1 Introduction

A table of frequently used symbols:

Symbol	Representation
g	the input graph
v	the set of nodes in g
e	the set of edges in g
n	a node in v
G	the constructed metagraph
V	the set of metanodes in G
E	the set of metaedges in G
N	a metanode in V of the form $\{n_i : x_i\}$ where $n_i \in v$ and x_i is the number of atoms at n_i

Each $N \in V$ is composed of i many nodes from v. A metanode takes the form $\{n_i : x_i\}$ where $n_i \in v$ and x_i is the number of atoms at n_i. The $\sum_0^i x_i = k$ at any given N ensuring that all atoms are accounted for at each metanode

2 Algorithms

Algorithm 1: Construct Meta-Graph

Input: $g = (v, e)$: the input graph, $\{s, t\} \in v$: the start and target compounds, k: flow/number of atoms to conserve

Output: $G = (V, E)$: the meta-graph

$MG \leftarrow (MV = \emptyset, ME = \emptyset)$ `/* initialize new metagraph */`

$start \leftarrow \{s : k\}$ `/* create a metanode with all` k `atoms at the start compound */`

$V \leftarrow V \cup start$ `/* Add the start state to the set of metanodes */`

Algorithm 2:

Input:

Output: