Exhaustive Generation: Backtracking and Branch-and-bound

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Knapsack Problem

Knapsack (Optimization) Problem

Instance: Profits $p_0, p_1, \ldots, p_{n-1}$
Weights $w_0, w_1, \ldots, w_{n-1}$
Knapsack capacity M

Find: and n-tuple $[x_0, x_1, \ldots, x_{n-1}] \in \{0,1\}^n$
such that $P = \sum_{i=0}^{n-1} p_i x_i$ is maximized,
subject to $\sum_{i=0}^{n-1} w_i x_i \leq M$.

Example

Objects:	1	2	3	4
weight (lb)	8	1	5	4
profit	$500	$1,000	$ 300	$ 210

Knapsack capacity: $M = 10$ lb.

Two feasible solutions and their profit:

x_1	x_2	x_3	x_4	profit
1	1	0	0	$ 1,500
0	1	1	1	$ 1,510

This problem is NP-hard.

Naive Backtracking Algorithm for Knapsack

Examine all 2^n tuples and keep the ones with maximum profit.

Global Variables $X, OptP, OptX$.
Algorithm $\textsc{Knapsack1}\ (l)$

```
if (l = n) then
    if Σ_{i=0}^{n-1} w_i x_i ≤ M then CurP ← Σ_{i=0}^{n-1} p_i x_i;
        if (CurP > OptP) then
            OptP ← CurP;
            OptX ← [x_0, x_1, ..., x_{n-1}];
else x_l ← 1; Knapsack1 (l + 1);
     x_l ← 0; Knapsack1 (l + 1);
```

First call: $OptP \leftarrow -1$; $\textsc{Knapsack1}\ (0)$.

Running time: 2^n n-tuples are checked, and it takes $\Theta(n)$ to check each solution. The total running time is $\Theta(n2^n)$.

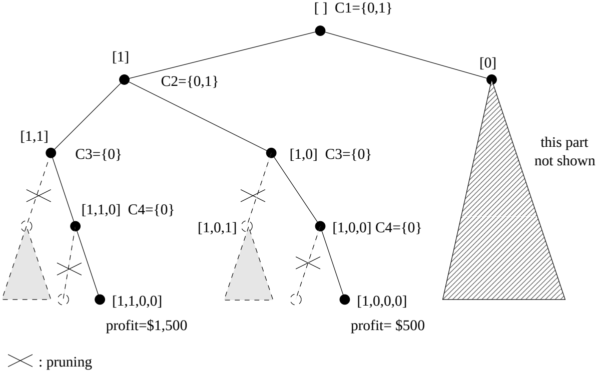
A General Backtracking Algorithm

- Represent a solution as a list: $X = [x_0, x_1, x_2, \ldots]$.
- Each $x_i \in P_i$ (possibility set)
- Given a partial solution: $X = [x_0, x_1, \ldots, x_{l-1}]$, we can use constraints of the problem to limit the choice of x_l to $\mathcal{C}_l \subseteq P_l$ (choice set).
- By computing $\mathcal{C}_l$ we prune the search tree, since for all $y \in P_l \setminus \mathcal{C}_l$ the subtree rooted on $[x_0, x_1, \ldots, x_{l-1}, y]$ is not considered.

Part of the search tree for the previous Knapsack example:

w_i	8	1	5	4
p_i	\$500	\$1,000	\$ 300	\$ 210

$M = 10.$



General Backtracking Algorithm with Pruning

Global Variables $X = [x_0, x_1, \ldots]$, $\mathcal{C}_l$, for $l = 0, 1, \ldots$).

Algorithm $\textsc{Backtrack}\ (l)$
- if ($X = [x_0, x_1, \ldots, x_{l-1}]$ is a feasible solution) then
  - "Process it"
- Compute $\mathcal{C}_l$;
- for each $x \in \mathcal{C}_l$ do
  - $x_l \leftarrow x$;
  - $\textsc{Backtrack}(l+1)$;

Backtracking with Pruning for Knapsack

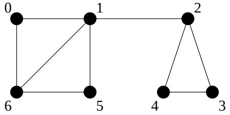
Global Variables $X, OptP, OptX$.
Algorithm $\textsc{Knapsack2}\ (l, CurW)$

if $(l = n)$ then if $(\sum_{i=0}^{n-1} p_i x_i > OptP)$ then
$OptP \leftarrow \sum_{i=0}^{n-1} p_i x_i$;
$OptX \leftarrow [x_0, x_1, \ldots, x_{n-1}]$;
if $(l = n)$ then $\mathcal{C}_l \leftarrow \emptyset$
else if $(CurW + w_l \leq M)$ then $\mathcal{C}_l \leftarrow \{0, 1\}$;
else $\mathcal{C}_l \leftarrow \{0\}$;
for each $x \in \mathcal{C}_l$ do
$x_l \leftarrow x$;
$\textsc{Knapsack2}\ (l + 1, CurW + w_l x_l)$;

First call: $\textsc{Knapsack2}\ (0, 0)$.

