

All Kinds of Behavior are Possible in Chemical Kinetics: A Theorem and Its Potential Applications to Chemical Computing

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Abstract

Until the late 1950s, it was believed that the processes described by the equations of chemical kinetics are simple: the process of each chemical reaction, concentrations of some chemical substances decrease while concentrations of other substances increases. This belief was shattered when the first periodic reaction – the famous Belousov-Zhabotinsky reaction – was discovered. Since then, it was shown that many other types of unusual behavior is possible for chemical systems. This discovery led to the possibility of finding chemical reactions that emulate non-trivial transformations that occur during computations – and thus, perform computations “in vitro”, by actually performing the corresponding chemical reactions. The potential advantages of such chemical computing are numerous, the main advantage is that with 10^{23} molecules performing computations in parallel, we have a potential for an unheard-of-parallelization – and thus, of an unheard-of speed-up. The possibility of computing “in vitro” was at first only theoretically conjectured, but then, in 1994, L. Adleman has actually performed successful chemical computations. This started a current boom in chemical computing, with many new ideas and devices appearing all the time.

From both practical and theoretical viewpoints, chemical computing has been a clear success story. However, one open problem remained in this area: while *many* types of behavior have been shown to occur in chemical kinetics, it has been not know whether *all* types of behavior are possible. In this paper, we prove that every possible behavior can indeed be implemented in an appropriate chemical kinetics system. This result has the following direct implication for chemical computing: no matter what computational device one invents, with whatever weird behavior, it is, in principle, possible to emulate this device by appropriate chemical reactions. In this sense, chemical computing is truly ubiquitous.

1 Introduction

Chemical computing: a brief reminder. No matter how fast our computers become, there are still problems – such as weather prediction – which still require a large amount of computation time. A natural way to speed up computations is to use many processors working in parallel: the more processors we use, the faster we come up with the answer. Parallelization is the main reason why we humans solve many problems such as face recognition faster than modern computers:

- in comparison with computers that can perform billions of operations per second, a neuron is a very slow computational device, performing only between 10 and 100 operations per second;
- however, because in the brain, we have billions of neurons working in parallel, the resulting image processing occurs much faster.

Once we decide on the amount of space allocated for computing, the desire to have more processors working in parallel can be reformulated as the need to make computational units smaller and smaller. In some modern computers, individual electronic units are already of the size of several hundred molecules. A natural next step is to reduce these units to a single molecule size. In this case, elementary computational operations consist of interactions between molecules. Such interactions are exactly what chemistry is about. Thus, the ideal case is when controlled chemical reactions perform computations for us. This is the main idea of *chemical computing*.

This idea sounds very promising, because with $\approx 10^{23}$ molecules, we have a potential of 10^{23} processors working in parallel – many orders of magnitude more than what we can achieve today. This idea also sounds promising because this is, in effect, how we humans process data: in the neurons, all the processes are performed by appropriate chemical reactions.

To the best of our knowledge, the idea of chemical computing was first proposed by Yuri Matiyasevich, a mathematician famous for having solved one of Hilbert’s problems (the tenth), in his paper [24]. This idea was noticed; for example, it was discovered that while the general idea is great, its specific implementation suggested by Matiyasevich did not fully explore the natural parallelism; see, e.g., [9]. After that, several alternative schemes were proposed that have theoretically better computation speed-up potential; see, e.g., [13, 14, 15, 16, 17, 20, 22].

The situation changed drastically when, in 1994, L. Adleman actually performed chemical computations “in vitro” [4]. Since then, chemical computing has become a thriving research area; see, e.g., [1, 2, 3, 10, 18, 19, 23, 26, 27].

Chemical computing: remaining theoretical challenge. From the practical viewpoint, in chemical computing, we have impressive results and even more impressive potential applications. However, from the theoretical viewpoint, there is still a challenge:

- every time we need to implement a new computations-related process in chemical computing,
- it is an intellectual challenge, and when a creative idea makes this implementation possible, it is a great result.

By applying all these creative ideas, for many processes, researchers have shown that there processes can be indeed implemented by appropriate chemical reactions. However, a more general question remains open: can *any* possible process (i.e., process described by a general system of differential equations) be implemented by an appropriate system of chemical reactions? or there are processes (behaviors) which chemical computing cannot directly emulate?

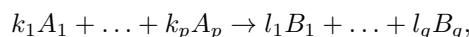
What we do. In this paper, we prove that every possible behavior is also possible in chemical kinetics – and thus, in principle, can be implemented by an appropriate system of chemical reactions.

Thus, whatever computational device with however weird behavior one can invent, it is, in principle, possible to implement this device chemically.

2 Main Result

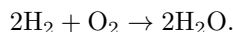
Chemical kinetics equations: a brief reminder. In order to formulate our result in precise terms, we need to recall the differential equations of chemical kinetics. Readers who are well familiar with the chemical kinetics equations can skip this subsection; we added it for the benefit of computer science readers who may be interested in chemical computing but not well acquainted with chemical equations.

When chemical reactions occur, concentrations of chemical substances change; see, e.g., [5, 6, 7]. General chemical reactions have the form



where A_i and B_j are molecules, and k_i and l_j describe how many molecules participate in an individual reaction.

For example, the standard reaction of combining hydrogen and oxygen into water has the form



Here, we have $p = 2$ input substances $A_1 = \text{H}_2$ and $A_2 = \text{O}_2$, with $k_1 = 2$ and $k_2 = 1$, and $q = 1$ output substance $B_1 = \text{H}_2\text{O}$, with $l_1 = 2$.

