

CS5800: Algorithms Spring 2018

Assignment 6.3

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April 2, 2018

The algorithm is based on the intuition that for an undirected graph, sum of degrees of all edges is equal to twice the number of edges in it.

Proof by induction:

Base case: let n be the number of edges. If $n=0$ then there is no edge in the graph. Hence, degree also would be zero. So, total degree $0 = 2 * 0 = 2 * \text{total number of edges}$.

Inductive step: Say the above theorem holds true for an undirected graph G with $n-1$ edges i.e. total degree of $G = 2(n-1)$. Now suppose there is an edge (u,v) which when added to the graph, makes the total count n . Since this is an undirected graph, every edge contributes twice in degree calculation.

So, total degree is $\text{degree}(G)+2 = 2(n-1)+2 = 2n$, which is twice the edge count. Hence proved.

Now to calculate number of carbon atoms from hydrogen atom, we can use the formula,
 $\text{total bonds} * 2 = \text{number of carbon atoms} * 4 + \text{number of hydrogen atoms} * 1$

Here atoms can represent nodes and the bonds between them are edges in a graph.

since we know, hydrogen atom will be in one bond, degree will be 1. For carbon, its 4. Now, because its given no sequence of atoms will form cycle, we can represent any hydrocarbon struture in the form of a connected tree. Hence, number of edges = total number of nodes-1.

Say we have k carbon atoms, l hydrogen atoms. total degree would be $k*4 + l*1$. which has $(k+l-1)$ edges. Hence,
 $2*(k+l-1) = 4k + l$

or $l-2 = 2k$

or $k = (l-2)/2$

Algorithm:

Step1: Get number of hydrogen atom.

Step 2: Subtract 2 from it.

Step 3: Divide the result by 2.

Step 4: return the result.

Analysis: Since the algorithm uses direct formula to derive number of carbon atoms from hydrogen atom, both the time and space complexity should be $O(1)$.