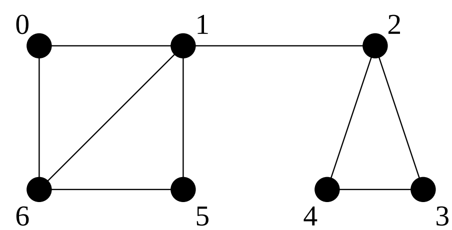
BACKTRACKING (CONT'D)

Backtracking: Generating all Cliques

PROBLEM: All Cliques
INSTANCE: a graph $G = (V, E)$.
FIND: all cliques of G without repetition



Cliques (and maximal cliques): $\emptyset, \{0\}, \{1\}, \ldots, \{6\}$, $\{0,1\}, \{0,6\}, \underline{\{1,2\}}, \{1,5\}, \{1,6\}, \{2,3\}, \{2,4\}, \{3,4\}, \{5,6\}$, $\underline{\{0,1,6\}}, \underline{\{1,5,6\}}, \underline{\{2,3,4\}}$.

DEFINITIONS:

Clique in $G(V, E)$: $C \subseteq V$ such that for all $x, y \in C$, $x \neq y$, $\{x, y\} \in E$.

Maximal clique: a clique not properly contained into another clique.

Many combinatorial problems can be reduced to finding cliques (or the largest clique):

1. Largest indepednent set in G (stable set): is the same as largest clique in $\overline{G}$.
2. Exact cover of sets by subsets: find clique with special property.
3. Find a Steiner triple sustem of order v: find a largest clique in a special graph.
4. Find all intersecting set systems: find all cliques in a special graph.
5. Etc.

In a Backtracking algorithm:
$X = [x_0, x_1, \ldots, x_{l-1}]$ is a partial solution
$\iff \{x_0, x_1, \ldots, x_{l-1}\}$ is a clique.
But we don't want ot get the same k-clique $k!$ times:
$[0, 1]$ extends to $[0, 1, 6]$
$[0, 6]$ extends to $[0, 6, 1]$

So we require partial solutions for be in sorted order:
$x_0 < x_1 < x_2 < \ldots < x_{l-1}$.

Let $S_{l-1} = \{x_0, x_1, \ldots, x_{l-1}\}$ for $X = [x_0, x_1, \ldots, x_{l-1}]$.

The **choice set** of this point is:
if $l = 0$ then $\mathcal{C}_0 = V$
if $l > 0$ then

$$\begin{aligned} \mathcal{C}_l &= \{v \in V \setminus S_{l-1} : v > x_{l-1} \text{ and } \{v, x\} \in E \text{ for all } x \in S_{l-1}\} \\ &= \{v \in \mathcal{C}_{l-1} \setminus \{x_{l-1}\} : \{v, x_{l-1}\} \in E \text{ and } v > x_{l-1}\} \end{aligned}$$

To compute $\mathcal{C}_l$, define:
$A_v = \{u \in V : \{u, v\} \in E\}$ (vertices adjacent to v)
$B_v = \{v + 1, v + 2, \ldots, n - 1\}$ (vertices larger than v)
$\mathcal{C}_l = A_{x_{l-1}} \cap B_{x_{l-1}} \cap \mathcal{C}_{l-1}$.

To **detect if a clique is maximal** (set inclusionwise):
Calculate N_l, the set of vertices that can extend S_{l-1}:
$N_0 = V$
$N_l = N_{l-1} \cap A_{x_{l-1}}$.
S_{l-1} is maximal $\iff N_l = \emptyset$.

Algorithm AllCliques(l)
Global: X, $\mathcal{C}_l (l = 0, \ldots, n-1)$, A_l, B_l pre-computed.

```
if (l = 0) then output ([ ]);
           else output ([x_0, x_1, ..., x_{l-1}]);
if (l = 0) then N_l ← V;
           else N_l ← A_{x_{l-1}} ∩ N_{l-1};
if (N_l = ∅) then output ("maximal");
if (l = 0) then C_l ← V;
           else C_l ← A_{x_{l-1}} ∩ B_{x_{l-1}} ∩ C_{l-1};
for each (x ∈ C_l) do
    x_l ← x;
    AllCliques(l + 1);
```

First call: AllCliques(0).

