

History and Evolution Equations in Mechanics and for Populations

What is a “dynamics”? A dynamics is a description of “what happens ‘a step after a step’”. It provides a logical, causal relationship. Such information is not in the usual statistical data. The confidence scientists have in their theories about the real world is derived from such models that provide a description of the reality, when idealized, with a high precision.

To understand something, to ask “why” and its causes (i.e., mechanism), one always has to ask “how did that happen”. This is essentially a question about *history*. In mathematical terms, it is a question about *dynamics*.

Even when one is not explicitly interested in how things changing with time, a dynamic perspective often provides a better understanding. We will see this in the modeling of the power law degree distribution for scale free networks based on preferential attachment, e.g., “the rich get richer”, mechanism.

To model dynamics in terms of mathematical equation(s) is one of the most important aspects of post Keplerian science. “Big data” is not the goal; it is only the very first, primitive step toward an *exact science*.

2.1 Non-dimensionalization procedure

A differential equation, or a system of differential equations, often contains parameters. By a parameter, we mean its value is unknown, but it is a constant independent of the variables in the equation. For example

$$\frac{dy}{dt} = ay, \quad y(0) = y_0, \quad (2.1)$$

has two parameters, a and y_0 . Note that the initial condition, which is not in the equation *per se*, can also be a parameter.

Variables in a differential equation are physical quantities; they have “dimensions”. If the y in Eq. (2.1) is concentration and t is time, then they have dimensions

$$\frac{[\text{number}]}{[\text{volume}]}, \quad \text{and} \quad [\text{time}],$$

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respectively. Noting the dimension of each additive term in an algebraic expression has to be the same, we immediately have the dimension for a being $1/[\text{time}]$.

The procedure of non-dimensionalization is such: redefine the dependent and independent variables in the equation in terms of the parameters with same dimensions:

non-dimensional time: $\tau = \frac{t}{1/b} = bt$, non-dimensional concentration: $u = \frac{y}{y_0}$.

Then the differential equation in (2.1) is simplified into

$$\frac{du}{d\tau} = u, \quad u(0) = 1. \quad (2.2)$$

This is a simpler, but mathematically identical equation.

Note that non-dimensionalization procedures usually are not unique.

2.2 Interest and compound interest (Ch. 3)

Today, we shall discuss dynamics, from discrete ‘time’, one step at a time, to continuous time, e.g., in terms of ordinary differential equation(s).

We first introduce two concepts: The *compound interest* for a bank account, and the Malthusian parameter for population growth per capita.

When you go to a bank, you might be told that “we pay an APR (annual percentage rate) of 6% and an APY (annual percentage yield) of 6.17%.” However, at another bank, you might be told that “we pay an APR of 6% and an APY of 6.18%.”

Is one of the banks made a mistake in their calculations? If you ask, you might find that the first bank pays its interest monthly, while the second one weekly. Therefore:

$$\left(1 + \frac{0.06}{12}\right)^{12} = 0.061678, \quad \text{but} \quad \left(1 + \frac{0.06}{52}\right)^{52} = 0.0618. \quad (2.3)$$

So the APY includes an important component: the compound interest.

Now the general formula: Let Δt be the time period for paying interest, r be the APR, then each period, the bank pays $(1 + r\Delta t)$ times the principle at the end of a period. Therefore, for the total time t , we have

$$P(t) = P(0) \left(1 + r\Delta t\right)^{t/\Delta t}. \quad (2.4)$$

The total fraction yield, then is

$$\frac{P(t) - P(0)}{P(0)} = \left(1 + r\Delta t\right)^{t/\Delta t} - 1. \quad (2.5)$$

2.2.0.1 Computing mortgage payments

This is certainly one of the most important pieces of “simple math” in your life! Even though there are plenty of webpages that allow you just type in some numbers and return

what you want, I think being a student in ACMS, it is important you are able to compute this yourself.

