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Aquatic Ecotoxicology: Theoretical Explanation of Empirical Formulas

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Abstract To analyze the effect of pollution on marine life, it is important to know how exactly the concentration of toxic substances decreases with time. There are several semi-empirical formulas that describe this decrease. In this paper, we provide a theoretical explanation for these empirical formulas.

1 Formulation of the Problem

Background. Pollution is ubiquitous, and oceans, lakes, and rivers are not immune from it. Good news is that many toxic substances are not stable, their concentration C in sea creatures decreases with time. It is important to be able to predict how this decrease will go.

What is known. Several semi-empirical equations

$$\frac{dC}{dt} = f(C)$$

describe this decrease (see, e.g., [2]):

- In most cases, $f(C)$ is a polynomial (mostly quadratic).
- In other cases, the formula is fractional-linear:

$$f(C) = \frac{a + b \cdot C}{1 + d \cdot C}.$$

Problem. How can we explain these formulas?

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What we do in this paper. In this paper, we use invariance ideas to provide a theoretical explanation for these empirical formulas.

2 Invariance Ideas

General idea. The numerical value of each physical quantity depends:

- on the selection of the measuring unit, and
- on the selection of the starting point.

Scaling and scale-invariance. If we replace the original measuring unit with the one which is λ times smaller, all numerical values multiply by λ:

$$x \mapsto \lambda \cdot x.$$

This transformation is known as *scaling*.

In many cases, there is no preferable measuring unit. In this case, it makes sense to assume that the formulas should remain the same if we change the measuring unit.

Shift and shift-invariance. If we replace the original starting point with the one which is x_0 units earlier, we add x_0 to all numerical values:

$$x \mapsto x + x_0.$$

This transformation is known as *shift*.

For quantities such as temperature or time, there is no preferred starting point. In this case, it makes sense to assume that the formulas should remain the same if we change the starting point.

More general invariance. If we change both the starting point and the measuring unit, we get a general linear transformation:

$$x \mapsto \lambda \cdot x + x_0.$$

A typical example of such a transformation is converting temperature from Celsius to Fahrenheit: $t_F = 1.8 \cdot t_C + 32$.

3 Let Us Apply Invariance Ideas to Our Problem

What we want. We want to find out how the reaction rate

$$r \stackrel{\text{def}}{=} \frac{dC}{dt}$$

depends on the concentration C.

We need a family of functions. In different places, this dependence is different. Thus:

- we cannot look for a *single* function $r = f(C)$,
- we should look for a *family* of functions.

Simplest types of families. The simplest type of family is:

- when we fix several functions $e_1(t), \ldots, e_n(t)$, and
- we consider all possible linear combinations of these functions:

$$C_1 \cdot e_1(t) + \ldots + C_n \cdot e_n(t).$$

Examples. For example:

- if we take $e_1(t) = 1$, $e_2(t) = t$, $e_3(t) = t^2$, etc.,
- then we get polynomials.

If we select sines and cosines, we get what is called trigonometric polynomials, etc.

Remaining problem. Which family should we select?

4 Let Us Apply Invariance Ideas to Our Case

Reminder. For time, there is no preferred measuring unit and no preferred starting point.

Resulting requirement. So, it makes sense to select a family which is invariant with respect to scalings and shifts.

This leads to the desired explanation of polynomial formulas. It is known that in all such invariant families, all the functions from these families are polynomials; see Appendix A. This explains why in most cases, the empirical dependence $r = f(C)$ is polynomial.

5 How to Explain Fractional-Linear Dependence?

Some natural transformations are non-linear. In the previous text, we only considered linear transformations. However, in some cases, we can also have natural non-linear transformations between different scales. For example:

- There are two natural scales for describing earthquakes: energy scale and logarithmic (Richter) scale.

- Our reaction to sound is best described not by its power, but the power's logarithms – decibels, etc.

How can we describe the class of all natural transformations?

