Chemistry 4010 Lecture 1: Introductory ideas

Marc R. Roussel

August 30, 2019

What is a dynamical system?

Three ingredients:

1. Time
2. Variables that describe the state of the system (state variables)
   - The state variables define a state space.
   - The phase space contains all the variables needed to compute the time evolution (in principle, if not in practice).
   - The phase space is not always the same as the state space.
3. A rule according to which the variables evolve in time
   - The rule may not be known.
   - It can be deterministic or stochastic (random).

Examples of dynamical systems

The time evolution operator

- Suppose that we have a dynamical system whose state at time t is given by $x(t)$.
- The time evolution operator φ^t is defined by

$$\varphi^t x(0) = x(t)$$

  Paraphrasing, the time evolution operator moves time forward by t.
- The time evolution operator is often not explicitly known.
- $\varphi^0 x(0) = x(0)$, so φ^0 is the identity operator.
- $\varphi^t x(s) = x(t+s)$
- Consequently, in operator notation, $\varphi(t+s) = \varphi^t \circ \varphi^s = \varphi^s \circ \varphi^t$.

The law of mass-action

- For (bio)chemists, one of the most important classes of dynamical systems are (perhaps obviously) chemically reacting systems.

- For well-mixed systems, the time evolution is described by the law of mass-action:

  The rate of an elementary reaction is proportional to the product of the concentrations of the reactants.

- The rate of reaction is the rate of change of a (possibly imaginary) substance with a stoichiometric coefficient of 1.