Let T be the total period of mortgage, e.g., 15 years, 30 years, etc. Let the repayment period be Δt . It is usually per month, or biweekly. At the time $t = 0$, you borrowed the amount of money $P(0)$. This amount should go down in time and eventually $P(T) = 0$. We shall assume that the interest is fixed at APR r :

Let M be the fixed per Δt repayment. Then for each Δt :

$$\boxed{P(t + \Delta t) = P(t)(1 + r\Delta t) - M.} \quad (2.6)$$

Following the steps in the textbook, we have

$$P(m\Delta t) = P(0)(1 + r\Delta t)^m + M \left(\frac{1 - (1 + r\Delta t)^m}{r\Delta t} \right). \quad (2.7)$$

To solve the M using $P(T) = 0$:

$$P(0)(1 + r\Delta t)^{T/\Delta t} + M \left(\frac{1 - (1 + r\Delta t)^{T/\Delta t}}{r\Delta t} \right) = 0. \quad (2.8)$$

$$M = \frac{P(0)(1 + r\Delta t)^{T/\Delta t}}{\frac{(1 + r\Delta t)^{T/\Delta t} - 1}{r\Delta t}} = P(0)r\Delta t \left(\frac{(1 + r\Delta t)^{T/\Delta t}}{(1 + r\Delta t)^{T/\Delta t} - 1} \right). \quad (2.9)$$

Now here is an interesting problem: Some bank decided to be greedy, so they are going to ask for daily interest(!) denoted by τ . However, the repayment is still Δt . Then in Eq. 2.9 we need to replace

$$1 + r\Delta t \longleftrightarrow (1 + r\tau)^{\Delta t/\tau}. \quad (2.10)$$

Now generalizing Eq. 2.10 to the extreme, one lets $\tau \rightarrow 0$:

$$r \longleftrightarrow \frac{(1 + r\tau)^{\Delta t/\tau} - 1}{\Delta t} \stackrel{\tau \rightarrow 0}{\cong} \frac{e^{r\Delta t} - 1}{\Delta t}. \quad (2.11)$$

You can prove that the right-hand-side of Eq. 2.11 is never smaller than r , because $e^{r\Delta t} = 1 + r\Delta t + \frac{1}{2}(r\Delta t)^2 + \dots$.

2.2.1 Some examples

See page 58.

2.2.2 Two mathematical results

(1)

$$\lim_{x \rightarrow 0} (1 + x)^{1/x} = ?$$

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Using the method of L'Hôpital rule

$$\lim_{x \rightarrow 0} \ln(1+x)^{1/x} = \lim_{x \rightarrow 0} \frac{\ln(1+x)}{x} = \lim_{x \rightarrow 0} \frac{\frac{1}{1+x}}{1} = 1.$$

Or, using Taylor expansion:

$$\lim_{x \rightarrow 0} \ln(1+x)^{1/x} = \lim_{y \rightarrow \infty} y \ln\left(1 + \frac{1}{y}\right) = \lim_{y \rightarrow \infty} y \left(\frac{1}{y} - \frac{1}{2y^2} + \frac{1}{3y^3} + \dots\right) = 1.$$

(2) Solving difference equation in (2.6):

$$u_{n+1} = au_n + b. \quad (2.12)$$

Note this is very similar to the differential equation

$$\frac{du}{dt} = \alpha u + \beta. \quad (2.13)$$

Recall how to solve the latter ODE: First, the general solution for the corresponding homogeneous equation; then solve a particular solution to the inhomogeneous equation; put add them together.

So, the general solution to the homogeneous equation $u_{n+1} = au_n$. Professor Qian has already discussed this. It is

$$u_n^{\text{homogeneous}} = Ca^n \quad (2.14)$$

Now to find a particular solution to $u_{n+1} = au_n + b$. Can we again gain some idea from how to solve the inhomogeneous ODE? The idea, called "variation of constant", is to assume the solution to the inhomogeneous equation in the form of $C_n a^n$. Then we have

$$\begin{aligned} C_{n+1} a^{n+1} &= C_n a^{n+1} + b, \\ C_{n+1} &= C_n + b a^{-n-1}. \end{aligned}$$

If we let $C_0 = b$ (since we are just interested in a particular solution, the choice for C_0 is arbitrary), then

$$\begin{aligned} C_n &= C_{n-1} + b a^{-n} = C_{n-2} + b(a^{-(n-1)} + a^{-n}) = C_0 + b \sum_{k=1}^{n-1} a^{-k} \\ &= b \frac{1 - a^{-n}}{1 - a^{-1}} = b \frac{a - a^{1-n}}{a - 1}. \end{aligned}$$

Putting all together, we have the general solution to $u_{n+1} = au_n + b$:

$$u_n = Ca^n + \left(\frac{a^n - 1}{a - 1}\right) ab. \quad (2.15)$$

in which $C = u_0$. To solve Eq. 2.6, we have n becomes m , $a = 1 + r\Delta t$ and $b = -M$. This yields exactly the result in Eq. 2.7.