Average Case Analysis of AllCliques

Let G be a graph with n vertices and let $c(G)$ be the number of cliques in G.
The running time for AllCliques for G is in $O(nc(G))$, since $O(n)$ is an upper bound for the running time at a node, and $c(G)$ is the number of nodes visited.

Let $\mathcal{G}_n$ be the set of all graphs on n vertices.
$|\mathcal{G}_n| = 2^{\binom{n}{2}}$
(bijection between $\mathcal{G}_n$ and all subsets of the set of unordered pairs of $\{1, 2, \ldots, n\}$).

Assume the graphs in $\mathcal{G}_n$ are equally likely inputs for the algorithm (that is, assume uniform probability distribution on $\mathcal{G}_n$).
Let $T(n)$ be the average running time of AllCliques for graphs in $\mathcal{G}_n$.
Let $\overline{c}(n)$ be the average number of cliques in a graph in $\mathcal{G}_n$.
Then, $T(n) \in O(n\overline{c}(n))$.

So, all we need to do is estimating $\overline{c}(n)$.

$$\overline{c}(n) = \frac{\Sigma_{G \in \mathcal{G}_n} c(G)}{|\mathcal{G}_n|} = \frac{1}{2^{\binom{n}{2}}} \sum_{G \in \mathcal{G}_n} c(G).$$

We will show that:

$$\overline{c}(n) \leq (n+1)n^{\log_2 n}, \text{ for } n \geq 4.$$

SKEETCH OF THE PROOF:
Define the indicator function, for each sunset $W \subseteq V$:

$$\mathcal{X}(G,W) = \begin{cases} 1, & \text{if } W \text{ is a clique of } G \\ 0, & \text{otherwise} \end{cases}$$

Then,

$$\begin{aligned} \overline{c}(n) &= \frac{1}{2^{\binom{n}{2}}} \sum_{G\in\mathcal{G}_n} c(G) \\ &= \frac{1}{2^{\binom{n}{2}}} \left(\sum_{W\subseteq V} \mathcal{X}(G,W) \right) \\ &= \frac{1}{2^{\binom{n}{2}}} \sum_{W\subseteq V} \sum_{G\in\mathcal{G}_n} \mathcal{X}(G,W) \end{aligned}$$

Now, for fixed W, $\Sigma_{G\in\mathcal{G}_n} \mathcal{X}(G,W) = 2^{\binom{n}{2}-\binom{|W|}{2}}$.
(Number of subsets of $\binom{V}{2}$ containing edges of W)

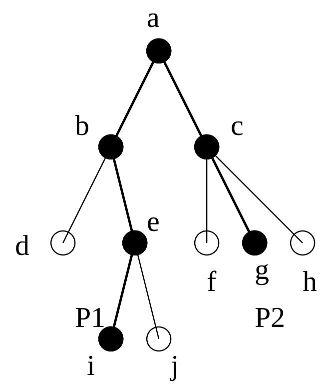
$$\begin{aligned} \overline{c}(n) &= \frac{1}{2^{\binom{n}{2}}} \sum_{W\subseteq V} 2^{\binom{n}{2}-\binom{|W|}{2}} \\ &= \frac{1}{2^{\binom{n}{2}}} \sum_{k=0}^{n} \binom{n}{k} 2^{\binom{n}{2}-\binom{k}{2}} \\ &= \sum_{k=0}^{n} \frac{\binom{n}{k}}{2^{\binom{k}{2}}}. \end{aligned}$$

So, $\overline{c}(n) = \Sigma_{k=0}^{n} t_k$, where $t_k = \frac{\binom{n}{k}}{2^{\binom{k}{2}}}$.
A technical part of the proof bounds t_k as follows: $t_k \leq n^{\log_2 n}$ (see the textbook for details).
So, $\overline{c}(n) = \Sigma_{k=0}^{n} t_k \leq \Sigma_{k=0}^{n} n^{\log_2 n} = (n+1)n^{\log_2 n} \in O(n^{\log_2 n+1})$.