The speed of each chemical reaction depends on the intensity i_r of this reaction r and on the concentrations of the substances that take part in this reaction. For a reaction to occur, the molecules of all the input substances have to meet. The probability of such encounter is proportional to all the concentrations C_{A_i} , so the reaction rate v_r is proportional to the product of all the concentrations:

$$v_r = i_r \cdot (C_{A_1})^{k_1} \cdot \dots \cdot (C_{A_p})^{k_p}.$$

Because of this reaction:

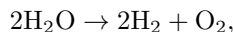
- the concentration of each input substance A_i decreases with a rate $k_i \cdot v_r$:
 $\dot{C}_{A_i} = -k_i \cdot v_r$, where, as usual, $\dot{C}$ means the time derivative $\frac{dC}{dt}$, while
- the concentration of each output substance B_j increases with a rate $l_j \cdot v_r$:
 $\dot{C}_{B_j} = l_j \cdot v_r$.

(It is worth mentioning that in some reaction, e.g., in catalysis, a substance A can be both an input and an output. In this case, we have $\dot{C}_{A_i} = (-k_i + l_i) \cdot v_r$.)

For example, for in the above reaction r , the reaction rate is equal to

$$v_r = i_r \cdot (C_{H_2})^2 \cdot C_{O_2}.$$

Usually, several chemical reactions $r, r', \dots$ are going on. In this case, to describe the rate with which the concentration C_A of each substance A changes, we simply add the rates of change corresponding to different reactions. For example, for water, there is also an inverse reaction r' :



whose reaction rate is equal to $V_{R'} = i_{r'} \cdot (C_{H_2O})^2$. Because of these two reactions, the concentrations of hydrogen, oxygen, and water change according to the following differential equations:

$$\dot{C}_{H_2} = -2 \cdot i_r \cdot (C_{H_2})^2 \cdot C_{O_2} + 2 \cdot i_{r'} \cdot (C_{H_2O})^2;$$

$$\dot{C}_{O_2} = i_r \cdot (C_{H_2})^2 \cdot C_{O_2} + i_{r'} \cdot (C_{H_2O})^2;$$

$$\dot{C}_{H_2O} = 2 \cdot i_r \cdot (C_{H_2})^2 \cdot C_{O_2} - 2 \cdot i_{r'} \cdot (C_{H_2O})^2.$$

Chemical kinetics until late 1950s. It is known that *general* differential equations can exhibit all kinds of behavior. Newton's equations describe the periodic motion of celestial bodies, Lorentz equations describe chaotic behavior, etc.

In comparison with the variety of behaviors that describe general differential equations, the behavior described by most *chemical* kinetics equations is simple: some concentrations decrease, other concentrations increase. Until the last 1950s, it was expected that all chemical systems behave in this simple manner.

Belousov-Zhabotinsky reaction and further discoveries. Our understanding of possible behavior of chemical systems changes drastically when it was discovered that, contrary to the original expectations, the equations of chemical kinetics can exhibit periodic behavior [8, 12, 28].

Later on, it was discovered that other chemical systems show an even more complex behavior, a chaotic behavior or a behavior corresponding to some of the patterns described by catastrophe theory; see, e.g., [6, 11, 25].

A natural hypothesis. Since many kinds of weird behaviors originally observed in general differential equations have been observed in actual chemical system, it is natural to conjecture that *all* kinds of general behaviors are possible in chemical systems as well. This is what we prove in this paper.

Dynamical systems. In this paper, we consider *dynamical systems*, i.e., systems of differential equations of the type $\dot{x}_i = f_i(x_1(t), \dots, x_n(t))$, where f_i are continuous functions. Such systems describe most physical phenomena.

We will prove that for each observed behavior of such a system, there exists a chemical system which has the exact same behavior.

Since a chemical system describes concentrations, and concentrations are always non-negative, we have to restrict ourselves to dynamical systems for which $x_i(t) \geq 0$ for all i and t .

Comment. In this paper, we consider “stationary” dynamical systems in which the rate is not explicitly depending on time t . If needed, we can also allow an explicit dependence on time, i.e., we can also allow systems of the type $\dot{x}_i = f_i(t, x_1(t), \dots, x_n(t))$.

Indeed, as it is well known in dynamical systems theory, we can easily this case to the stationary case if we introduce a new auxiliary variables x_0 (whose meaning is time) with the corresponding differential equation $\dot{x}_0 = 1$ and initial value $x_0(0) = 0$. Then, the system consisting of the equations $\dot{x}_0 = 1$ and $\dot{x}_i = f_i(x_0(t), x_1(t), \dots, x_n(t))$ is stationary and describes the exact same solutions.

W.l.o.g., we start at time $t = 0$. Without losing generality, we can assume that our observations started at moment $t = 0$.

Indeed, if we started at some other moment of time t_0 , then we can take this moment as a new starting point for measuring time. With this new starting point, what was originally time t becomes $t' = t - t_0$. Thus, in the new time scale, we do start at the moment $t' = t_0 - t_0 = 0$.

Limited time. At any moment, we only have observations corresponding to finitely many *trajectories* – i.e., finitely many processes whose dynamics is described by the given system of differential equations.

For each trajectory, at any given moment of time, we have only finitely many observations. Thus, we have only finitely many moments of time at which one of these processes was observed – and we also have finitely many moments of time at which we want to predict these values.

Let T denote the largest of all these moments of time. In these terms, when comparing the chemical system with the original dynamical system, it is sufficient to consider values $t \in [0, T]$.

Limited values of x_i . In each of the finitely many observed processes, we have some initial values $x_i(0)$. If we denote the largest of these values by X_0 ,

then we can conclude that all the initial conditions satisfy the inequalities

$$0 \leq x_i(0) \leq X_0, \quad i = 1, \dots, n.$$

For each of these processes, each function $x_i(t)$ is differentiable – we have an explicit expression for its derivative – and thus, it is a continuous function of time $t \in [0, T]$. Each continuous function on a closed interval is bounded; thus, each of the components x_i is bounded for each of the observed trajectories. Let X denote the largest of these bounds. So, we are guaranteed that for all moments of time $t \in [0, T]$, all the values $x_i(t)$ are bounded by X : $x_i(t) \leq X$.

Limited accuracy. Observations are never absolutely accurate, there is always some measurement uncertainty. Once we upper bound $\varepsilon > 0$ on the corresponding inaccuracy, then:

- the results $x'_i(t)$ of the chemical system are indistinguishable from the results $x_i(t)$ of the original dynamical systems
- if for all moments $t \in [0, T]$, these results differ by no more than ε :

$$|x'_i(t) - x_i(t)| \leq \varepsilon.$$

Need to consider auxiliary chemical substances. In the above text, we provided a somewhat simplified description of chemical kinetics. This simplified description corresponds to the ideal case when the input substance are directly transformed into the output ones. In reality, in most real-life chemical reactions, there are intermediate stages in which some auxiliary chemical substances are formed.

For example, when hydrogen and oxygen combine into water, we have intermediate reactions like $\text{H}_2 \rightarrow \text{H} + \text{H}$ or reactions of the type $\text{H}_2 + \text{Cat} \rightarrow \text{CatH}_2$ for some catalyst Cat.

To adequately describe chemical kinetics, we thus need to consider not only concentrations of the original substances, but also concentrations of these auxiliary substances as well. In other words, in order to describe how the concentrations of chemical substances change during chemical reactions, we need to also consider auxiliary variables.

Since auxiliary variables are needed even for a correct description of *chemical* dynamics, we will allow auxiliary variables in the *general* case as well.

Thus, we arrive at the following definition.

Definition 1. Let $T > 0$, $X_0 > 0$, and $X > 0$ be positive real numbers, and let n be a positive integer. By a (T, X_0, X) -dynamical system (or simply dynamical system, for short), we mean a tuple $f = (f_1, \dots, f_n)$ consisting of n continuously differentiable functions $f_i : [0, X]^n \rightarrow \mathbb{R}$, $i = 1, \dots, n$ with the

following property: For all initial values $x_1(0), \dots, x_n(0) \in [0, X_0]$, the solution $x_1(t), \dots, x_n(t)$ of the corresponding system of differential equations

$$\frac{dx_i}{dt} = f_i(t, x_1(t), \dots, x_n(t)), \quad i = 1, \dots, n,$$

satisfies the inequality $0 \leq x_i(t) \leq X$ for all $t \in [0, T]$ and for all $i = 1, \dots, n$. The values $x_i(t)$ are called the solution to the dynamical system (corresponding to the given initial conditions).

Comment. The requirement that the functions $f_i(x_1, \dots, x_n)$ are continuously differentiable is introduced to make sure that the trajectory is uniquely determined by the initial conditions. If this requirement is not satisfied, we may have non-uniqueness.

Let us give a simple example of this non-uniqueness: $n = 1$, and the function $f_1(x_1)$ is defined as follows:

- $f_1(x_1) = \sqrt{x_1}$ when $x_1 \geq 0$, and
- $f_1(x_1) = 0$ when $x_1 \leq 0$.

In this case, both $x_1(t) = 0$ and $x_1'(t) = \frac{1}{2} \cdot t^2$ are solutions of the equation $\dot{x}_1 = f_1(x_1)$ with the same initial condition $x_1(0) = x_1'(0) = 0$.

Let us now formally describe the notion of chemical equations. To the previous description, we must add the need to avoid “ex nihil” (“from nothing”) reactions of the type $A \rightarrow A + B$, by requiring that a *conservation law* is satisfied: in each reaction, the total atomic mass of the input should be equal to the total atomic mass of the output.

Definition 2. Let $S = \{A_1, \dots, A_N\}$ be a finite set. Its elements will be called substances. Let $m_1 > 0, \dots, m_N > 0$ be integers called atomic masses of the corresponding substances.

- By a state of the system of substances, we mean a non-negative vector

$$x = (x_1, \dots, x_N).$$

For each i from 1 to N , the i -th component x_i of the state is called the concentration of the substance A_i .

- By a reaction, we mean a triple $r = \langle k_r, l_r, i_r \rangle$ consisting of two non-negative integer vectors $k_r = (k_{r,1}, \dots, k_{r,N})$ and $l_r = (l_{r,1}, \dots, l_{r,N})$ and a positive real number i_r for which $\sum_{i=1}^N k_{r,i} \cdot m_i = \sum_{i=1}^N l_{r,i} \cdot m_i$. A reaction will also be denoted as

$$k_{r,1}A_1 + \dots + k_{r,N}A_N \xrightarrow{i_r} l_{r,1}A_1 + \dots + l_{r,N}A_N.$$

- By a system of chemical reactions, we mean a finite set R of reactions.
- By a reaction speed v_r corresponding to the reaction r and concentrations $x = (x_1, \dots, x_n)$, we mean a number $v_r(x) = i_r \cdot \prod_{i=1}^N (x_i)^{k_{r,i}}$.
- For each set R of reactions, once we fix N initial values

$$x_1(0) \geq 0, \quad \dots, \quad x_N(0) \geq 0,$$

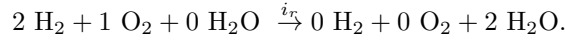
we can then find the solution $x_i(t)$ to the system of differential equations

$$\frac{dx_i}{dt} = \sum_{r \in R} (l_{r,i} - k_{r,i}) \cdot v_r(x)$$

with the given initial values $x_1(0), \dots, x_N(0)$. For each real number $t \geq 0$ and for each integer $i = 1, \dots, N$, the value $x_i(t)$ is called the solution to the chemical system.

Comment. In the description of a chemical reaction, terms corresponding to $k_{r,i} = 0$ or to $l_{r,j} = 0$ can be omitted. Also, the coefficients $k_{r,i} = 1$ and $l_{r,j} = 1$ can also be omitted.

For example, we will simply write $2\text{H}_2 + \text{O}_2 \xrightarrow{i_r} 2\text{H}_2\text{O}$, while, strictly speaking, Definition 2 requires us to write



Theorem. For all positive numbers $T > 0$, $X_0 > 0$, and $X > 0$, and for every (T, X_0, X) -dynamical system f , there exists an integer N , a system R of chemical reactions, and values $x_{n+1}(0), \dots, x_N(0)$ such that for all initial conditions $x_1(0), \dots, x_n(0) \in [0, X_0]$, the solution $x_i(t)$ of the dynamical system f and the solution $x'_i(t)$ of the chemical system are ε -close for all $i \leq n$ and for all $t \in [0, T]$:

$$|x_i(t) - x'_i(t)| \leq \varepsilon.$$

Comment. This result was first announced in [21].

3 Proof

1°. We want to approximate trajectories of a dynamical system by the trajectories of a corresponding chemical system. Let us show that if we can approximate the original functions $f_i(x_1, \dots, x_n)$ by sufficiently close functions $f'_i(x_1, \dots, x_n)$, then the trajectories of the new system will be close to the trajectories of the original system corresponding to the same initial conditions $x'_i(0) = x_i(0)$.

For this proof, we will assume that the functions f_i and f'_i differ by no more than some small number α , i.e., that

$$|f_i(x_1, \dots, x_n) - f'_i(x_1, \dots, x_n)| \leq \alpha$$

for all possible values $x = (x_1, \dots, x_n)$ from the given box $[0, X]^n$.

We will then find the bound on the absolute value of the difference

$$\Delta x_i(t) \stackrel{\text{def}}{=} x'_i(t) - x_i(t)$$

in terms of α . From this bound, it will be clear that, by choosing α to be sufficiently small, we can make the bound on $|\Delta x_i(t)|$ also as small as possible. In other words, we will prove what we intended to: that if the dynamical systems f_i and f'_i are sufficiently close, then we can guarantee that their trajectories will be close as well.

By definition of the trajectories, we have

$$\dot{x}_i = f_i(x_1, \dots, x_n) \text{ and } \dot{x}'_i = f'_i(x'_1, \dots, x'_n).$$

Thus, for the difference Δx_i , we have

$$\frac{d}{dt}(\Delta x_i) = f'_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n).$$

To use the fact that the functions f' and f are close, we represent the right-hand side as the sum of the two terms, one of which describes the difference between f' and f :

$$\frac{d}{dt}(\Delta x_i) = (f'_i(x'_1, \dots, x'_n) - f_i(x'_1, \dots, x'_n)) + (f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n)).$$

The absolute value of the first term is bounded by α . To estimate the value of the second term – in which all n variables change – we will represent it, in turn, as the sum of several terms corresponding to a change in a single variable. First, we change x_1 , then we change x_2 , etc.:

$$\begin{aligned} f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n) = & \\ & (f_i(x'_1, x_2, \dots, x_n) - f_i(x_1, \dots, x_n)) + \\ & (f_i(x'_1, x'_2, x_3, \dots, x'_n) - f_i(x'_1, x_2, x_3, \dots, x_n)) + \\ & \dots + \\ & (f_i(x'_1, \dots, x'_{n-1}, x_n) - f_i(x'_1, \dots, x'_{n-1}, x'_n)). \end{aligned}$$

To estimate each of these differences, we can use the fact that all the functions $f_i(x_1, \dots, x_n)$ are continuously differentiable, i.e., that each partial derivative (exists and) is continuous. Every continuous function on a bounded closed box is bounded. Let M denote the largest of the maxima of all these partial derivatives.

Then, for all points x in this box and for all i and j , we have $\left| \frac{\partial f_i}{\partial x_j} \right| \leq M$.

For a function of one variable whose derivative is bounded by some number M , from

$$f(x') - f(x) = \int_x^{x'} \frac{df}{dx} dx,$$

we conclude that

$$|f(x') - f(x)| = \left| \int_x^{x'} \frac{df}{dx} dx \right| \leq M \cdot |x' - x|.$$

In the general case of a function of several variables, we can apply this argument to the dependence on x_1 and conclude that

$$|f_i(x'_1, x_2, \dots, x_n) - f_i(x_1, x_2, \dots, x_n)| \leq M \cdot |\Delta x_1|.$$

By similarly considering a change in x_2 , we conclude that

$$|f_i(x'_1, x'_2, \dots, x_n) - f_i(x'_1, x_2, \dots, x_n)| \leq M \cdot |\Delta x_2|,$$

and so on until we reach the last variable:

$$|f_i(x'_1, \dots, x'_{n-1}, x_n) - f_i(x'_1, \dots, x'_{n-1}, x'_n)| \leq M \cdot |\Delta x_n|.$$

From the above equality

$$\begin{aligned} f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n) = & \\ & (f_i(x'_1, x_2, \dots, x_n) - f_i(x_1, \dots, x_n)) + \\ & (f_i(x'_1, x'_2, x_3, \dots, x'_n) - f_i(x'_1, x_2, x_3, \dots, x_n)) + \\ & \dots + \\ & (f_i(x'_1, \dots, x'_{n-1}, x_n) - f_i(x'_1, \dots, x'_{n-1}, x'_n)), \end{aligned}$$

we can now conclude that

$$\begin{aligned} |f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n)| \leq & \\ & |f_i(x'_1, x_2, \dots, x_n) - f_i(x_1, \dots, x_n)| + \\ & |f_i(x'_1, x'_2, x_3, \dots, x'_n) - f_i(x'_1, x_2, x_3, \dots, x_n)| + \\ & \dots + \\ & |f_i(x'_1, \dots, x'_{n-1}, x_n) - f_i(x'_1, \dots, x'_{n-1}, x'_n)|. \end{aligned}$$

We already know bounds for each terms in the right-hand side, so we conclude that

$$|f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n)| \leq M \cdot |\Delta x_1| + M \cdot |\Delta x_2| + \dots + M \cdot |\Delta x_n|,$$

i.e.,

$$|f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n)| \leq M \cdot \sum_{i=1}^n |\Delta x_i|.$$

For every i , from the above formula

$$\frac{d}{dt}(\Delta x_i) = (f'_i(x'_1, \dots, x'_n) - f_i(x'_1, \dots, x'_n)) + (f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n)),$$

we conclude that

$$\left| \frac{d}{dt}(\Delta x_i) \right| \leq |f'_i(x'_1, \dots, x'_n) - f_i(x'_1, \dots, x'_n)| + |f_i(x'_1, \dots, x'_n) - f_i(x_1, \dots, x_n)|.$$

We know that the first term is bounded by α and the second by $M \cdot \Delta$, where we denoted $\Delta \stackrel{\text{def}}{=} \sum_{i=1}^n |\Delta x_i|$. Thus, we have

$$\left| \frac{d}{dt}(\Delta x_i) \right| \leq \alpha + M \cdot \Delta.$$

Based on these inequalities, we want to deduce an inequality in terms of $\Delta = \sum_{i=1}^n |\Delta x_i|$ and its derivative. By the chain rule,

$$\frac{d}{dt}(|\Delta x_i|) = \text{sign}(\Delta x_i) \cdot \frac{d}{dt}(\Delta x_i),$$

where $\text{sign}(z) = \frac{d}{dz}(|z|)$ is equal to 1 for $z \geq 0$ and to -1 for $z \leq 0$. Since the absolute value of $\text{sign}(z)$ is always equal to 1, we get

$$\left| \frac{d}{dt}(|\Delta x_i|) \right| = \left| \frac{d}{dt}(\Delta x_i) \right|,$$

hence

$$\left| \frac{d}{dt}(|\Delta x_i|) \right| \leq \alpha + M \cdot \sum_{i=1}^n |\Delta x_i|.$$

By definition of $\Delta = \sum_{i=1}^n |\Delta x_i|$, we have

$$\frac{d}{dt}(\Delta) = \sum_{i=1}^n \frac{d}{dt}(|\Delta x_i|).$$

We have already shown that each term in the sum is bounded by $\alpha + M \cdot \Delta$, so we conclude that

$$\dot{\Delta} = \frac{d}{dt}(\Delta) \leq n \cdot \alpha + n \cdot M \cdot \Delta.$$

Therefore, to estimate the difference Δ , we must make conclusions based on this differential inequality.

The process of finding solutions of an inequality usually starts with solving the corresponding equality

$$\frac{d\Delta}{dt} = n \cdot \alpha + n \cdot M \cdot \Delta.$$

To simplify this expression, we can move all the terms containing Δ to the left-hand side – by dividing both sides by the original right-hand side $n \cdot \alpha + n \cdot M \cdot \Delta$. As a result, we get

$$\frac{1}{dt} \cdot \frac{d\Delta}{n \cdot \alpha + n \cdot M \cdot \Delta} = 1.$$

This expression can be simplified if we take into account that for the denominator

$$\tilde{\Delta} \stackrel{\text{def}}{=} n \cdot \alpha + n \cdot M \cdot \Delta,$$

we have $d\tilde{\Delta} = n \cdot M \cdot d\Delta$. Thus, multiplying both sides of the above inequality by $n \cdot M$, we get

$$\frac{1}{dt} \cdot \frac{d\tilde{\Delta}}{\tilde{\Delta}} = n \cdot M.$$

The left-hand side is equal to the derivative $\frac{d}{dt}(\ln(\tilde{\Delta}))$ of the logarithm of $\tilde{\Delta}$. The derivative is constant, so the logarithm is a linear function of time: $\ln(\tilde{\Delta}(t)) = C + n \cdot M \cdot t$ for some constant C .

To find the integration constant, let us consider the initial moment of time $t = 0$. For $t = 0$, we have $\tilde{\Delta}(0) = n \cdot \alpha + n \cdot M \cdot \Delta(0)$. Here,

$$\Delta(0) = \sum_{i=1}^n |\Delta x_i(0)| = \sum_{i=1}^n |x'_i(0) - x_i(0)|.$$

Since we start with the same initial conditions, we have $|x'_i(0) - x_i(0)| = 0$ and thus, $\Delta(0) = 0$ and $\tilde{\Delta}(0) = n \cdot \alpha$. Hence, $\ln(\tilde{\Delta}(0)) = C = \ln(n \cdot \alpha)$ and thus, $\ln(\tilde{\Delta}(t)) = \ln(n \cdot \alpha) + n \cdot M \cdot t$. Therefore,

$$\tilde{\Delta}(t) = \exp(\ln(\tilde{\Delta}(t))) = n \cdot \alpha \cdot \exp(n \cdot M \cdot t).$$

So, for $\Delta(t) = \frac{\tilde{\Delta}(t) - n \cdot \alpha}{n \cdot M}$, we get

$$\Delta(t) = \frac{n \cdot \alpha \cdot (\exp(n \cdot M \cdot t) - 1)}{n \cdot M} = \frac{\alpha}{M} \cdot (\exp(n \cdot M \cdot t) - 1).$$

Similarly, from the above inequality $\frac{d}{dt}(\Delta) \leq n \cdot \alpha + n \cdot M \cdot \Delta = \tilde{\Delta}$, we conclude that

$$\frac{d\tilde{\Delta}}{dt} = n \cdot M \cdot \frac{d\Delta}{dt} \leq n \cdot M \cdot \tilde{\Delta},$$

hence for

$$\frac{d(\ln(\tilde{\Delta}))}{dt} = \frac{1}{\tilde{\Delta}} \cdot \frac{d\tilde{\Delta}}{dt},$$

we get

$$\frac{d(\ln(\tilde{\Delta}))}{dt} \leq n \cdot M.$$

Thus,

$$\begin{aligned} \ln(\tilde{\Delta}(t)) &= \ln(\tilde{\Delta}(0)) + \int_0^t \frac{d(\ln(\tilde{\Delta}))}{dt} dt \leq \\ \ln(\tilde{\Delta}(0)) + n \cdot M \cdot t &= \ln(n \cdot \alpha) + n \cdot M \cdot t. \end{aligned}$$

