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Abstract

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1 Method

1.1 Algorithm

Our algorithm begins by reading in and expected amino acid order and the NMR carbon shift data from a data file. It then changes the amino acids to there expected C_α and C_β values and stores them in an list that represents the protein chain. Next, the carbon shift values for a single amino acid is placed in a tile. A tile contains the C_α and C_β values for the amino acid residue i and residue $i - 1$. Next, missing data is accounted for. If there are less tiles than the number of amino acids in the protein chain, place holder tiles are generated to make up the difference. Before the search for the best solution begins, the tiles are grouped by the type of amino acids they could represent to accelerate the assignment process. Tiles that do not match a group are grouped with the place holder tiles

To start the search, tiles in the place holder group and tiles in the same amino acid group as the first amino acid in the protein chain are placed in the first position in a node. The tile is then compared to the first amino acid in the protein chain, and a cost is generated. All of the generated nodes are place in a frontier array.

The node in the frontier with the lowest cost is removed from the frontier and used to generate child nodes. To generate a child node, a tile is added to the end of the node. A child node is generated for all unplaced tiles that are either in the place holder group or in the group matching the corresponding amino acid in the protein chain. A cost of placing the tile is then generated. The cost is a sum of the cost of placing the previous tiles in the node, how well the current tile matched the corresponding amino acid in the protein chain and how well the tile's residue $i - 1$ values match the residue i values of the tile placed before it. The child nodes are then added to the frontier, and the process of generating child nodes is repeated.

Once a node has every tile placed, it is said to be in the goal state. The first node that reaches goal state is stored as the current best solution. Every node that hits goal state is compared to the current best solution. The node with the lower cost is saved as the current best solution.

A solution has been found once the current best solution's cost is lower than the cost of any nodes in the frontier. The search is then ended. The algorithm then outputs the cost of the best solution followed by the assigned carbon shift values.

References

[1] Babak Alipanahi, Xin Gao, Emre Karakoc, Frank Balbach, Shuai Cheng Li, Guangyu Feng, Logan Donaldson and Ming Li, "IPASS: error tolerant NMR backbone resonance assignment by linear programming," technical report, 2009.