Backtracking: Generating all Cliques

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



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

Definition

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):

- Largest independent set in G (stable set): is the same as largest clique in $\overline{G}$.

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- Find a Steiner triple system of order v: find a largest clique in a special graph.
- Find all intersecting set systems: find all cliques in a special graph.
- 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

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

So,
$\mathcal{C}_0 = V$
$\mathcal{C}_l = \{v \in \mathcal{C}_{l-1} \setminus \{x_{l-1}\} : \{v, x_{l-1}\} \in E \text{ and } v > x_{l-1}\}$, for $l > 0$

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

if $(l = 0)$ then output $([\ ])$;
  else output $([x_0, x_1, \ldots, x_{l-1}])$;
if $(l = 0)$ then $N_l \leftarrow V$;
  else $N_l \leftarrow A_{x_{l-1}} \cap N_{l-1}$;
if $(N_l = \emptyset)$ then output ("maximal");
if $(l = 0)$ then $\mathcal{C}_l \leftarrow V$;
  else $\mathcal{C}_l \leftarrow A_{x_{l-1}} \cap B_{x_{l-1}} \cap \mathcal{C}_{l-1}$;
for each $(x \in \mathcal{C}_l)$ do
  $x_l \leftarrow x$;
  $\textsc{AllCliques}(l+1)$;

First call: $\textsc{AllCliques}(0)$.

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 $\mathcal{G}_n$.
We will calculate $T(n)$.

$T(n) =$ 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 $\overline{c}(n)$.

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

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,

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

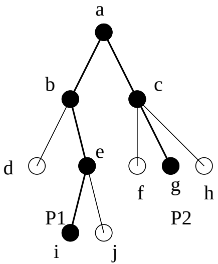
Now, for fixed W, $\sum_{G \in \mathcal{G}_n} \mathcal{X}(G, W) = 2^{\binom{n}{2} - \binom{|W|}{2}}$.
(Number of subsets of $\binom{V}{2}$ containing edges of W)

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

So, $\overline{c}(n) = \sum_{k=0}^{n} t_k$, 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, $\overline{c}(n) = \sum_{k=0}^{n} t_k \leq \sum_{k=0}^{n} n^{\log_2 n} = (n+1) n^{\log_2 n} \in O(n^{\log_2 n + 1})$.
Thus, $T(n) \in O(n \overline{c}(n)) \subseteq O(n^{\log_2 n + 2})$.

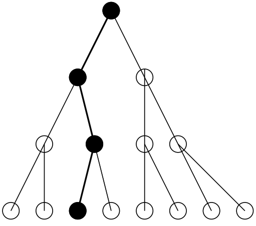
Estimating the size of a Backtrack tree

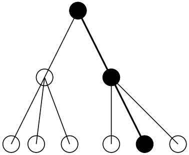
State Space Tree: tree size $= 10$



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

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





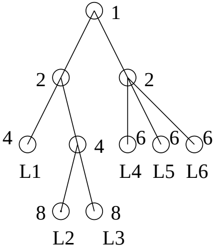
Probing path P_1:
Estimated tree size: $N(P_1) = 15$

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

Game for chosing a path (probing):
At each node 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 (number is estimated number of nodes at this level)



$P(L_1) = 1/4$, $P(L_2) = P(L_3) = 1/8$, $P(L_4) = P(L_5) = P(L_6) = 1/6$
$N(L_1) = 1 + 2 + 4 = 7$ $N(L_2) = N(L_3) = 1 + 2 + 4 + 8 = 15$
$N(L_4) = N(L_5) = N(L_6) = 1 + 2 + 6 = 9$

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

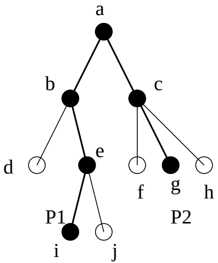
In practice, to **estimate** $\overline{N}$, do k probes $L_1, L_2, \ldots, L_k$, and calculate the average of $N(L_i)$:

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

Algorithm $\textsc{EstimateBacktrackSize}()$

```
s ← 1; N ← 1; l ← 0;
Compute C_0;
while C_l ≠ ∅) do
    c ← |C_l|;
    s ← c ∗ s;
    N ← N + s;
    x_l ← a random element of C_l;
    Compute C_{l+1} for [x_0, x_1, ..., x_l];
    l ← l + 1;
return N;
```

In the example below, doing only 2 probes:



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	c	2	3
	1	f, g, h	3	g	6	$\underline{9}$
	2	$\emptyset$				

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 following 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: $N(P) = \sum_{Y \in P} S(Y)$.

$P = P(X)$ 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 $P(X)$ 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: $\sum_{\{X \in \mathcal{L}(T): Y \in P(X)\}} \frac{1}{S(X)} = \frac{1}{S(Y)}$.

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

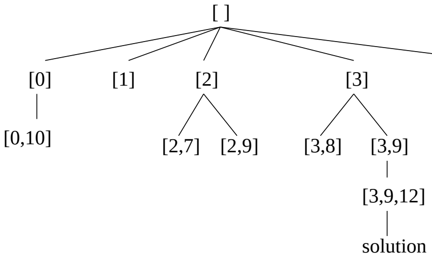
$$\begin{aligned} A_x &= \{y \in V : S_y \cap S_x = \emptyset\} \quad \text{(vertices adjacent to } x\text{)} \\ B_x &= \{y \in V : S_x >_{lex} S_y\} \end{aligned}$$

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	∅	∅	∅



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

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

Procedure $\textsc{ExactCoverBT}(l, r')$

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

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

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

$x_l \leftarrow x$;

$\textsc{ExactCoverBT}(l + 1, r)$;

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
  $H_i \leftarrow \{j : S_j \cap \{0, 1, \ldots, i\} = \{i\}\}$;
$H_n \leftarrow \emptyset$;
$\textsc{ExactCoverBT}(0, 0)$;

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

Backtracking with bounding

When applying backtracking for an **optimization** problem, we use **bounding** for prunning the tree.
Let us consider a **maximization** problem.
Let $\text{profit}(X)$ = profit for a feasible solution X.
For a partial soluion $X = [x_0, x_1, \ldots, x_{l-1}]$, define

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

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

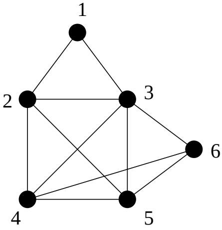
Algorithm $\textsc{Bounding}(l)$

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
  $P \leftarrow \text{profit}([x_0, x_1, \ldots, x_{l-1}])$;
  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;
  $x_l \leftarrow x$;
  $\textsc{Bounding}(l + 1)$

Maximum Clique Problem

PROBLEM: Maximum Clique (optimization)
INSTANCE: a graph $G = (V, E)$.
FIND: a maximum clique of G.

This problem is NP-complete.



Maximum cliques:

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

Modification of ALLCLIQUES to find the maximum clique (no bounding).
Blue 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
  $OptSize \leftarrow l$;
  $OptClique \leftarrow [x_0, x_1, \ldots, x_{l-1}]$;
if $(l = 0)$ then $\mathcal{C}_l \leftarrow V$;
  else $\mathcal{C}_l \leftarrow A_{x_{l-1}} \cap B_{x_{l-1}} \cap \mathcal{C}_{l-1}$;
$\mathbf{M} \leftarrow \mathbf{B}([\mathbf{x_0}, \mathbf{x_1}, \ldots, \mathbf{x_{l-1}}])$;
for each $(x \in \mathcal{C}_l)$ do
  if $(\mathbf{M} \leq \mathbf{OptSize})$ **then return;**
  $x_l \leftarrow x$; MAXCLIQUE($l + 1$);

Main
  $OptSize \leftarrow 0$; 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

General bounding function: $B(X) = l + ub[l]$.

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

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

Bounds based on colouring

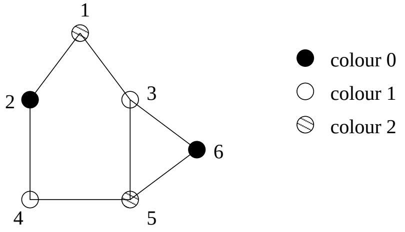
Definition (Vertex Colouring)

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

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

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

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

```
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 $\textsc{GreedyColour}(G)$, determining k and $\textsc{Colour}[x]$ for all $x \in V$.

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

Greedy Bound:
Call $\textsc{GreedyColour}$ dynamically.

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

Number of nodes of the backtracking tree: random graphs with edge density 0.5

# vertices	50	100	150	200	250
# edges	607	2535	5602	9925	15566
max clique size	7	9	10	11	11
bounding function:					
none	8687	257145	1659016	7588328	26182672
size bound	3202	57225	350310	1434006	5008757
sampling bound	2268	44072	266246	1182514	4093535
greedy bound	430	5734	22599	91671	290788

Branch-and-bound

The book presents branch-and-bound as a variation of backtracking in which the choice set is tried in decreasing order of bounds.

However, branch-and-bound is usually a more general scheme.

It often involves keeping all active nodes in a priority queue, and processing nodes with higher priority first (priority is given by upper bound).

Next we look at the book's version of branch-and-bound.

Algorithm $\text{BranchAndBound}(l)$

external $B()$, $\text{profit}()$; global $\mathcal{C}_l$ $(l = 0, 1, \ldots)$

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

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

if $(P > OptP)$ then $OptP \leftarrow P$;

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

Compute $\mathcal{C}_l$; $count \leftarrow 0$;

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

$nextchoice[count] \leftarrow x$;

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

$count \leftarrow count + 1$;

Sort $nextchoice$ and $nextbound$ by decreasing order of $nextbound$;

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

if $(nextbound[i] \leq OptP)$ then return;

$x_l \leftarrow nextchoice[i]$;

$\text{BranchAndBound}(l + 1)$;