Therefore,

$$\tilde{\Delta}(t) = \exp(\ln(\tilde{\Delta}(t))) \leq n \cdot \alpha \cdot \exp(n \cdot M \cdot t).$$

Thus, for $\Delta(t) = \frac{\tilde{\Delta}(t) - n \cdot \alpha}{n \cdot M}$, we get

$$\Delta(t) \leq \frac{n \cdot \alpha \cdot (\exp(n \cdot M \cdot t) - 1)}{n \cdot M} = \frac{\alpha}{M} \cdot (\exp(n \cdot M \cdot t) - 1).$$

The right-hand side of this inequality is an increasing function of time t , so its largest value is attained for the largest possible value $t = T$, thence

$$\Delta(t) \leq \frac{\alpha}{M} \cdot (\exp(n \cdot M \cdot T) - 1).$$

Since $\Delta(t) = \sum_{i=1}^n |\Delta x_i(t)| = \sum_{i=1}^n |x'_i(t) - x_i(t)|$, this implies that for every t and for every i , we have

$$|x'_i(t) - x_i(t)| \leq \frac{\alpha}{M} \cdot (\exp(n \cdot M \cdot T) - 1).$$

So, for any $\varepsilon > 0$, if we want to make sure that $|x'_i(t) - x_i(t)| \leq \varepsilon$ for all i and t , it is sufficient to choose α for which $\frac{\alpha}{M} \cdot (\exp(n \cdot M \cdot T) - 1) \leq \varepsilon$, i.e., to choose

$$\alpha = \frac{M}{\exp(n \cdot M \cdot T) - 1} \cdot \varepsilon.$$

The statement is proven.

2°. We want to prove that an arbitrary dynamical system can be approximated by an appropriate chemical system. Our proof of this approximation result consists of two stages:

- first, we will prove this result for a certain class of dynamical systems, a class selected because for systems from this class, the desired approximation is easier to construct;

- after that, we will prove that an arbitrary dynamical system can be approximated by a system of this simpler type, and how the chemical approximation of this simpler system can be modified into a chemical approximation to the original dynamical system.

3°. The definition of a special class of dynamical systems – with which we start the approximation result – is based on the fact that for every i , and for all points $x = (x_1, \dots, x_n)$ for which $x_i > 0$, the ratio $g_i(x_1, \dots, x_n) \stackrel{\text{def}}{=} \frac{f_i(x_1, \dots, x_n)}{x_i}$ is continuous – as a ratio of two continuous functions.

As a special class, we will consider all dynamical systems for which each of these functions $g_i(x_1, \dots, x_n)$ can be continuously extended to the values $x_i = 0$. In this case, $f_i(x_1, \dots, x_n) = x_i \cdot g_i(x_1, \dots, x_n)$ for some continuous function $g_i(x_1, \dots, x_n)$.

In this case, to construct the desired α -approximation $f'_i(x_1, \dots, x_n)$ to the given function $f_i(x_1, \dots, x_n)$, it is sufficient to find, for an appropriate small $\beta > 0$, a β -approximation $g'_i(x_1, \dots, x_n)$ to the ratio $g_i(x_1, \dots, x_n)$; then, for $f'_i(x_1, \dots, x_n) = x_i \cdot g'_i(x_1, \dots, x_n)$, the inequality

$$|g'_i(x_1, \dots, x_n) - g_i(x_1, \dots, x_n)| \leq \beta$$

implies that

$$|f'_i(x_1, \dots, x_n) - f_i(x_1, \dots, x_n)| = x_i \cdot |g'_i(x_1, \dots, x_n) - g_i(x_1, \dots, x_n)| \leq X \cdot \beta.$$

Thus, it is sufficient to take β for which $X \cdot \beta \leq \alpha$: e.g., to take $\beta = \frac{\alpha}{X}$.

4°. It is known that an arbitrary continuous function on a box can be approximated, with any given accuracy, by a polynomial.

We will use this result and approximate the original ratio $g_i(x_1, \dots, x_n)$ by a polynomial $g'_i(x_1, \dots, x_n)$. A polynomial is, in general, a linear combination of monomials:

$$g'_i(x_1, \dots, x_n) = \sum_m a_m \cdot P_m(x_1, \dots, x_n),$$

where each a_m is a constant, and

$$P_m(x_1, \dots, x_n) = x_1^{d_{m,1}} \cdot \dots \cdot x_n^{d_{m,n}},$$

with $d_{m,j} \geq 0$. In this case,

$$f'_i(x_1, \dots, x_n) = x_i \cdot g'_i(x_1, \dots, x_n) = \sum_m a_m \cdot (x_i \cdot P_m(x_1, \dots, x_n)),$$

where each term $x_i \cdot P_m(x_1, \dots, x_n)$ has the form

$$x_i \cdot P_m(x_1, \dots, x_n) = x_1^{d_{m,1}} \cdot \dots \cdot x_{i-1}^{d_{m,i-1}} \cdot x_i^{d_{m,i}+1} \cdot x_{i+1}^{d_{m,i+1}} \cdot \dots \cdot x_n^{d_{m,n}}.$$

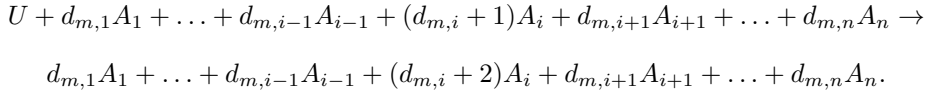
5°. For each monomial $P_m(x_1, \dots, x_n)$, we will find a reaction r for which its intensity v_r is close to the corresponding term $a_m \cdot x_i \cdot P_m(x_1, \dots, x_n)$.

To form these reaction, to each variable x_i we assign a substance A_i whose concentration will be described by x_i . In addition to the resulting n substances, we will use an auxiliary “universal” substance U – a substance that can be, in principle, transformed into any other substance. The concentration of the universal substance U will be denoted by u .

We assume that all $n + 1$ substances $A_1, \dots, A_n, U$ have the same atomic weight $m_1 = \dots = m_n = m_U$.

