
  - Then consider removing v from A and P_a.


1
2
6
3
5
4

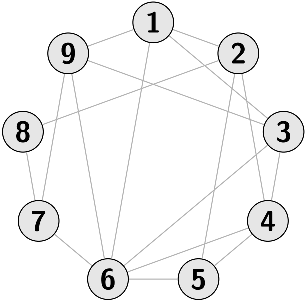
. . . and Bound

- Keep track of the best solution found so far, (A_{max}, B_{max}). We call this the *incumbent*.
- Careful! The balance condition means feasibility is not quite hereditary. At leaf nodes, either $|A| = |B|$ or $|A| = |B| + 1$.
- If $|A| + |P_a| \leq |A_{max}|$, or $|B| + |P_b| \leq |B_{max}|$, then we cannot unseat the incumbent, so we backtrack.
- A much better bound can be found using clique covers.

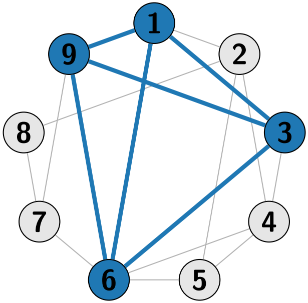
A Bound using Clique Covers

- If we can colour a graph using k colours, it cannot contain a clique with more than k vertices (each vertex in a clique must be given a different colour).
- Dually, if we can cover a graph using k cliques, its independence number is at most k.

A Bound using Clique Covers



A Bound using Clique Covers



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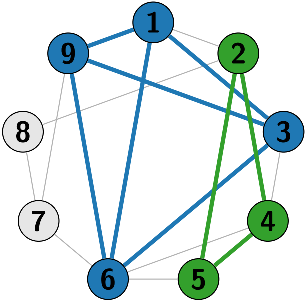

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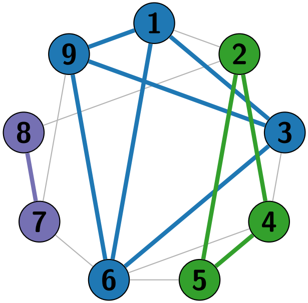


A Bound using Clique Covers

- We use a greedy clique cover.
- Vertices are permuted at the top of search, for a static variable ordering.
- We only need to perform one clique cover per recursive call, not one per vertex selection.

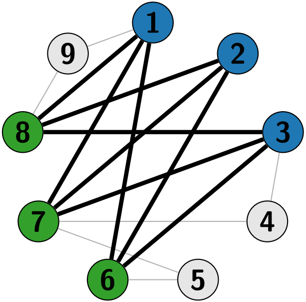
Dealing with Bipartite Graphs

- This bound knows about independent sets on each side, but not about compatibility.
- This bound is useless if the graph is bipartite, or becomes bipartite during search.
- We can detect this: a greedy clique cover uses k cliques iff the input is an independent set.
- Open problem: find a bound for this case which is both useful and quick to compute.

