Optimizing Molecular-based Reservoir Computers with NSGA-II

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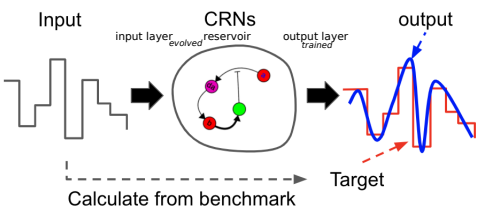
In this work, we use NSGA-II[1], a multiobjective evolutionary algorithm, to find Chemical Reaction Networks (CRNs) able to perform well as reservoirs.

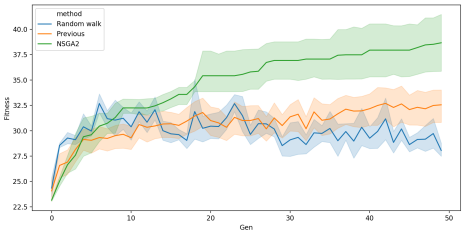
Reservoir computing [2] is a design approach originally proposed for Recurrent Neural Networks (RNNs). In this approach, the input layer is fully connected to a large RNN, called reservoir. Both parts are then connected to the output through the output layer. Contrary to standard neural networks, in the reservoir computing approach, only the output layer gets trained, while other weights are generated randomly. That approach transforms the training phase in a simple linear regression, which can be solved efficiently.

In practice, the reservoir can be any kind of complex dynamical system rather than an explicit RNN, which makes reservoir computing a well-suited approach to work with molecular programming systems. We recently demonstrated[3] its applicability to a molecular programming paradigm called the PEN toolbox[4]. However, further testing showed that the systems evolved in our previous work only performed efficiently on the specific benchmark task we used for evolution, and thus lacked generality.

In this work, we switched to a multi-objective algorithm, using three different objectives: two different benchmark tasks (short- and long-term memory) plus a small size objective. That last objective is motivated by the fact that small PEN networks are less subject to the reality gap when simulated, and are easier to implement *in-vitro*.

Our multi-objective approach allowed us to evolve reservoirs that performed better on a variety of benchmark task (green line below) than reservoirs evolved on a single task (orange) and randomly generated networks (blue).





References

[1] Kalyanmoy Deb, Amrit Pratap, Sameer Agarwal, and TAMT Meyarivan. A fast and elitist multiobjective genetic algorithm: Nsga-ii. *IEEE transactions on evolutionary computation*, 6(2):182–197, 2002.

[2] Herbert Jaeger and Harald Haas. Harnessing nonlinearity: Predicting chaotic systems and saving energy in wireless communication. *science*, 304(5667):78–80, 2004.

[3] Wataru Yahiro, Nathanael Aubert-Kato, and Masami Hagiya. A reservoir computing approach for molecular computing. In *Artificial Life Conference Proceedings*, pages 31–38. MIT Press, 2018.

[4] Kevin Montagne, Raphael Plasson, Yasuyuki Sakai, Teruo Fujii, and Yannick Rondelez. Programming an in vitro dna oscillator using a molecular networking strategy. *Molecular systems biology*, 7(1):466, 2011.