Applied Topology: DNA topology, Material Science, Topological Data Analysis
Topologie appliquée : Topologie de l'ADN, science des matériaux, analyse des données topologiques
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JAVIER ARSUAGA, University of California, Davis
Using liquid crystal models to study DNA knotting in bacteriophages

Bacteriophages, viruses that propagate in bacteria, packed their genome in a protein container called capsid. Inside the capsid the viral genome is at a such high concentration and pressure that it is best described as a liquid crystal. This liquid crystal structure of DNA is characterized by ordered layers near the capsid and an isotropic phase at the center of the capsid.

Topological studies have shown that DNA extracted from P4 bacteriophages (P4 DNA) is knotted and the observed knots are very complex (i.e. high average crossing number). Interestingly, the distribution of knots of low average crossing number show an absence of the four crossing knot and a prevalence of the toroidal five crossing knot (5_1) over the twist crossing knot (5_2).

In this work we use cryo-electron microscopy to determine the layer organization of DNA in bacteriophage P4, and the continuum theory of liquid crystals to model its liquid crystal structure. The model shows that the experimentally observed structure is a minimizer of the proposed energy and that the experimental knot distribution can be reproduced by perturbing the minimizer. We therefore propose a new liquid crystal model based on cryoEM observations that is consistent with topological studies of P4 DNA.

MARTIN FRANKLAND, University of Regina
Multiparameter persistence modules in the large scale

A persistence module with m discrete parameters is a diagram of vector spaces indexed by the poset $\mathbb{N}^m$. If we are only interested in the large scale behavior of such a diagram, then we can consider two diagrams equivalent if they agree outside of a "negligeable" region. In the 2-dimensional case, we classify the indecomposable diagrams up to finitely supported diagrams. In higher dimension, we partially classify the indecomposable diagrams up to suitably finite diagrams. We also relate the decomposition to the rank invariant. This is joint work with Don Stanley.

KAI ISHIHARA, Hiroshima University
Spatial graphs confined to tubes in the simple cubic lattice

Knots, links, and spatial graphs in the simple cubic lattice can be considered as models for polymers such as DNA and proteins. Previous research has shown that knots and links confined to a tube in the simple cubic lattice are restricted depending on the size of the tube. In this talk, we will consider spatial theta-curves and spatial handcuff graphs confined to tubes in the simple cubic lattice. This is a joint work with Koya Shimokawa.

E J JANSE VAN RENSBURG, York University
Knot probabilities in confined lattice knots

A lattice knot is a model of ring polymer entropy in three dimensions, and has become a standard theoretical model for quantifying the entropy of a knotted ring polymer. An advantage of the model is that there are efficient Monte Carlo algorithms for sampling lattice knots, even of fixed knot or link type, in various three dimensional lattices. These models may give qualitative insights in the knotting probabilities and entanglement complexity of polymers. For example, the increase in knot probability, as a lattice polygon increases in length, suggests that long ring polymers will likely have a high degree of entanglement complexity. In this talk I shall briefly consider confined lattice knots, and in particular relative knotting probabilities when lattice knots are confined in a cube (as a model of confined knotted ring polymers). I shall review what is

known about confined lattice knots, and how to approximately enumerate them using the GAS algorithm. Two ensembles of confined lattice knots will be (briefly) examined, namely a grand canonical ensemble model where lattice knots are weighted by length (by introducing a chemical potential in the model), and secondly, a canonical ensemble model with lattice knots approximately enumerated as a function of concentration in the confining volume. Results on the relative incidence of knots of various types will be presented as a function of the chemical potential, or as a function of concentration.

PETER LIU, UC Davis
Analyzing RNA structure data with tree polynomials

Advancements in innovative technology such as high-throughput sequencing, cryogenic electron microscopy and artificial intelligence have enabled production of myriad data of RNA structures. Analyzing these data allows us to better understand the functions of RNAs and their roles in various biological processes. However, studying extensive RNA structure data poses challenges without proper representations. Polynomial invariants, such as the Tutte polynomial for graphs and the Jones polynomial for knots, are essential mathematical objects in algebraic combinatorics and algebraic topology. They encode structural information and are compatible with modern data analytic tools. In this talk, we introduce a computationally efficient, interpretable and complete polynomial invariant for trees. We apply this tree polynomial and its generalizations to the study of RNA secondary structures.

ALLISON MOORE, Virginia Commonwealth University
Unknotting numbers and invariants of trivalent spatial graphs

The unknotting number of a knot is a topological invariant that is notoriously difficulty to calculate. Unknotting numbers of knots, links, and theta curves (a type of spatial trivalent planar graph) is externally motivated by modeling problems arising in molecular biology. Generalizing the theorem of Scharlemann that unknotting number one knots are prime, we prove that if a composite theta-curve has unknotting number one, then it is the order 2 sum of an unknotting number one knot and a trivial theta-curve. We also will discuss some recent results in which we bound the unknotting numbers of spatial trivalent planar graphs by their signature and a certain slice orbifold Euler characteristic. This reports on works joint with Baker, Buck, O'Donnol and Taylor.

PUTTIPONG PONGTANAPAISAN, Arizona State University
Random 2-component links which span a lattice tube

Atapour, Ernst, Soteros, and Whittington showed that all but exponentially few sufficiently large pairs of self-avoiding polygons, each confined to and spanning a lattice tube, are topologically linked. These systems are of interest because they can be used to model the entanglements of ring polymers in nanochannels. In this talk, we turn our attention to small tube sizes that still allow for interesting linking behaviors. These tube size constraints will enable us to compare the exponential growth rates of various families of links. This is joint work with Jeremy Eng, Rob Scharein, and Chris Soteros.

ANDREW RECHNITZER, UBC
On BFACF and stick numbers

The BFACF algorithm has been the standard approach to sampling self-avoiding polygons of fixed topology for over 40 years. In this talk we describe adapting BFACF to random polygons in R3.

One immediate application of this method is to improve bounds on stick-numbers - both for equilateral polygons and non-equilateral polygons. In particular, we find upper bounds for both the stick and equilateral-stick numbers for all knots of 13 or fewer crossings. In some cases these upper bounds on stick-numbers actually give exact stick-number.

In many cases there remains a gap between the equilateral-stick and stick number bounds. By adapting the move set of BFACF we can try to "equilateralise" polygons. This is sometimes sufficient to infer the existence of an equilateral conformation

without actually producing it. We also apply the recent CoBarS method of Cantarella and Schumacher to produce equilateral conformations.

This is work together with Jason Cantarella and Clayton Shonkweiler, building on some earlier work with Nick Beaton and Nathan Clisby. Of course, any errors are entirely my own.

ROB SCHAREIN, Hypnagogic Software

Minimal Step Numbers for Knotted θ-curves and Handcuff Graphs on the Simple Cubic Lattice

We use Moriuchi's enumeration of prime θ-curves and handcuff graphs up to seven crossings to create instantiations of these on the simple cubic lattice. From there an implementation of the BFACF algorithm on the lattice for trivalent graphs is used to find minimal step number (MSN) candidates. This algorithm implements the exhaustive set of moves found by Tamaki. Preliminary MSN results will be shown.

MATTHEW SCHMIRLER, University of Saskatchewan

Optimizing Lattice Polygon Models to DNA Experimental Knotting Probabilities

We present here the results of optimizing two different lattice models of DNA, where model parameters are tuned by fitting to DNA experimental knotting probabilities obtained by Shaw and Wang (Science, 1993). The resulting knotting probability fits are of similar quality for both models; however, we observe that the model containing a short-range bending potential has a persistence length that is much more agreeable to that of DNA. We next study how knotting probabilities in this optimized bending model change with varying DNA length, where we find remarkable agreement with knotting probability results obtained from an optimized off-lattice freely-jointed chain model.

KOYA SHIMOKAWA, Ochanomizu University

Interlocking molecules and polyhedral links

Knots and links are ubiquitous in chemical systems. Their structure can be responsible for a variety of physical and chemical properties, making them very important in materials development. We analyze the topological structures of interlocking molecules composed of metal-peptide rings using the concept of polyhedral links. To that end, we discuss the topological classification of alternating polyhedral links. We show that the alternating link diagrams of polyhedral links of certain types do not admit nontrivial flypes. Hence, by the affirmative answer of the Tait flyping conjecture, the classification of the topology of these interlocking structures can be achieved by simply analyzing their alternating diagrams.