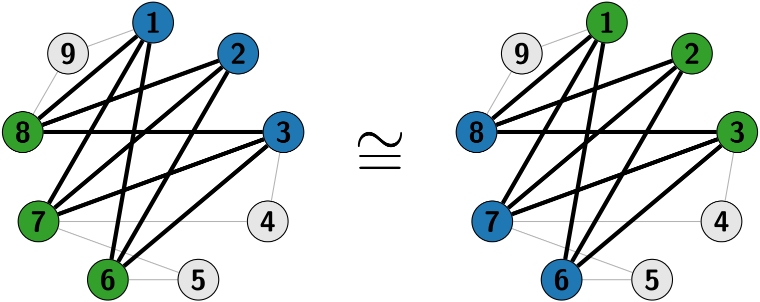
Symmetries

$$(A, B) \cong (B, A)$$

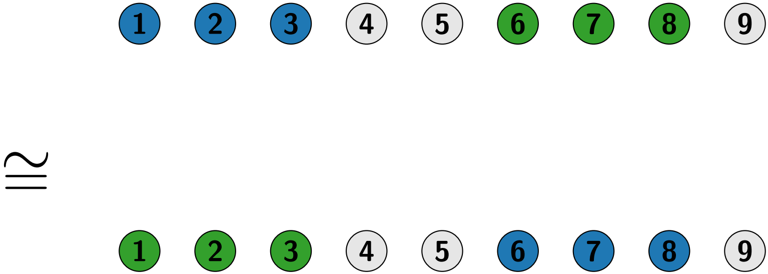
Symmetries



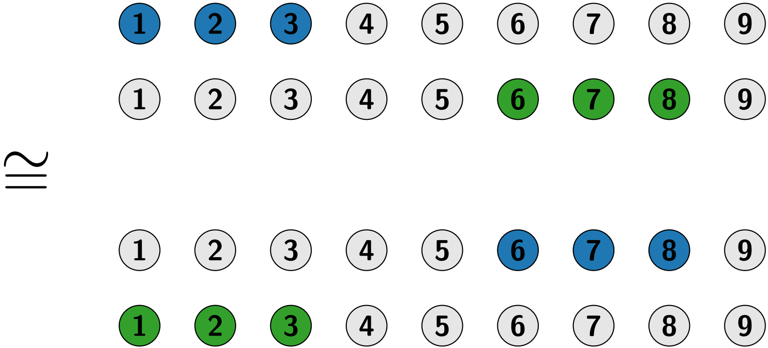
Symmetries



Excluding Symmetries



Excluding Symmetries



Excluding Symmetries

1	1	1	0	0	0	0	0	0
0	0	0	0	0	1	1	1	0

$\cong$

0	0	0	0	0	1	1	1	0
1	1	1	0	0	0	0	0	0

Excluding Symmetries

$$\begin{array}{ccccccccc} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}$$

$\geq_{lex}$

$$\begin{array}{ccccccccc} 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{array}$$

$\cong$

$$\begin{array}{ccccccccc} 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{array}$$

$\leq_{lex}$

$$\begin{array}{ccccccccc} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}$$

Excluding Symmetries using Lex

- Idea: only find solutions (A, B) where $A \geq_{lex} B$.
  - Don't swap the roles of A and B when recursing for the purposes of this test.
- We remove half of the solutions (not half of the search space).
- If we can prove that $B \geq_{lex} A$ must hold based upon the decisions made so far, backtrack.
- The most significant set bit in A must be more significant than the most significant bit set in B.
- If the first k bits of A are zero, then the first k bits of B must be zero.

Excluding Symmetries: What Could Possibly Go Wrong?

- We may have to explore deep into the search tree before the rule kicks in: so long as the most significant bit is undecided, we can't filter anything.
- Worse, we may exclude a solution which we would otherwise find quickly.

Excluding Symmetries, Second Attempt

- We have fixed an arbitrary order for the bits. This order may not be the same as the decision order.
- Idea: allow the algorithm to select the arbitrary order for the lex comparison.
- So we select the most significant bit first.
- When we reject a vertex v from A, if B is empty, then reject v from P_b.

Excluding Symmetries, with Two Lines of Code

`expand` :: (Graph G, Set A, Set B, Set P_a, Set P_b, Set A_{max}, Set B_{max})

begin
  $(bounds, order) \leftarrow$ `cliqueSort`(G, P_a)
  for $i \leftarrow |P_a|$ **downto** 1 **do**
    if $bounds[i] + |A| > |A_{max}|$ **and** $|P_b| + |B| > |B_{max}|$ **then**
      $v \leftarrow order[i]$
      $A \leftarrow A \cup \{v\}$ // Consider $v \in A$
      $P_a \leftarrow P_a \setminus \{v\}$
      $P'_a \leftarrow P_a \cap \overline{\mathrm{N_G}(v)}$ // Remove vertices adjacent to v
      $P'_b \leftarrow P_b \cap \mathrm{N_G}(v)$ // Remove vertices not adjacent to v
      if $|A| = |B|$ **and** $|A| > |A_{max}|$ **then**
        $(A_{max}, B_{max}) \leftarrow (A, B)$ // We've found a better solution
      if $P'_b \neq \emptyset$ **then**
        `expand`$(G, B, A, P'_b, P'_a, B_{max}, A_{max})$ // Swap and recurse
      $A \leftarrow A \setminus \{v\}$ // Now consider $v \notin A$
      if $B = \emptyset$ **then**
        $P_b \leftarrow P_b \setminus \{v\}$ // Avoid symmetric solutions

