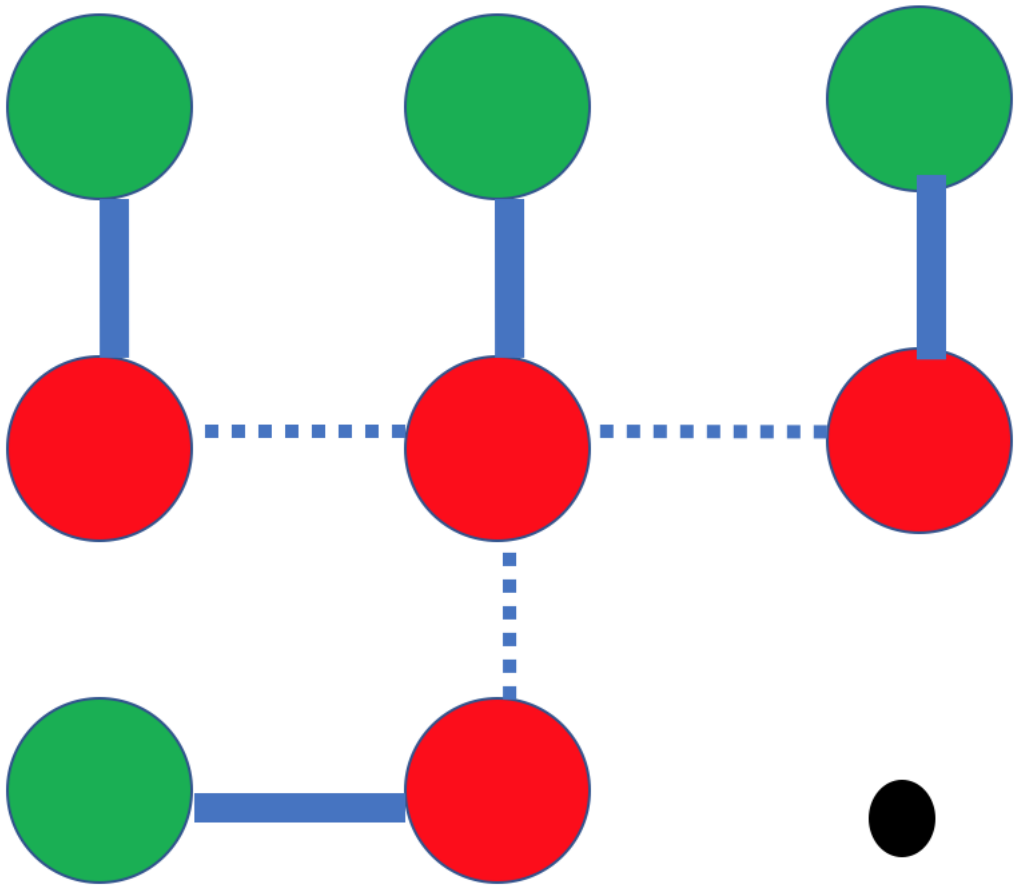
Bisphere Problem Description

The problem we are trying to solve is a simplification of a protein folding problem. Namely, we simplified a protein alpha carbon and sidechain pair to a bisphere segment with a backbone sphere and a sidechain sphere. This problem is set up as follows:

We are given a y by x grid with n bisphere segments that must be placed on it. Each bisphere segment has a backbone sphere and a sidechain sphere that are connected by an edge. The segments must be placed on the board in such a way that maximizes the number of contacts between sidechain spheres. In other words, we must arrange the segments on the grid in such a way that gives us the largest possible number of adjacent side chain spheres.

With 4 bispheres on a 3 by 3 grid, one optimal configuration is shown below:



In the diagram above, the green spheres correspond to backbone spheres, the red spheres correspond to sidechain spheres, the solid blue lines correspond to edges, and the dotted blue lines correspond to contacts. In this example, the optimal contact number of 3 is attained.

SAT Solver Approach

To do this with a SAT solver, the following Boolean matrices will need to be implemented:

1. B_{ij} : Indicates whether a spot on the grid has a backbone sphere or not.
2. S_{ij} : Indicates whether a spot on the grid has a sidechain sphere or not.
3. E_i : Indicates whether a space between two grid spots has a edge present or not.
4. E_i : Indicates whether a space between two grid spots has a contact present or not.

We must now add the following constraints to ensure that these matrices hold values that maximize the number of contacts on the grid:

1. Prevent a backbone sphere and a sidechain sphere from overlapping on the grid, and also prevent edges from overlapping with contacts.
2. Limit the number of backbone spheres, sidechain spheres, and edges on the grid to the number of bisphere segments.
3. Add a constraint that prevents standalone spheres. Namely, make it so that a sphere existing means that an edge must also exist coming out of it.
4. Limit it so that an edge can only exist between a backbone sphere and a sidechain sphere, and there can only be one edge per sphere.
5. Limit it so that a contact is present only when two sidechain spheres are adjacent to one another, and vice versa.
6. Use a for loop to increase the number of contacts desired by updating a constraint. More specifically, start from 0 contacts, see if it is possible, and keep going up until it is impossible to attain a certain number of contacts with the current grid dimensions and number of bispheres.