Algorithms and Data Structures for Biology
6 May 2019 — Lab Session

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1 Average Case Analysis

Please refine the average case analysis of the branch-and-bound algorithm you have defined as part of the Fifth Assignment. More specifically, you are asked to consider the following situations:

- The utility is not a random number, but is somehow correlated to the size: the greater the size, the greater the utility. Suppose, in particular, that once the size has been generated randomly between 1 and 10, the utility is twice as big as the size, plus some "noise" produced itself randomly between -3 and $+3$. Can you think of a better algorithm which can take advantage of this specific form of distribution? Please implement it.
- n is not only $3m$ or $7m$ but can be any expression between in the form im where $i \in \{1, \dots, 10\}$ For each of these expression, repeat the whole experiment. What's the worst possible value of im?

2 On the Fifth Assignment

Below, you can find *one possible* solution to the Fifth assignment. Of course, this is not the only possible way the assignment could be carried out.

2.1 Formal Problem

Given two positive integers m and n and two families of posititve integers $S_1, \dots, S_m$ and $U_1, \dots, U_m$, we want to find a set $\mathcal{D}$ of integers between 1 and m such that $\sum_{j \in \mathcal{D}} S_j \leq n$ and $\sum_{j \in \mathcal{D}} U_j$ is maximal.

2.2 Exhaustive Search

First of all we define a method SumIndex to compute the sum of all elements in a family L whose indices are in a set D. This way given sizes S and utilities U, the total size associated to a set of databases D is SumIndex(D, S) and the total utility is SumIndex(D, U).

Algorithm 1 SumIndex(D, L)

Require: L family of integers, D set of indices of L.
Ensure: Returns the sum of all element of L with indices in D

```
s ← 0
for j in D do
    s ← s + L_j
end for
return s
```

Then to perform an exhaustive search we need to enumerate all possible sets $\mathcal{D}$ of integers between 1 and m. Then we just need to compute their total sizes and utilities and pick a valid one maximising utility. To do so we use an intermediate method RestrictedExhaustiveSearch which computes the best solution for the parameters m, n, S and U with an additional constraint: we have already decided whether we want to pick each of the first i databases, and D is the set of databases with index smaller than i which we decided to pick.

Algorithm 2 RestrictedExhaustiveSearch(m, n, S, U, i, D)

Require: m,n integers, S,U families of integers of size m, $i \leq m$ and D set of integers smaller than i.
Ensure: Returns a set D' of integers between 1 and m such that all $j \leq i$ is in D' if and only if it is in D, $\sum_{j\in\mathcal{D}'} S_j \leq n$ and $\sum_{j\in\mathcal{D}'} U_j$ is maximal if such a set exists, and returns the emptyset otherwise.

```
if i = m then
  if SumIndex(D, S) ≤ n then
    return D
  else
    return ∅
  end if
else
  D1 = RestrictedExhaustiveSearch(m, n, S, U, i + 1, D)
  D1 = RestrictedExhaustiveSearch(m, n, S, U, i + 1, D ∪ {i + 1})
  if SumIndex(D1, U) ≥ SumIndex(D2, U) then
    return D1
  else
    return D2
  end if
end if
```

To find a general solution to our problem we simply use the previous method with 0 for i and an empty set as D.

Algorithm 3 ExhaustiveSearch(m, n, S, U)

```
return RestrictedExhaustiveSearch(m, n, S, U, 0, ∅)
```

2.3 Complexity

We will show that the complexity of the method ExhaustiveSearch is $O(m2^m)$.

First remark that the auxiliary function SumIndex performs $|D| + 2$ computations. Then we prove that the method RestrictedExhaustiveSearch executes at most $(m + 5)(2^{m-i} + 2^{m-i+1} - 2)$ instructions if D has size at most i. We reason by induction on $m - i$.

Initialisation. If $m = i$ then we compute SumIndex(D, S) in $O(|D|)$, with by assumption $|D| \leq i = m$, and we perform three more operations (two ifs and one return) so the complexity is bounded by $m + 5$.

Preservation. If $m > i$ then we call RestrictedExhaustiveSearch twice, with the parameters m, n, S, U, $i + 1$ and either D or $D \cup \{i + 1\}$. By assumption we have $|D| \leq i$ so we have both $|D| \leq i + 1$ and $|D| \cup \{i + 1\} \leq i + 1$ and we can apply the induction hypothesis to both calls, which terminates in at most $(m + 5)(2^{m-i-1} + 2^{m-i} - 2)$ instructions each for a total of $(m + 5)(2^{m-i} + 2^{m-i+1} - 4)$. Moreover the sets $D1$ and $D2$ have at most size m so each calls to SumIndex terminates in at most $m + 2$ operations, and we perform three more operations (two ifs and one return, again) for a total of $2m + 7$ additional operations. To conclude we have $(m+5)(2^{m-i}+2^{m-i+1}-4)+2m+7 \leq (m+5)(2^{m-i}+2^{m-i+1}-2)$, which is the expected result.

Finally the method ExhaustiveSearch calls RestrictedExhaustiveSearch with $i = 0$ and D empty (hence of size at most 0), so its complexity is $(m+5)(2^m + 2^{m+1} - 2)$, or $O(m2^m)$.

2.4 Branch and Bound

The basic structure of our branch-and-bound algorithm is the same as the exhaustive search. The difference is that we keep track of the size we use while building the set D, and we make sure never to consider a set whose size exceeds the limit n. The method RestrictedBranchAndBound finds the best solution under the constraint that we already decided whether to pick the databases with index small than i (and this choice is described by D), and n is *the remaining size after picking the elements in* D, which is always kept positive.

Algorithm 4 RestrictedBranchAndBound(m, n, S, U, i, D)

Require: m,n integers, S,U families of integers of size m, $i \leq m$ and D set of integers smaller than i.
Ensure: Returns a set D' of integers between 1 and m such that all $j \leq i$ is in D' if and only if it is in D, $\sum_{j \in \mathcal{D}', j > i} S_j \leq n$ and $\sum_{j \in \mathcal{D}'} U_j$ is maximal.

if $i = m$ **then**
  return D
else
  if $S_{i+1} > n$ **then**
    return RestrictedBranchAndBound$(m, n, S, U, i+1, D)$
  else
    $D1 =$ RestrictedBranchAndBound$(m, n, S, U, i+1, D)$
    $D1 =$ RestrictedBranchAndBound$(m, n - S_{i+1}, S, U, i+1, D \cup \{i+1\})$
    if SumIndex$(D1, U) \geq$ SumIndex$(D2, U)$ **then**
      return $D1$
    else
      return $D2$
    end if
  end if
end if

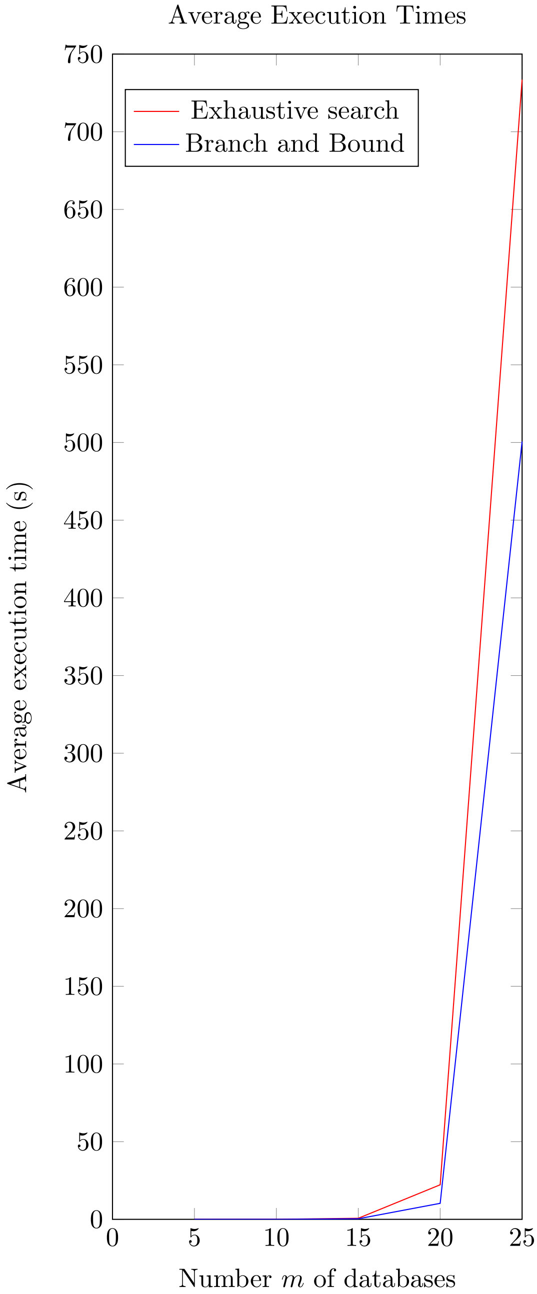
Again the method BranchAndBound just calls the previous method with no constraint.

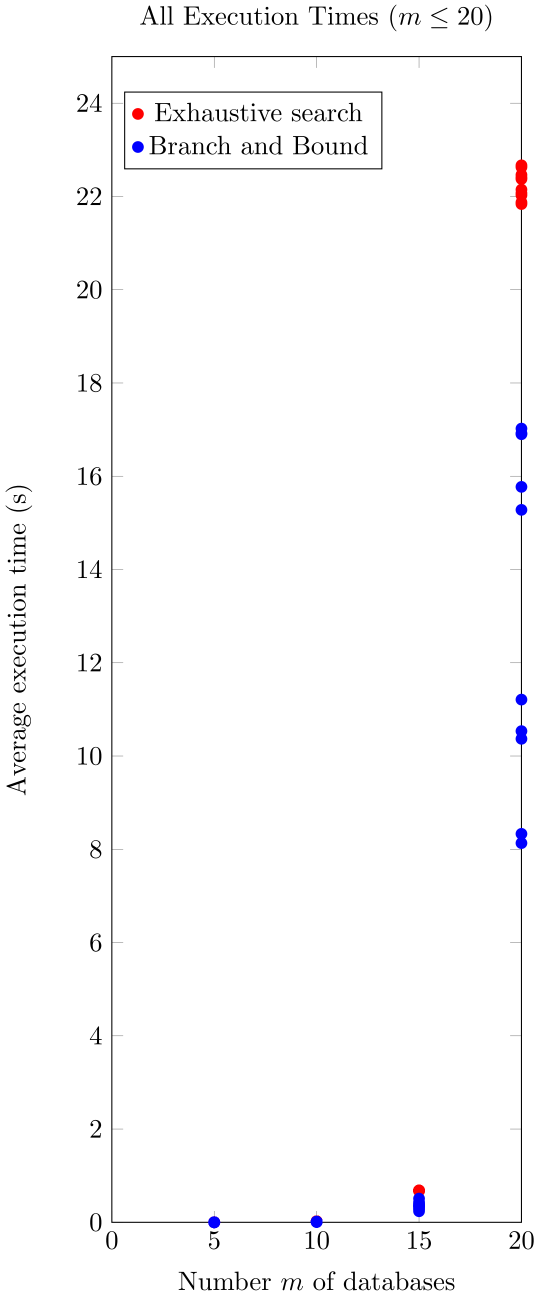
Algorithm 5 BranchAndBound(m, n, S, U)

return RestrictedBranchAndBound$(m, n, S, U, 0, \emptyset)$

2.5 Testing

We present below the experimental execution times of our algorithms when m takes the values 5, 10, 15, 20 and 25, n is $3m$ and S and U are both families of random elements between 1 and 10. The first graph shows the evolution of the average times of 10 executions of each algorithm over the same 10 choices of random families S and U (except for $m = 25$ where each algorithm has been tested only once). The second graph shows all the experimental results.





We can observe that although the branch-and-bound algorithm is faster, it does not appear immensely more efficient than the exhaustive search : it still seems to have an exponential complexity. We can also observe that the execution time of the exhaustive search algorithm does not depend much on the families S and U, whereas the execution time of the branch-and-bound algorithm varies a lot when we run it on different families.