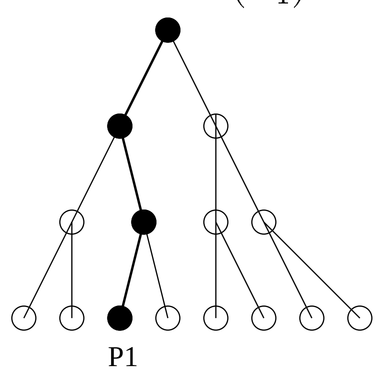
Thus, $T(n) \in O(n\overline{c}(n)) \subseteq O(n^{\log_2 n+2})$.

Estimating the size of a Backtrack tree

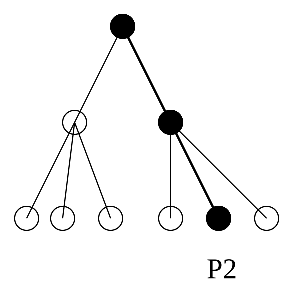
State Space Tree: tree size = 10



Probing path P_1:
Estimated tree size: $N(P_1) = 15$



Probing path P_2:
Estimated tree size: $N(P_2) = 9$



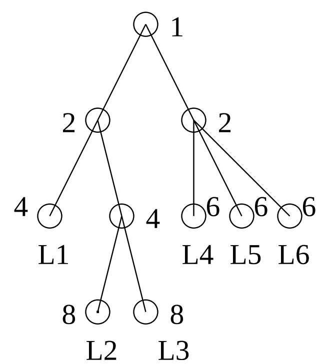
Game for chosing a path (probing):
At each nde of the tree, pick a child node uniformly at random.

For each leaf L, calculate $P(L)$, the probability that L is reached.

We will prove later that the expected value of $\overline{N}$ of $N(L)$ turns out to be the size of the space state tree. Of course,

$$\overline{N} = \sum_{L \text{ leaf}} P(L)N(L) \qquad \text{(by definition)}$$

In the previous example, consider T:



The numbers besides the nodes represent the estimated number of nodes at this level of the tree if this node is in the path to the chosen leaf.
$P(L_1) = 1/4$, $P(L_2) = P(L_3) = 1/8$,
$P(L_4) = P(L_5) = P(L_6) = 1/6$
$N(L_1) = 1 + 2 + 4 = 7$
$N(L_2) = N(L_3) = 1 + 2 + 4 + 8 = 15$
$N(L_4) = N(L_5) = N(L_6) = 1 + 2 + 6 = 9$

$$\overline{N} = \sum_{i=1}^{6} P(L_i)N(L_i) = \frac{1}{4} \times 7 + 2 \times (\frac{1}{8} \times 15) + 3 \times (16 \times 9) = 10 = |T|$$

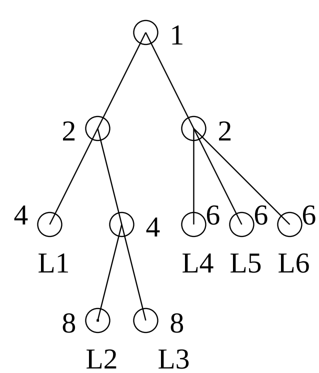
In practice, to **estimate** $\overline{N}$, do k probes $L_1, L_2, \ldots, L_k$, and calculate the average of $N(L_i)$:

$$N_{est} = \frac{\Sigma_{i=1}^{k} N(L_i)}{k}$$

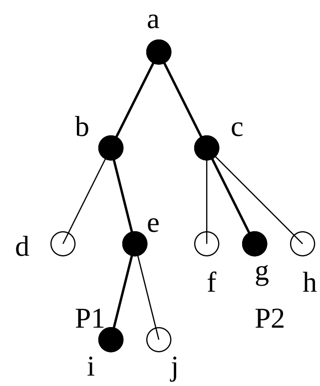
Each probe is performed by running the following algorithm:

Algorithm EstimateBacktrackSize()

