Nikolaus Awtrey

Beckstein Lab

Arizona State University

02/20/2020

Kinetic Diagram Analyzer Algorithm Verbalization

Generate partial diagrams for G:

* 1. Calculate the number of edges needed for each partial diagram. This happens to be the number of nodes minus 1.
  2. Get list of all possible combinations of unique edges using the number of unique edges needed for each partial diagram, and the number of unique edges in G. For example, a 4-state diagram with leakage requires 3 unique edges for every partial diagram (4 minus 1), and there are 5 unique edges in the input diagram G, so the number of ways of putting 3 lines in 5 positions is 5 choose 3 (10).
  3. Generate list of all possible partial diagrams. For a given combination of possible edges:
     1. Make a copy of G.
     2. Remove all edges from G.
     3. Reassign particular combination of edges.
     4. Repeat for all combinations of edges.
  4. From the list of all possible diagrams, remove the diagrams with closed loops since, by definition, a partial diagram cannot have a closed loop. For the same example mentioned above, 2 of the total 10 diagrams have closed loops and thus only 8 are considered valid.

1. Generate directional partial diagrams:
   1. Calculate the number of target states (just equal to the number of states).
   2. For a given target and partial diagram:
      1. Make a copy of the partial diagram.
      2. Find the unique edges of the partial diagram.
      3. Generate directional connections of the partial diagram:
         1. For a given target, make a list of all the unique edges in the partial diagram that neighbor the target state, store those states, and remove those edges from the list.
         2. Repeat this process until there are no more edges left in the list.
      4. Using the stored neighbors, generate list of directional edges by working backwards (towards the target).
      5. Remove all edges from the given partial diagram.
      6. Add the directional edges to the partial diagram.
      7. Repeat for every partial diagram.
      8. Repeat for every target (state).
2. Calculate state probabilities:
   1. For a given state and directional partial diagram, read the rate constant associated with every process that has a direction associated with it and multiply these values together.
   2. For the same given state, sum all the directional partial diagram terms generated from i. to obtain the multiplicity of that given state.
   3. Repeat for every state in G.
   4. Sum all state multiplicities to obtain the normalization factor for the state probabilities.
3. Assign probability values to state nodes in G.
4. Generate diagrams for all possible cycles in G:
5. Calculate cycle fluxes for every cycle: