# Computer scientists develop new way to study molecular networks

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Computer scientists at Virginia Tech developed a new approach to address the shortcomings in the computational analysis of the multiple ways interactions can occur within cells. Their award winning work may lead to further understanding of the interactions between molecules.

In biology, molecules can have multi-way interactions within cells, and until recently, computational analysis of these links has been "incomplete," according to T. M. Murali, associate professor of computer science in the College of Engineering at Virginia Tech.

His group authored an article on their new approach to address these shortcomings, titled "Reverse Engineering Molecular Hypergraphs," that received the Best Paper Award at the recent 2012 ACM Conference on Bioinformatics, Computational Biology and Biomedicine.

Intricate networks of connections among molecules control the processes that occur within cells. The "analysis of these interaction networks has relied almost entirely on graphs for modeling the information. Since a link in a graph connects at most two molecules (e.g., genes or proteins), such edges cannot accurately represent interactions among multiple molecules. These interactions occur very often within cells," the computer scientists wrote in their paper.

To overcome the limitations in the use of the graphs, Murali and his students used hypergraphs, a generalization of a graph in which an hyperedge can connect multiple molecules.

"We used hypergraphs to capture the uncertainty that is inherent in reverse engineering gene to gene networks from systems biology datasets ," explained Ahsanur Rahman, the lead author on the paper. "We believe hypergraphs are powerful representations for capturing the uncertainty in a network's structure."

They developed reliable algorithms that can discover hyperedges supported by sets of networks. In ongoing research, the scientists seek to use hyperedges to suggest new experiments. By capturing uncertainty in network structure, hyperedges can directly suggest groups of genes for which further experiments may be required in order to precisely discover interaction patterns. Incorporating the data from these experiments might help to refine hyperedges and resolve the interactions among molecules, resulting in fruitful interplay and feedback between computation and experiment.

Murali, and his students Ahsanur Rahman and Christopher L. Poirel, both doctoral candidates, and David L. Badger, a software engineer in Murali's group, all of Blacksburg, Va., and all in the computer science department, used funding from the National Institutes of Health and the National Science Foundation to better understand this uncertainty in these various forms of interactions.

Murali is also the co-director of the Institute for Critical Technology and Applied Science's Center for Systems Biology of Engineered Tissues and the associate program director for the computational tissue engineering interdisciplinary graduate education program at Virginia Tech.

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