Chemical Computers as Universal Approximators

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I. Introduction to chemical computing

There has been recent interest in using molecular reactions for doing computations. This interest stems from Leonard Adleman's paper [?] in which he demonstrated how to use reactions between DNA molecules to solve a computationally difficult problem. He solved an instance of the Hamilitonian Path problem, a problem that has been shown to be NP-complete, by encoding the edges and vertices of a directed graph with strands of DNA such that when they were combined, the resulting DNA strands encoded the possible paths in the graph. He then seperated the resulting strands to find those strands which encoded paths that are solutions to the problem.

Soon afterwards, the computational ability of Adleman's set of chemical operations on the DNA were analysed [?, ?]. It was shown that Adleman's original operations do not form a universal computer, but if we add certain additional chemical operations, DNA molecules become a *universal computer* in the sense that all discrete computations can be performed by it (see, for e.g., [?]). As of now, these additional chemical operations are purely theoretical in the sense that it is not clear how to implement them in practice.

II. Formulation of the Problem and Main Result

Existing computers consist of binary elements. Therefore, the only way to perform computations on real numbers is to reduce these computations to processing binary data. Chemical computers are different in this respect: at any moment in time, the state of a chemical computer (i.e., the state of the chemical system) is characterized by several continuous variables (such as concentrations of different substances).

We show that a chemical computer can not only perform all possible discrete computations, but all possible *continuous* computations as well. In other words, we show that chemical computers are universal *approximators*, meaning that whatever behavior we can obtain by an arbitrary dynamical system can also be obtained (with arbitrary precision) with appropriate chemical reactions. By a dynamical system we mean a system of (generally nonlinear) differential equations

$$\frac{dx_i(t)}{dt} = f_i(t, x_1(t), ..., x_n(t)).$$

Following [?], Ch. 4, we assume that the region of physical interest is always limited, so we are interested only in initial concentrations x_i that do not exceed some limit values X, and only in the moments of time limited by some value T where f_i are arbitrary smooth functions. This leads to our main result.

Theorem. *For every dynamical system and for every $\varepsilon > 0$, T and X, there exists a set of reactions with $N > n$ substances, such that if we fix the initial concentrations of $N - n$ substances, then for all t from the interval $[0, T]$ and for all initial values $x_i(0)$ from $[0, X]$ the difference between the solutions of the system and the concentrations of the first n substances is $< \varepsilon$.*

III. Idea of the Proof

The proof for this theorem involves reconsiling the differences between an arbitrary dynamic system and kinetic equations of a chemical reaction by adding chemical reactions that can arbitrarily approximate each difference. There are four differences that we have to address:

1. time coordinate t does not enter explicitly into the equations of chemical kinetics; while in the general case we allowed the right-hand side of the equations to depend explicitly on t;
2. the values of the chemical concentrations can never be negative;
3. the equations of chemical kinetics are polynomial (functions f_k are polynomials); while in the general case the functions f_k can be arbitrary;
4. in the equations of chemical kinetics, the functions f_k are not arbitrary polynomials, but only

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the polynomials that stem from the chemical reactions: if, e.g., the term $+kab$, where k is a constant, appears in the right-hand side of the equations for dc/dt, this means that the list of reactions includes the reaction $a+b \to c$ or $\to$ c+something and therefore, the terms $-kab$ must appear in the equations for da/dt and db/dt.

We will approximate the general case with kinetics equations by first approximating with equations that do not contain time, and with equations whose values can never become negative, then with polynomial equations and finally with the polynomial equations stemming from chemical kinetics.

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