RNA Folding: Beyond The Thermodynamic Hypothesis

Max Ward and Amitava Datta
Computer Science and Software Engineering, University of Western Australia

Introduction & Motivation

RNA is a biologically active molecule with many poorly understood functions. For example, it is,

- Involved in regulation of DNA expression
- Implicated in developmental pathways
- A catalyst for many biological processes

Quick and accurate prediction of RNA structure is therefore essential. RNA folding algorithms are currently not able to reliably predict correct structures. These algorithms typically globally optimize some scoring function, usually thermodynamic stability. However, there is evidence that many RNAs fold into suboptimal states.

My Contribution

I hypothesized that local interactions are stronger than global interactions during RNA structure formation. To test this, a sliding window was used to generate locally optimal structures, then various algorithms were devised to merge these substructures. For some window sizes, the resulting complete structures were more accurate than those predicted by state of the art algorithms, which globally optimize. This constitutes strong support for my hypothesis. In addition, a new algorithm called '*ab*-splat', which was based on the computation of locally optimal windows, was introduced.

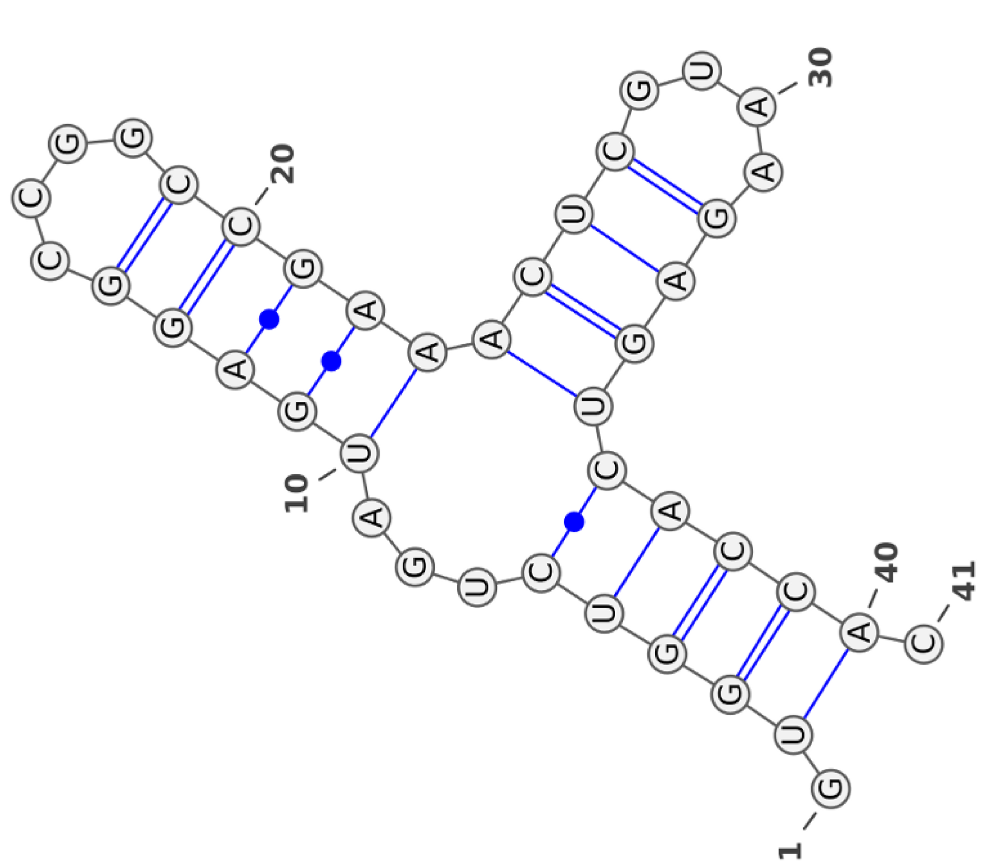

Figure 1: A RNA molecule

Unitarily-Correctable Codes

A correctable subsystem $\mathcal{B}$ is said to be a *unitarily-correctable code* (UCC) for $\mathcal{E}$ if the recovery operation is simply a conjugation-by-unitary channel $\mathcal{U}(\cdot) := U(\cdot)U^*$.

- Since finding correctable subsystems in full generality is an extremely difficult problem, restricting our attention to unitarily-correctable codes seems potentially wise.
- These codes are of physical interest; they are codes in which the two-step process of recovery only involves the conjugation-by-unitary step (and not the projective measurement step).
- It has been shown [3] that if a quantum channel $\mathcal{E}$ is unital, then we can unambiguously define *the unitarily-correctable code algebra* of $\mathcal{E}$, denoted $UCC(\mathcal{E})$, to be the albebra composed of the direct sum of all of the unitarily-correctable codes.
- In terms of Figure 1, unitarily-correctable codes are those for which $p_1 = 1$ and $p_2 = p_3 = 0$ (i.e., there is just one block on the right).

The Multiplicative Domain

The *multiplicative domain* of $\mathcal{E}$ [4], denoted $MD(\mathcal{E})$, is defined to be the following set:

$$\big\{a \in \mathcal{L}(\mathcal{H}) : \mathcal{E}(a)\mathcal{E}(b) = \mathcal{E}(ab) \text{ and } \mathcal{E}(b)\mathcal{E}(a) = \mathcal{E}(ba)\ \forall\, b \in \mathcal{L}(\mathcal{H})\big\}.$$

- $\mathcal{E}$ behaves particularly nicely when restricted to $MD(\mathcal{E})$ (as a $*$-homomorphishm, in fact).
- $MD(\mathcal{E})$ was first studied by operator theorists over thirty years ago.
- $MD(\mathcal{E})$ is an algebra, and hence [5] is unitarily equivalent to a direct sum of tensor blocks:

$$MD(\mathcal{E}) \cong \oplus_k \big(I_{\mathcal{A}_k} \otimes \mathcal{L}(\mathcal{B}_k)\big) \oplus 0_{\mathcal{K}}. \qquad (1)$$

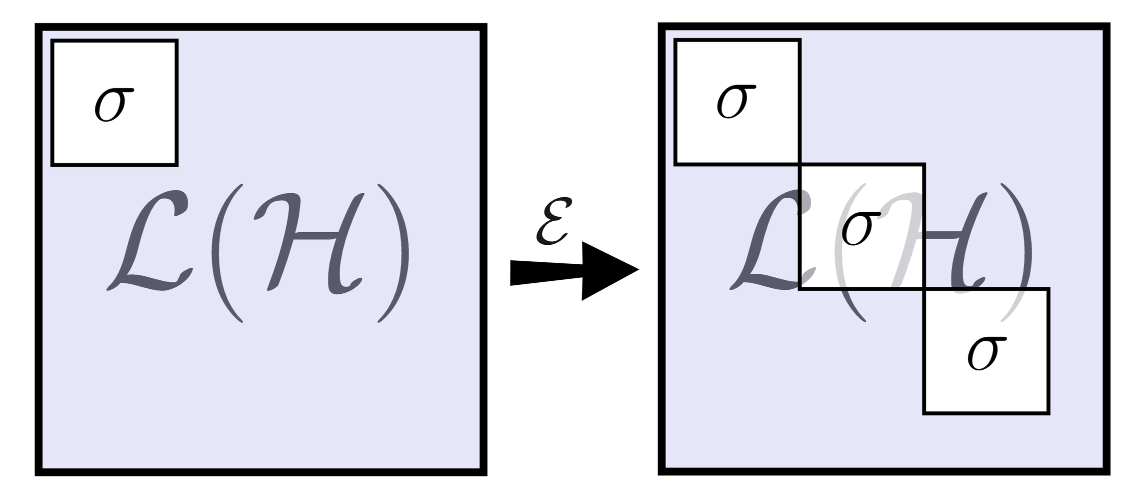

Figure 2: The action of a quantum channel on its multiplicative domain.

The Great Connection

By looking at Figures 1 and 2, we expect that there might be some connection between correctable subsystems for a channel $\mathcal{E}$ and its multiplicative domain. Indeed, one of our main results is that the two situations coincide when $\mathcal{E}$ is unital and the subsystem is unitarily-correctable.

Main Result

Theorem. *Let $\mathcal{E}$ be a unital quantum channel. Then $MD(\mathcal{E}) = UCC(\mathcal{E})$.*

- This theorem says that when we write $MD(\mathcal{E})$ in the form of Equation (1), the $\mathcal{B}_k$'s are exactly the unitarily-correctable codes for $\mathcal{E}$.
- When $\mathcal{E}$ is not unital, $MD(\mathcal{E})$ in general only captures a subclass of the unitarily-correctable codes for $\mathcal{E}$.
- Because $MD(\mathcal{E})$ is easy to compute, this provides a concrete method of finding some UCCs.

Generalization

In the same spirit as the multiplicative domain, we can define "generalized multiplicative domains" for channels by requiring not that the channel be multiplicative with itself, but rather that it be multiplicative with some $*$-homomorphism.

- Generalized multiplicative domains capture *all* correctable codes for *arbitrary* channels.
- Unlike the multiplicative domain, these algebras in general are very difficult to compute.

Conclusions and Outlook

This characterization provides a simple way to find all unitarily-correctable codes for unital channels and even some codes for non-unital channels. General correctable subsystems can be characterized in terms of algebras that are analogous to the multiplicative domain, though in general it is not clear how to calculate them – further research in this area would be of great interest.

For Further Information

For the details of our work:

- Choi, M.-D., Johnston, N., and Kribs, D. W.. Journal of Physics A: Mathematical and Theoretical **42**, 245303 (2009).
- Johnston, N., and Kribs, D. W., *Generalized Multiplicative Domains and Quantum Error Correction* (2009, preprint).

Preprints and this poster can be downloaded from:

- www.arxiv.org
- www.nathanieljohnston.com

References

[1] D. W. Kribs, R. Laflamme, D. Poulin, M. Lesosky, Quantum Inf. & Comp. **6** (2006), 383-399.

[2] P. Zanardi, M. Rasetti, Phys. Rev. Lett. **79**, 3306 (1997).

[3] D. W. Kribs, R. W. Spekkens, Phys. Rev. A **74**, 042329 (2006).

[4] M.-D. Choi, Illinois J. Math., **18** (1974), 565-574.

[5] K. R. Davidson, *C^*-algebras by example*, Fields Institute Monographs, 6. American Mathematical Society, Providence, RI, 1996.

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