

Loop homology of bi-secondary structures

Andrei C. Bura^{1,*}, Qijun He², Christian M. Reidys^{2,3}

¹*Department of Mathematics, Virginia Tech, 225 Stanger Street, Blacksburg, VA 24061-1026*

²*Biocomplexity Institute and Initiative, University of Virginia, 995 Research Park Boulevard, Charlottesville, VA 2291*

³*Department of Mathematics, University of Virginia, 141 Cabell Dr, Charlottesville, VA 22903*

anbur12@vt.edu

Bi-secondary structures were introduced by Haslinger and Stadler and are pairs of RNA secondary structures, i.e. diagrams with non-crossing arcs in the upper half-plane. A bi-secondary structure is represented by drawing its respective secondary structures in the upper and lower half-plane. An RNA secondary structure has a loop decomposition, where a loop corresponds to a boundary component, when the secondary structure is interpreted as an orientable fatgraph. The loop-decomposition of secondary structures facilitates the computation of its free energy and any two loops intersect either trivially or in exactly two vertices. In bi-secondary structures the intersection of loops is more complex and is of importance in current algorithmic work in bio-informatics and evolutionary optimization. We constructed a simplicial complex capturing the intersection relations of a bi-secondary structure's loops. We showed that only the zeroth and second homology groups are nontrivial and, furthermore, that the second homology group is free. We identified certain distinct combinatorial structures in the arc diagram of the bi-secondary structure which we called crossing components. We showed that the total number of these crossing components equals the rank of the second homology group. Thus we can give the generators of the second homology group a bio-physical interpretation: they correspond to pairs of mutually exclusive secondary substructures.