A specific rule corresponding to the monomial $P_m(x_1, \dots, x_n)$ will be different depending on the whether the coefficient a_m is positive or negative.

6°. For monomials for which $a_m > 0$, we take the reaction



In this reaction, for all the substances except for the i -th substance A_i and the auxiliary universal substance U , the number of molecules entering the reaction is the same as the number of molecules leaving this reaction. The only difference is that a molecule of the universal substance is transformed into a molecule of A_i . In this transformation, all the other substances play the role of catalysts – in the sense that

- while the presence of these other substances is necessary for the reaction to occur, and
- while the speed of this reaction depends on the concentrations of these other substances,
- in the long run, each of this other substances is neither consumed nor produced – in this reaction their concentration does not change.

A precise description of the corresponding terms in chemical equations confirms this qualitative analysis. Indeed, according to the general formula for the chemical equations (as given in Definition 2), the speed v_r of this reaction is equal to

$$v_r = i_r \cdot u \cdot x_1^{d_{m,1}} \cdot \dots \cdot x_{i-1}^{d_{m,i-1}} \cdot x_i^{d_{m,i}+1} \cdot x_{i+1}^{d_{m,i+1}} \cdot \dots \cdot x_n^{d_{m,n}},$$

where i_r denotes the intensity of this reaction and u denotes the concentration of the universal substance U . In terms of the monomial $P_m(x_1, \dots, x_n)$, this formula takes the form

$$v_r = i_r \cdot u \cdot x_i \cdot P_m(x_1, \dots, x_n).$$

According to the same Definition 2, as a result of this reaction, there is no contribution to differential equations describing $\frac{dx_j}{dt}$ for $j \neq i$. The only

contributions are to the terms $\frac{dx_i}{dt}$ and $\frac{du}{dt}$: namely, we get the terms

$$\begin{aligned}\frac{dx_i}{dt} &= \dots + i_r \cdot u \cdot x_i \cdot P_m(x_1, \dots, x_n) + \dots, \\ \frac{du}{dt} &= \dots - i_r \cdot u \cdot x_i \cdot P_m(x_1, \dots, x_n) + \dots\end{aligned}$$

When $i_r \cdot u = a_m$, the term corresponding to $\frac{dx_i}{dt}$ is exactly the desired term $a_m \cdot x_i \cdot P_m(x_1, \dots, x_n)$. However, this does not mean that we have solved our problem; indeed:

- we can select the initial concentration $u(0)$ of the universal quantity U to satisfy the equality $i_r \cdot u(0) = a_m$;
- however, due to the differential equation describing u , the amount u decreases with time, so at the next moments of time, this amount will be smaller, and the equality $i_r \cdot u(t) = a_m$ will no longer be satisfied.

Let us show that by selecting $u(0)$ to be large enough – and by correspondingly selecting $i_r = \frac{a_m}{u(0)}$ – we will be able to guarantee that the approximate equality $i_r \cdot u(t) \approx a_m$ holds for all moments $t \in [0, T]$ with a given accuracy.

Indeed, for $i_r = \frac{a_m}{u(0)}$, the product $i_r \cdot u(t)$ takes the form $\frac{u(0)}{u(t)} \cdot a_m$. Thus, if we find $u(0)$ for which the ratio $\frac{u(0)}{u(t)}$ is close to 1 for all t , we get the desired approximate equality $i_r \cdot u(t) \approx a_m$ for all moments $t \in [0, T]$.

In the ideal case when $i_r \cdot u \approx a_m$, the corresponding term in $\frac{du}{dt}$ takes the form

$$\frac{du}{dt} = \dots - a_m \cdot x_i \cdot P_m(x_1, \dots, x_n) + \dots$$

Equations corresponding to different monomials lead to other such terms (and other terms comes from monomials with $a_m < 0$, see the following part of the proof). Good news for us is that these terms do not depend on the selected value $u(0)$, so we have

$$\frac{du}{dt} = d(t),$$

for some function $d(t)$ which does not depend on $u(0)$. Thus,

$$u(t) = u(0) + D(t),$$

where we denoted

$$D(t) \stackrel{\text{def}}{=} \int_0^t d(s) ds.$$

The function $D(t)$ is a (differentiable hence) continuous function of t , so its absolute value $|D(t)|$ has the largest possible value D . Thus, for all t , we have

$|u(0) - u(t)| \leq D$, hence $u(0) - D \leq u(t) \leq u(0) + D$. Thus, the ratio $\frac{u(0)}{u(t)}$ satisfies the inequality

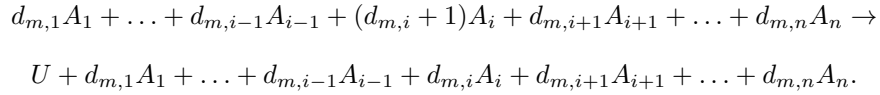
$$\frac{u(0)}{u(0) + D} \leq \frac{u(0)}{u(t)} \leq \frac{u(0)}{u(0) - D},$$

or, equivalently,

$$\frac{1}{1 + \frac{D}{u(0)}} \leq \frac{u(0)}{u(t)} \leq \frac{1}{1 - \frac{D}{u(0)}}.$$

When $u(0)$ increases, both the left-hand side and the right-hand side terms in this inequality tend to 1. So, whatever accuracy we want in approximating the original monomial term by the corresponding chemical term, we can indeed guarantee it by selecting an approximately large value $u(0)$.

7°. For monomials for which $a_m < 0$, we take the reaction



In this reaction, for all the substances except for the i -th substance A_i and the auxiliary universal substance U , the number of molecules entering the reaction is the same as the number of molecules leaving this reaction. The only difference is that a molecule of the i -th substance A_i is transformed into a molecule of the universal substance U . In this transformation, all the other substances play the role of catalysts – in the sense that

- while the presence of these other substances is necessary for the reaction to occur, and
- while the speed of this reaction depends on the concentrations of these other substances,
- in the long run, each of this other substances is neither consumed nor produced – in this reaction their concentration does not change.