$s \leftarrow 1$; $N \leftarrow 1$; $l \leftarrow 0$;
Compute $\mathcal{C}_0$;
while $\mathcal{C}_l \neq \emptyset$) do
    $c \leftarrow |\mathcal{C}_l|$;
    $s \leftarrow c * s$;
    $N \leftarrow N + s$;
    $x_l \leftarrow$ a random element of $\mathcal{C}_l$;
    Compute $\mathcal{C}_{l+1}$ for $[x_0, x_1, \ldots, x_l]$;
    $l \leftarrow l + 1$;
return N;



In the example below, doing only 2 probes:



we get:

P_1:	l	$\mathcal{C}_l$	c	x_l	s	N
					1	1
	0	b, c	2	b	2	3
	1	d, e	2	e	4	7
	2	i, j	2	i	8	$\underline{15}$
	3	$\emptyset$				

P_1:	l	$\mathcal{C}_l$	c	x_l	s	N
					1	1
	0	b, c	2	b	2	3
	1	f, g, h	3	g	6	$\underline{9}$
	2	$\emptyset$				

Based on these 2 probes the estimated size of the tree is:

$$N_{est} = \frac{15+9}{2} = 12.$$

Theorem.
For a state space tree T, let P be the path probed by the algorithm EstimateBacktrackSize.
If $N = N(P)$ is the value returned by the algorithm, then the expected value of N is $|T|$.
Proof.
Define the folwing function on the nodes of T:

$$S([x_0, x_1, \ldots, x_{l-1}]) = \begin{cases} 1, & \text{if } l = 0 \\ |\mathcal{C}_{l-1}| \times S([x_0, x_1, \ldots, x_{l-2}]) & \end{cases}$$

($s \leftarrow c * s$ in the algorithm)
The algorithm computes: $N(P) = \Sigma_{Y \in P} S(Y)$.
$P = P(X)$ is a path in T from root to leaf X, say $X = [x_0, x_1, \ldots, x_{l-1}]$.
Call $X_i = [x_0, x_1, \ldots, x_i]$.
The probability that $P(X)$ is chosen is:

$$\frac{1}{\mathcal{C}_0(x_0)} \times \frac{1}{\mathcal{C}_1(x_1)} \times \ldots \times \frac{1}{\mathcal{C}_{l-1}(x_{l-1})} = \frac{1}{S(X)}.$$

So,

$$\begin{aligned} \overline{N} &= \sum_{X \in \mathcal{L}(T)} prob(P(X)) \times N(P(X)) \\ &= \sum_{X \in \mathcal{L}(T)} \frac{1}{S(X)} \sum_{Y \in P(X)} S(Y) \\ &= \sum_{Y \in T} \sum_{\{X \in \mathcal{L}(T) : Y \in P(X)\}} \frac{S(Y)}{S(X)} \\ &= \sum_{Y \in T} S(Y) \sum_{\{X \in \mathcal{L}(T) : Y \in P(X)\}} \frac{1}{S(X)} \end{aligned}$$

We claim that: $\Sigma_{\{X \in \mathcal{L}(T): Y \in P(X)\}} \frac{1}{S(X)} = \frac{1}{S(Y)}$.

Proof of the claim:
Let Y be a non-leaf. If Z is a child of Y and Y has c children, then $S(Z) = c \times S(Y)$.
So,

$$\sum_{\{Z:Z \text{ is a child of } Y\}} \frac{1}{S(Z)} = c \times \frac{1}{c \times S(Y)} = \frac{1}{S(Y)}$$

Iterating this equation until all Z's are leafs:

$$\frac{1}{S(Y)} = \sum_{\{X:X \text{ is a leaf descendant of } Y\}} \frac{1}{S(X)}$$

So the claim is proved!

Thus,

$$\begin{aligned} \overline{N} &= \sum_{Y \in T} S(Y) \sum_{\{X \in \mathcal{L}(T): Y \in P(X)\}} \frac{1}{S(X)} \\ &= \sum_{Y \in T} S(Y) \frac{1}{S(Y)} \\ &= \sum_{Y \in T} 1 = |T|. \end{aligned}$$

The theorem is thus proved!

