Extremal Problems on the Steiner k-Distance and the Steiner k-Wiener Index

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Distance-based indices on graphs are of interest to chemical graph theorists for their connections to the chemical properties of molecules. In this paper, I study several extremal properties of the Steiner k-distance, Steiner k-centroid, and Steiner Wiener Index. More specifically, I show that the Steiner k-distance, Steiner k-leaf-distance, and Steiner k-internal-distance are all concave along a path. I also calculate distances between the Steiner k-median, Steiner k-internal-median, and Steiner k-leaf-median. Finally, I bound the ratios between the Steiner k-distances of similar and unlike vertices and the ratio between the Steiner Wiener Index and the Steiner k-distance of a Steiner 2-centroid. The extremal graphs that produce these bounds are included. These results help identify centralized points within graphs, which correlate to centralized atoms within molecules. The properties I find for these centralized atoms can improve our understanding of interactions between molecules. Additionally, the bounds provided in this paper measure how evenly arranged the points in a graph are, and how connected specific vertices are with the rest of the graph. When performed on molecules, these measurements can help predict chemical properties such as the boiling point and other phase transition temperatures.

Awards Won:
American Mathematical Society: Honorable Mention and One-Year Membership to AMS (for 5 projects with up to 3 team members per project)