2.3 Two perspectives on the world

As discussed in Sec. 1.2, mechanics considers a world made of point masses; but chemistry deals a world made of molecules, each of which is already infinitely complex, with nearly infinite internal degrees of freedom. To study a system made of many individuals, one first has to classify them into “dynamic species” and then represent the system in terms the population sizes

$$(x_1, x_2, \dots, x_n) \quad (2.16)$$

where x_i is the population of the i^{th} species. Note strictly speaking, the x_i has to be a non-negative integer. However, if the population size is sufficiently large, then it is acceptable to treat the x_i as a non-negative real value. In solution chemistry, one usually uses *concentration* or *number density* to represent a population size.

Another important application of mathematical modeling is in population dynamics. This can be about populations of biological organisms, chemical species inside a test tube, or sociological and economical agents. As long as one has the notion of different “individuals”, there is the concept of a “population”.

This population dynamic view is much more general than just in chemistry. The “species” can also be bacteria, human cells, or populations in ecology, and players in infectious epidemics. Population dynamics usually starts with an equation like this:

$$\text{rate of population increase} = \text{birth rate} - \text{death rate} + \text{immigration rate}. \quad (2.17)$$

If we use $x(t)$ to denote the population at time t , then the above equation becomes

$$\frac{dx}{dt} = x(b(x) - d(x)) + i(x), \quad (2.18)$$

in which b and d are the *per capita* birth and death rates, respectively. Note that one of the most important aspects of birth and death is that if $x = 0$, then there will be no possibility of further birth or death. Without immigration, an extinct population will remain extinct. The immigration term $i(x)$, however, has a very different feature: It needs not to be zero when $x = 0$.

Clearly, down to individual and very small population size, the above deterministic differential equation cannot be really valid. Eq. 2.18 becomes true when the population size is sufficiently large, when the statistical uncertainties can be neglected. Therefore, equations like (2.18) should be understood as a consequence of a statistical result.

Population dynamics, though appears to be deterministic mechanistic modeling, is actually a result of probabilistic mechanistic models. We shall discuss this important aspect in a later time.

2.4 A fundamental theorem in population dynamics with independent species

Dynamical models can be, for example, about “money in your bank account” or “the numbers of individuals in the various species in a wild forest”. It can also be about

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the number of individuals in each and every subpopulation of an entire population, such as the case in the next section.

Consider a population with many subpopulations $\vec{x} = (x_1, x_2, \dots, x_n)$, all $x_i \geq 0$. In the absence of immigration, if we denote $r_i(\vec{x}) = b_i(\vec{x}) - d(\vec{x})$, then

$$\frac{dx_i}{dt} = x_i r_i(\vec{x}), \quad (2.19)$$

and the per capita growth rate for the entire population, which is also the mean per capita growth rate,

$$\bar{r} = \frac{\sum_{i=1}^n \frac{dx_i}{dt}}{\sum_{i=1}^n x_i} = \frac{\sum_{i=1}^n x_i r_i(\vec{x})}{\sum_{i=1}^n x_i}, \quad x_i \geq 0. \quad (2.20)$$

Then,

$$\frac{d\bar{r}(\vec{x})}{dt} = \left[\frac{\sum_{i=1}^n x_i r_i^2}{\sum_{i=1}^n x_i} - \left(\frac{\sum_{i=1}^n x_i r_i}{\sum_{i=1}^n x_i} \right)^2 \right] + \frac{\sum_{i,j=1}^n x_i x_j r_j \left(\frac{\partial r_i}{\partial x_j} \right)}{\sum_{i=1}^n x_i} \quad (2.21)$$

We note that the term inside $[\dots]$ on the right-hand-side is never negative:

$$\frac{\sum_{i=1}^n x_i r_i^2}{\sum_{i=1}^n x_i} - \left(\frac{\sum_{i=1}^n x_i r_i}{\sum_{i=1}^n x_i} \right)^2 = \frac{\sum_{i=1}^n x_i (r_i - \bar{r})^2}{\sum_{i=1}^n x_i} \geq 0, \quad (2.22)$$

In fact, it is actually the variance of r_i among the different subpopulations. Therefore, it is always positive if there are variations among r_i . This mathematical result is a part of the ideas of both Adam Smith, on economics, and Charles Darwin, on the natural selection. In fact, the term $[\dots]$ in Eq. (2.21) has been identified by R. A. Fisher, the British statistician and evolutionary biologist, as the “growth of fitness due to natural selection”.* And here is a quote from Smith’s *magnum opus* “An Inquiry into the Nature and Causes of the Wealth of Nations” (1776):

“As every individual, therefore, endeavours as much as he can both to employ his capital in the support of domestic industry, and so to direct that industry that its produce may be of the greatest value; every individual necessarily labours to render the annual revenue of the society as great as he can. He generally, indeed, neither intends to promote the public interest, nor knows how much he is promoting it. By preferring the support of domestic to that of foreign industry, he intends only his own security; and by directing that industry in such a manner as its produce may be of the greatest value, he intends only his own gain, and he is in this, as in many other cases, led by an invisible hand to promote an end which was no part of his intention. Nor is it always the worse for the society that it was no part of it. By pursuing his own interest he frequently promotes that of the society more effectually than when he really intends to promote it. I have never known much good done by those who affected to trade for the public good. It is an affectation, indeed, not very common among merchants, and very few words need be employed in dissuading them from it.”

* Edwards, A.W.F (1994) The fundamental theorem of natural selection. *Biol. Rev.* 69, 443–474.

Eq. 2.21 can be written as:

$$\frac{d}{dt} \left(\frac{\sum_{i=1}^n x_i r_i}{\sum_{i=1}^n x_i} \right) - \frac{\sum_{i=1}^n x_i \frac{dr_i(\vec{x})}{dt}}{\sum_{i=1}^n x_i} = \frac{\sum_{i=1}^n x_i (r_i - \bar{r})^2}{\sum_{i=1}^n x_i}. \quad (2.23)$$

This equation can be phrased as “the change in the per capita growth rate of an entire population is never less than the average change in per capita growth rate of the subpopulations”.[†] Eq. 2.21 also shows that $d\bar{r}/dt$ could be negative if the last term on the right-hand-side is large and negative. Therefore, it is interesting to investigate under what circumstances it is positive or negative.

First, we note that if all r_i are constant, independent of \vec{x} , then this last term is zero since $(\partial r_i / \partial x_j) = 0$.

Second, if r_i is a linear function of \vec{x} : $r_i(\vec{x}) = \sum_{k=1}^n w_{ik} x_k$. Furthermore, one can always decompose a matrix into a symmetric and an anti-symmetric parts: $w_{ij} = w_{ij}^S + w_{ij}^A$. Then

$$\begin{aligned} \frac{\sum_{i,j=1}^n x_i x_j r_j \left(\frac{\partial r_i}{\partial x_j} \right)}{\sum_{i=1}^n x_i} &= \frac{\sum_{i,j,k=1}^n x_i w_{ij} x_j w_{jk} x_k}{\sum_{i=1}^n x_i} \\ &= \frac{\sum_{i,j,k=1}^n x_i w_{ij}^S x_j w_{jk}^S x_k}{\sum_{i=1}^n x_i} + \frac{\sum_{i,j,k=1}^n x_i w_{ij}^A x_j w_{jk}^A x_k}{\sum_{i=1}^n x_i} \\ &= \frac{\sum_{j=1}^n x_j \left(\sum_{i=1}^n x_i w_{ij}^S \right)^2}{\sum_{i=1}^n x_i} - \frac{\sum_{j=1}^n x_j \left(\sum_{i=1}^n x_i w_{ij}^A \right)^2}{\sum_{i=1}^n x_i}. \end{aligned} \quad (2.24)$$

Hence, a symmetric interaction between subpopulations i and j increases the \bar{r} , and an anti-symmetric interaction between subpopulations i and j decreases the \bar{r} . Competition and symbiosis are the former type, and predator and prey are the latter type.

[†] Price, G.R. (1972) Fishers fundamental theorem made clear. *Ann. Hum. Genet. Lond.* **36**, 129–140.