Exact Cover

PROBLEM: Exact Cover
INSTANCE: a collection $\mathcal{S}$ of subsets of $\mathcal{R} = \{0, 1, \ldots, n-1\}$.
QUESTION: Does $\mathcal{S}$ contain an exact cover of $\mathcal{R}$

Rephrasing the question:
Does there exist $\mathcal{S}' = \{S_{x_0}, S_{x_1}, \ldots, S_{x_{l-1}}\} \subseteq \mathcal{S}$ such that every element of $\mathcal{R}$ is contained in exactly one set of $\mathcal{S}'$?

Transforming into a clique problem:

$\mathcal{S} = \{S_0, S_1, \ldots, S_{m-1}\}$

Define: $G(V, E)$ in the following way: $V = \{0, 1, , \ldots, m-1\}$
$\{i, j\} \in E \iff S_i \cap S_j = \emptyset$

An exact cover of $\mathcal{R}$ is a clique of G that covers $\mathcal{R}$.

Good ordering on $\mathcal{S}$ for prunning:
$\mathcal{S}$ sorted in decreasing lexicographical ordering.
Choice set:

$$\begin{aligned} \mathcal{C}'_0 &= V \\ \mathcal{C}'_l &= A_{x_{l-1}} \cap B_{x_{l-1}} \cap \mathcal{C}'_{l-1}, \text{ if } l > 0, \end{aligned}$$

where

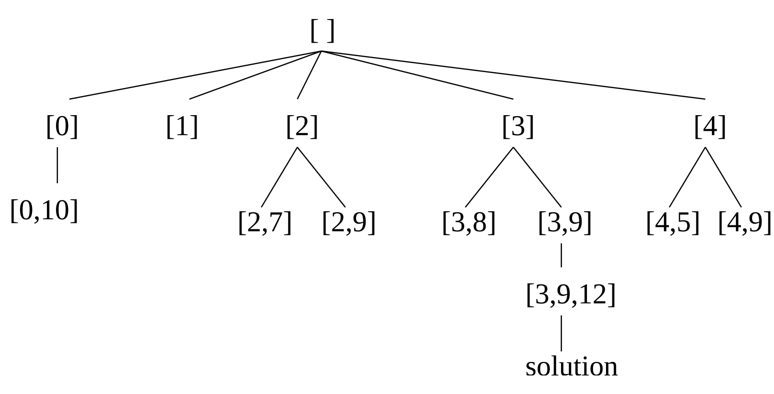
$$\begin{aligned} A_x &= \{y \in V : S_y \cap S_x = \emptyset\} \quad \text{(vertices adjacent to } x) \\ B_x &= \{y \in V : S_x >_{lex} S_y\} \end{aligned}$$

Further pruning will be used to reduce $\mathcal{C}'_l$ by removing H_r's, which will be defined later.

Example: (corrected from book page 121)

j	S_j	rank(S_j)	$A_j \cap B_j$	corrected?
0	0,1,3,	104	10	Y
1	0,1,5	98	12	
2	0,2,4	84	7,9	Y
3	0,2,5	82	8,9,12	Y
4	0,3,6	73	5,9	Y
5	1,2,4	52	$\emptyset$	
6	1,2,6	49	11	Y
7	1,3,5	42	$\emptyset$	Y
8	1,4,6	37	$\emptyset$	
9	1	32	10,11,12	
10	2,5,6	19	$\emptyset$	
11	3,4,5	14	$\emptyset$	
12	3,4,6	13	$\emptyset$	

i	0	1	2	3	4	5	6
H_i	0,1,2,3,4	5,6,7,8,9	10	11,12	$\emptyset$	$\emptyset$	$\emptyset$



ExactCover $(n, \mathcal{S})$

Global X, $\mathcal{C}_l$, $l = (0, 1, \ldots)$

Procedure ExactCoverBT(l, r')

if $(l = 0)$ then $U_0 \leftarrow \{0, 1, \ldots, n-1\}$;

$r \leftarrow 0$;

else $U_l \leftarrow U_{l-1} \setminus S_{x_{l-1}}$;

$r \leftarrow r'$;

while $(r \notin U_l)$ and $(r < n)$ do $r \leftarrow r + 1$;

if $(r = n)$ then output $([x_0, x_1, \ldots, x_{l-1}])$.

if $(l = 0)$ then $\mathcal{C}'_0 \leftarrow \{0, 1, \ldots, m-1\}$;

else $\mathcal{C}'_l \leftarrow A_{x_{l-1}} \cup B_{x_{l-1}} \cup \mathcal{C}'_{l-1}$;

$\mathcal{C}_l \leftarrow \mathcal{C}'_l \cap H_r$;

for each $(x \in \mathcal{C}_l)$ do

$x_l \leftarrow x$;

ExactCoverBT$(l + 1, r)$;

Main

$m \leftarrow |\mathcal{S}|$;

Sort $\mathcal{S}$ in decreasing lexico order

for $i \leftarrow 0$ to $m - 1$ do

$A_i \leftarrow \{j : S_i \cap S_j = \emptyset\}$;

$B_i \leftarrow \{i + 1, i + 2, \ldots, m - 1\}$;

for $i \leftarrow 0$ to $n - 1$ do

$H_i \leftarrow \{j : S_j \cap \{0, 1, \ldots, i\} = \{i\}\}$;

$H_n \leftarrow \emptyset$;

ExactCoverBT$(0, 0)$;

(U_i contains the uncovered elements at level i.
r is the smallest uncovered in U_i.)

BACKTRACKING WITH BOUNDING

Backtracking with bounding

Bounding functions:

When applying backtracking for an **optimization** problem, we use **bounding** for prunning the tree.

Let us consider a **maximization** problem.

Let profit(X) = profit for a feasible solution X.

For a partial soluion $X = [x_0, x_1, \ldots, x_{l-1}]$, define

$$P(X) = \max \{ \text{ profit}(X') : \text{ for all feasible solutions } X' = [x_0, x_1, \ldots, x_{l-1}, x'_l, \ldots, x'_{n-1}] \}.$$

A bounding function B is a real valued function defined on the nodes of the space state tree, such that for any feasible solution X, $B(X) \geq P(X)$.

$B(X)$ is an upper boud on the profit of any feasible solution that is descendant of X in the state space tree.

If the current best solution found has value $OptP$, then we can prune nodes X with $B(X) \leq OptP$, since $P(X) \leq B(X) \leq OptP$, that is, no descendant of X will improve on the current best solution.

General Backtracking with Bounding

Algorithm BOUNDING(l)

Global X, $OptP$, $OptX$, $\mathcal{C}_l$, $l = (0, 1, \ldots)$

if ($[x_0, x_1, \ldots, x_{l-1}]$ is a feasible solution) then

  $P \leftarrow$ profit($[x_0, x_1, \ldots, x_{l-1}]$);

  if ($P > OptP$) then

    $OptP \leftarrow P$;

    $OptX \leftarrow [x_0, x_1, \ldots, x_{l-1}]$;

Compute $\mathcal{C}_l$;

$B \leftarrow B([x_0, x_1, \ldots, x_{l-1}])$;

for each ($x \in \mathcal{C}_l$) do

  if $B \leq OptP$ then return;

  $x_l \leftarrow x$;

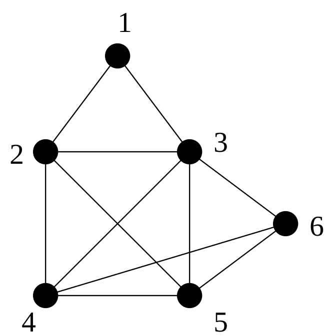
  BOUNDING($l + 1$)

Maximum Clique Problem

Problem: Maximum Clique (optimization)
Instance: a graph $G = (V, E)$.
Find: a maximum clique of G.

This problem is NP-complete.

Example:



Maximum cliques:

{2,3,4,5}, {3,4,5,6}

Modification of AllCliques in order to find the maximum clique (no bounding).

Boldface adds **bounding** to this algorithm.

