VCU Discrete Mathematics Seminar

Intrinsic Graph Metrics

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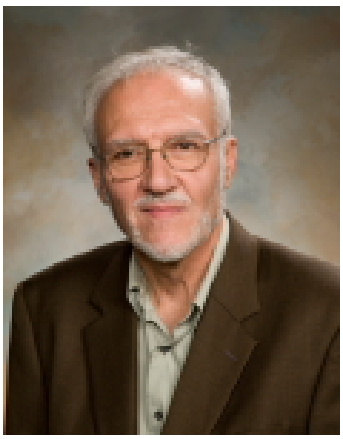
Thursday, Mar. 19
12:30–1:20
4119 Harris Hall (or 4145 Harris, TBA)

As molecular representations, graphs seemingly retain incomplete information of a molecules character—in particular, they seem to suppress molecular geometry. Thus identification of intrinsic limitations to graph representations is of interest, and there is a question of intrinsic metrics on graphs, independently of their use.

Yet there are other possible intrinsic graph metrics besides the most common shortest-path distance. We will examine several other candidate graph metrics that arise from various considerations: wave-like, combinatorial, probabilistic, linear-algebraic, and electric.

Granted a metric, there are associated graph invariants, e.g., to be used in molecular structure/property correlations. As the proposed metrics treat cycles differently than the shortest-path metric ρ, a comparison to ρ might measure "graph cyclicity". A variation of overall distances with respect to changes in weight of an edge might be used to measure centrality of that edge. Invariants may be defined via analogy to classical Euclidean-geometric quantities, including: linear curvature, torsion, Gaussian curvature, and mean volumina. One might surmise a possibility of a kind of intrinsic graph geometry.



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