Excluding Symmetries, with Two Lines of Code

```
expand :: (Graph G, Set A, Set B, Set Pa, Set Pb, Set Amax, Set Bmax)
begin
    (bounds, order) ← cliqueSort(G, Pa)
    for i ← |Pa| downto 1 do
        if bounds[i] + |A| > |Amax| and |Pb| + |B| > |Bmax| then
            v ← order[i]
            A ← A ∪ {v}                                  // Consider v ∈ A
            Pa ← Pa \ {v}
            P'a ← Pa ∩ ‾N_G(v)‾                          // Remove vertices adjacent to v
            P'b ← Pb ∩ N_G(v)                            // Remove vertices not adjacent to v
            if |A| = |B| and |A| > |Amax| then
                (Amax, Bmax) ← (A, B)                    // We've found a better solution
            if P'b ≠ ∅ then
                expand(G, B, A, P'b, P'a, Bmax, Amax)    // Swap and recurse
            A ← A \ {v}                                  // Now consider v ∉ A
            if B = ∅ then
                Pb ← Pb \ {v}                            // Avoid symmetric solutions
```

Excluding Symmetries, with Two Lines of Code

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  $(bounds, order) \leftarrow$ cliqueSort(G, P_a)
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      $v \leftarrow order[i]$
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begin
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    for i ← |P_a| downto 1 do
        if bounds[i] + |A| > |A_max| and |P_b| + |B| > |B_max| then
            v ← order[i]
            A ← A ∪ {v}                                  // Consider v ∈ A
            P_a ← P_a \ {v}
            P'_a ← P_a ∩ overline(N_G(v))                // Remove vertices adjacent to v
            P'_b ← P_b ∩ N_G(v)                          // Remove vertices not adjacent to v
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Excluding Symmetries, with Two Lines of Code

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  - **if** $bounds[i] + |A| > |A_{max}|$ **and** $|P_b| + |B| > |B_{max}|$ **then**
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    - **if** $P'_b \neq \emptyset$ **then**
      - $\texttt{expand}(G, B, A, P'_b, P'_a, B_{max}, A_{max})$ — // Swap and recurse
    - $A \leftarrow A \setminus \{v\}$ — // Now consider $v \notin A$
    - **if** $B = \emptyset$ **then**
      - $P_b \leftarrow P_b \setminus \{v\}$ — // Avoid symmetric solutions

The Rest of the Algorithm

`improvedBiclique` :: (Graph G) $\rightarrow$ (Set **of** Integer, Set **of** Integer)
begin
    $(A_{max}, B_{max}) \leftarrow (\emptyset, \emptyset)$
    permute G so that the vertices are in non-increasing degree order
    `expand`$(G, \emptyset, \emptyset, \mathrm{V}(G), \mathrm{V}(G), A_{max}, B_{max})$
    return (A_{max}, B_{max}) (unpermuted)

`cliqueSort` :: (Graph G, Set P) $\rightarrow$ (Array **of** Integer, Array **of** Integer)
begin
    bounds $\leftarrow$ an Array **of** Integer
    order $\leftarrow$ an Array **of** Integer
    $P' \leftarrow P$ `// vertices yet to be allocated`
    $k \leftarrow 1$ `// current clique number`
    while $P' \neq \emptyset$ **do**
        $Q \leftarrow P'$ `// vertices to consider for the current clique`
        while $Q \neq \emptyset$ **do**
            $v \leftarrow$ the first element of Q `// get next vertex to allocate`
            $P' \leftarrow P' \setminus \{v\}$
            $Q \leftarrow Q \cap \mathrm{N}(G, v)$ `// remove non-adjacent vertices`
            append k to *bounds*
            append v to *order*
        $k \leftarrow k + 1$ `// start a new clique`
    return (*bounds*, *order*)

The Rest of the Algorithm

```
improvedBiclique :: (Graph G) → (Set of Integer, Set of Integer)
begin
    (A_max, B_max) ← (∅, ∅)
    permute G so that the vertices are in non-increasing degree order
    expand(G, ∅, ∅, V(G), V(G), A_max, B_max)
    return (A_max, B_max) (unpermuted)

cliqueSort :: (Graph G, Set P) → (Array of Integer, Array of Integer)
begin
    bounds ← an Array of Integer
    order ← an Array of Integer
    P′ ← P                                  // vertices yet to be allocated
    k ← 1                                   // current clique number
    while P′ ≠ ∅ do
        Q ← P′                              // vertices to consider for the current clique
        while Q ≠ ∅ do
            v ← the first element of Q      // get next vertex to allocate
            P′ ← P′ \ {v}
            Q ← Q ∩ N(G, v)                 // remove non-adjacent vertices
            append k to bounds
            append v to order
        k ← k + 1                           // start a new clique
    return (bounds, order)
```

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            append k to bounds
            append v to order
        k ← k + 1                            // start a new clique
    return (bounds, order)
```

Results

Results

- We can solve all but four DIMACS problems in under a day.
- Usually, but not always, easier than maximum clique.
- Usually, but not always, easier than maximum independent set.
- Large sparse graphs with $|V| > 15,000$ and $|E| > 250,000$ take under 20 seconds.
- Excluding symmetries gains us between 0% and 50%.

Results

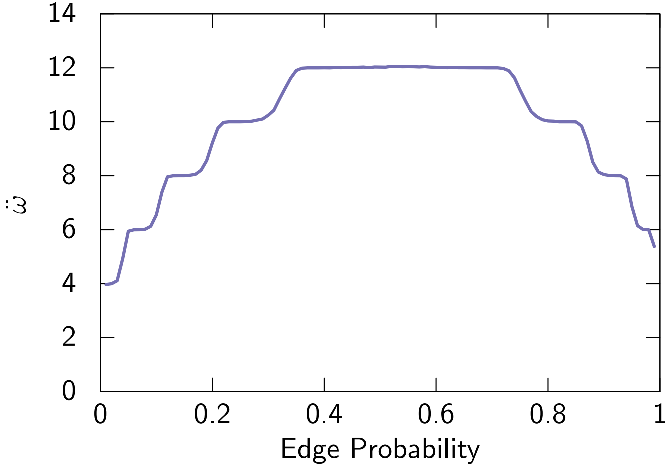
- We can solve all but four DIMACS problems in under a day.
- Usually, but not always, easier than maximum clique.
- Usually, but not always, easier than maximum independent set.
- Large sparse graphs with $|V| > 15,000$ and $|E| > 250,000$ take under 20 seconds.
- Excluding symmetries gains us between 0% and 50%.
    - Unless you look closely...
    - The bound function can get worse for subproblems ("misleading"), and is not invariant under isomorphism ("evil"). Occasionally this gives wild results.

Future Work

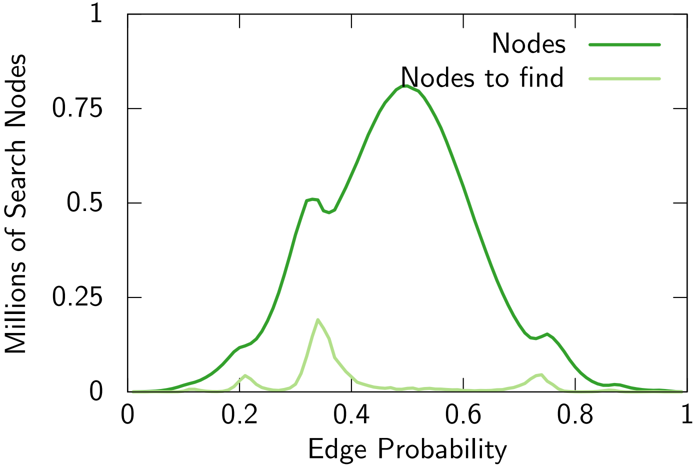
Is an Algorithm Worth It?

- A naïve constraint programming model is easy, but slow.
- What about a better constraint programming model?
- What about MIP?

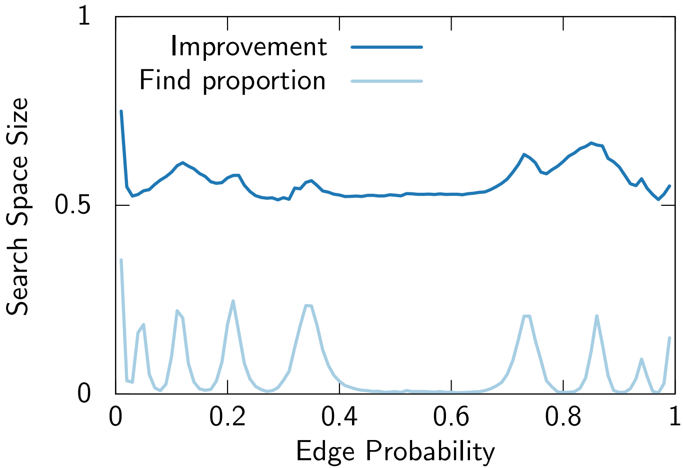
Random Graphs G(250, x)



Difficulty of G(250, x)



Effects of Symmetry Exclusion in G(250, x)



Parallel Branch and Bound

- For maximum clique, parallel branch and bound typically gives us close to linear speedups, and sometimes much better.
- We do the same here. But how do symmetries interact with parallelism?

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