Algorithm MaxClique(l)
Global: X, $\mathcal{C}_l (l = 0, \ldots, n-1)$, A_l, B_l pre-computed.

```
if (l > OptSize) then
    OptSize ← l;
    OptClique ← [x_0, x_1, ..., x_{l-1}];
if (l = 0) then C_l ← V;
            else C_l ← A_{x_{l-1}} ∩ B_{x_{l-1}} ∩ C_{l-1};
M ← B([x_0, x_1, ..., x_{l-1}]);      (bold: bounding)
for each (x ∈ C_l) do
    if (M ≤ OptSize) then return;      (bold: bounding)
    x_l ← x;
    MaxClique(l + 1);
```

Main

```
    OptSize ← 0;
    MaxClique(0);
    output OptClique;
```

Bounding Functions for MaxClique

Definition. Induced Subgraph
Let $G = (V, E)$ and $W \subseteq V$. The subgraph induced by W, $G[W]$, has vertex set W and edgeset: $\{\{u, v\} \in E : u, v \in W\}$.

If we have:
partial solution: $X = [x_0, x_1, \ldots, x_{l-1}]$ with choice set $\mathcal{C}_l$,
extension solution $X = [x_0, x_1, \ldots, x_{l-1}, x_l, \ldots, x_j]$,
Then $\{x_l, \ldots, x_j\}$ must be a clique in $G[\mathcal{C}_l]$.

Let $mc(l)$ denote the size of a maximum clique in $G[\mathcal{C}_l]$, and let $ub(l)$ be an upper bound on $mc(l)$.

Then, a general bounding function is $B(X) = l + ub[l]$.

Bound based on size of subgraph

Since $mc(l) \leq |\mathcal{C}_l|$, we derive the bound:

$$B_1(X) = l + |\mathcal{C}_l|.$$

Bounds based on colouring

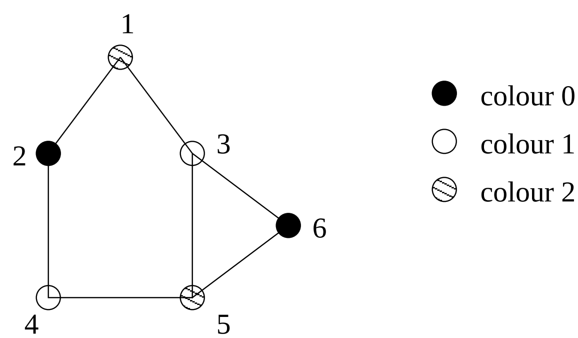
Definition. Vertex Colouring

Let $G = (V, E)$ and k a positive integer. A (vertex) k-colouring of G is a function

$$\text{Color}: V \rightarrow \{0, 1, \ldots, k-1\}$$

such that, for all $\{x, y\} \in E$, $\text{Color}(x) \neq \text{Color}(y)$.

Example: a 3-colouring of a graph:



Lemma. If G has a k-colouring, then the maximum clique of G has size at most k.

Proof. Let C be a clique. Each $x \in C$ must have a distinct colour. So, $|C| \leq k$. This is true for any clique, in particular for the maximum clique.

Finding the minimum colouring gives the best upper bound, but it is a hard problem. We will use a **greedy heuristic** for finding a small colouring.

Define $\textsc{ColourClass}[h] = \{i \in V : \textsc{Colour}[i] = h\}$.

```
GreedyColour(G = (V, E))
        Global Colour
        k ← 0; // colours used so far
        for i ← 0 to n − 1 do
                h ← 0;
                while (h < k) and (A_i ∩ ColourClass[h] ≠ ∅) do
                        h ← h + 1;
                if (h = k) then k ← k + 1;
                                ColourClass[h] ← ∅;
                ColourClass[h] ← ColourClass[h] ∪ {i};
                Colour[i] = h;
        return k;
```

Sampling Bound:

Statically, beforehand, run GreedyColour(G), determining k and Colour[x] for all $x \in V$.

SamplingBound($X = [x_0, x_1, \ldots, x_{l-1}]$)
    Global $\mathcal{C}_l$, Colour
    return $l + |\{\text{Colour}[x] : x \in \mathcal{C}_l\}|$;

Greedy Bound:

Call GreedyColour dynamically.

GreedyBound($X = [x_0, x_1, \ldots, x_{l-1}]$)
    Global $\mathcal{C}_l$
    $k \leftarrow$GreedyColour($G[\mathcal{C}_l]$);
    return $l + k$;

Here I discuss the performance for random graphs, comparing the 3 bounds seen.

Please, refer to Tables 4.4 and 4.5 in the textbook.