A precise description of the corresponding terms in chemical equations also confirms this qualitative analysis. Indeed, according to the general formula for the chemical equations (as given in Definition 2), the speed v_r of this reaction is equal to

$$v_r = i_r \cdot x_1^{d_{m,1}} \cdot \dots \cdot x_{i-1}^{d_{m,i-1}} \cdot x_i^{d_{m,i}+1} \cdot x_{i+1}^{d_{m,i+1}} \cdot \dots \cdot x_n^{d_{m,n}},$$

where i_r denotes the intensity of this reaction. In terms of the monomial $P_m(x_1, \dots, x_n)$, this formula takes the form

$$v_r = i_r \cdot x_i \cdot P_m(x_1, \dots, x_n).$$

According to the same Definition 2, as a result of this reaction, there is no contribution to differential equations describing $\frac{dx_j}{dt}$ for $j \neq i$. The only contributions are to the terms $\frac{dx_i}{dt}$ and $\frac{du}{dt}$: namely, we get the terms

$$\begin{aligned}\frac{dx_i}{dt} &= \dots - i_r \cdot x_i \cdot P_m(x_1, \dots, x_n) + \dots, \\ \frac{du}{dt} &= \dots + i_r \cdot x_i \cdot P_m(x_1, \dots, x_n) + \dots\end{aligned}$$

When $i_r = |a_m|$, the term corresponding to $\frac{dx_i}{dt}$ is exactly the desired term $a_m \cdot x_i \cdot P_m(x_1, \dots, x_n)$. The corresponding term for $\frac{du}{dt}$ takes the form

$$\frac{du}{dt} = \dots + |a_m| \cdot x_i \cdot P_m(x_1, \dots, x_n) + \dots$$

8°. Thus, the desired approximation result is proven for the case when each ratio $g_i(x_1, \dots, x_n) = \frac{f_i(x_1, \dots, x_n)}{x_i}$ can be continuously extended to values $x = (x_1, \dots, x_n)$ for which $x_i = 0$.

9°. Let us now show how a general dynamical system can be reduced to this special case. The main idea of this reduction is to avoid the zone $x_i \approx 0$ where the above ratio condition is not satisfied. For this purpose, we will add, to each substance, a small amount $\delta > 0$, and perform all the dynamics after that as before; the dynamics for the zone $x_i < \delta$ – which does not affect our processes, except for the short first period of time when the concentrations are increases – will then be defined in such a way that the above condition about the ratio $g_i(x_1, \dots, x_n)$ is satisfied.

To implement this idea, we will introduce new functions $\tilde{f}_i(x_1, \dots, x_n)$ which for $x_i \geq \delta$ have the form

$$\tilde{f}_i(x_1, \dots, x_n) = f_i(x_1 - \delta, \dots, x_n - \delta).$$

The meaning of this definition is that, in describing the changes in all the variables x_i , we do not take into account the extra amount δ that we added to the concentrations x_i . Thus, trajectories of the new system have the form $\tilde{x}_i(t) = \delta + x_i(t)$, where $x_i(t)$ is a trajectory of the original dynamical system. When δ is small, these trajectories are close.

For values $x_i < \delta$, the above formula does not work, since the original function $f_i(x_1, \dots, x_n)$ is only defined for $x_i \geq 0$. Thus, we need to extend the above expression to cover such values. We want to make sure that there is a limit of the ratio $\tilde{g}_i(x_1, \dots, x_n) = \frac{\tilde{f}_i(x_1, \dots, x_n)}{x_i}$ when $x_i \rightarrow 0$. When

such a limit exists, then $\tilde{f}_i(x_1, \dots, x_n) = x_i \cdot \tilde{g}_i(x_1, \dots, x_n)$ for some continuous function $\tilde{g}_i(x_1, \dots, x_n)$; in this case, for $x_i = 0$, we have

$$\tilde{f}_i(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n) = 0.$$

Vice versa, if $\tilde{f}_i(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n) = 0$, then the limit of the desired ratio takes the following form:

$$\lim_{x_i \rightarrow 0} \frac{\tilde{f}_i(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n)}{x_i} = \lim_{x_i \rightarrow 0} \frac{\tilde{f}_i(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n) - \tilde{f}_i(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n)}{x_i}.$$

One can easily check that this exactly the definition of the partial derivative $\frac{\partial \tilde{f}_i}{\partial x_i}$ at the point where $x_i = 0$. So, when we extend the above expression $\tilde{f}_i(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n)$ to a continuously differentiable function that is defined for all $x_i \geq 0$, all we need to do to satisfy the above limit condition is to make sure that

$$\tilde{f}_i(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n) = 0.$$

for all i . For each i , we thus extend the original smooth functions $\tilde{f}_i(x_1, \dots, x_n)$ defined for $x_i \geq \delta$ to the zone $x_i \geq 0$ in such a way that $\tilde{f}_i(x_1, \dots, x_n) = 0$ for $x_i = 0$. The existence of such extension is well known in mathematical analysis.

To move the behavior into the zone $x_i \geq \delta$, we add – very fast – the amount δ to the concentrations of each of n substances $A_1, \dots, A_n$. This can be done, e.g., if we introduce n new auxiliary substances $U_1, \dots, U_n$ each of which has the initial concentration $u_i(0) = \delta$, and add n very fast reactions $U_i \rightarrow A_i$ for each i from 1 to n . As a result of these reactions, each substance A_i indeed acquires an additional concentration δ . When the time is short enough, this transition does not affect the remaining dynamics, so the new trajectories $x_i(t)$ will be close to the original ones.

10°. The reduction of a generic dynamical system to a dynamical system of a special type is explained. Since we have already proven that dynamical systems of the special type can be approximated by chemical systems, we can thus also approximate a generic dynamical system by a chemical system. The theorem is proven.

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