What are natural nonlinear transformations? As we have mentioned, linear transformations are natural. Also:

- If we have a natural transformations between scales A and B, then the inverse transformation should also be natural.
- If we apply two natural transformations one after another, then the resulting composition should also be natural.

Thus, the class of all natural transformations should be closed under composition and inverse. Such classes are known as *transformation groups*.

Also, we want to describe all these transformation in a computer. In each computer, we can only store finitely many parameters. Thus, we should restrict ourselves to finite-parametric transformation groups that contain all linear transformations.

A known result about such groups explains fractional-linear dependence. It is known that every element of finite-parametric transformation groups that contain all linear transformations is a fractional-linear function; see, e.g., [1, 3, 5]. This explains why the dependence $r = f(C)$ is sometimes described by a fractional-linear function: r and C can be viewed as two different scales for describing the same phenomena.

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References

1. V. M. Guillemin and S. Sternberg, "An algebraic model of transitive differential geometry", *Bulletin of American Mathematical Society*, 1964, Vol. 70, No. 1, pp. 16–47.
2. M. C. Newman, *Quantitative Methods in Aquatic Ecotoxicology*, Lewis Publishers. Boca Raton, Ann Arbor, London, and Tolyo, 1995.

3. H. T. Nguyen and V. Kreinovich, *Applications of Continuous Mathematics to Computer Science*, Kluwer, Dordrecht, 1997.
4. J. C. Robinson, *An Introduction to Ordinary Differential Equations*, Cambridge University Press, Cambridge, UK, 2004.
5. I. M. Singer and S. Sternberg, "Infinite groups of Lie and Cartan, Part 1", *Journal d'Analyse Mathematique*, 1965, Vol. XV, pp. 1–113.
6. M. Tenenbaum and H. Pollard, *Ordinary Differential Equations*, Dover Publ., New York, 2022.

7 How to Prove the Result about the Invariant Families

This result is easy to prove when the functions $e_i(t)$ are differentiable.

Let us first use shift-invariance. Shift-invariance implies that for each function $e_i(t)$, its shift $e_i(t+t_0)$ belongs to the same family. So, for some coefficients $C_{ij}(t_0)$, we get:

$$e_i(t+t_0) = C_{i1}(t_0)\cdot e_1(t) + \ldots + C_{in}(t_0)\cdot e_n(t).$$

If we differentiate both sides with respect to t_0, we get

$$e_i'(t+t_0) = C_{i1}'(t_0)\cdot e_1(t) + \ldots + C_{in}'(t_0)\cdot e_n(t).$$

In particular, for $t_0 = 0$, we get

$$e_i'(t) = c_{i1}\cdot e_1(t) + \ldots + c_{in}\cdot e_n(t),$$

where we denoted $c_{ij} \stackrel{\text{def}}{=} C_{ij}'(0)$. So, we get a system of linear differential equations with constant coefficients. It is known (see, e.g., [4, 6]) that its solutions are linear combinations of terms

$$t^m \cdot \exp(k\cdot t),$$

where k is an eigenvalue of the matrix c_{ij}, and m is a non-negative integer which is smaller than k's multiplicity.

Let us now use scale-invariance. Similarly, scale-invariance implies that for each function $e_i(t)$, its scaling $e_i(\lambda\cdot t)$ belongs to the same family. So, for some coefficients $C_{ij}(\lambda)$, we get:

$$e_i(\lambda\cdot t) = C_{i1}(\lambda)\cdot e_1(t) + \ldots + C_{in}(\lambda)\cdot e_n(t).$$

If we differentiate both sides with respect to λ, we get

$$t\cdot e_i'(\lambda\cdot t) = C_{i1}'(\lambda)\cdot e_1(t) + \ldots + C_{in}'(\lambda)\cdot e_n(t).$$

In particular, for $\lambda = 1$, we get

$$t\cdot \frac{de_i(t)}{dt} = c_{i1}\cdot e_1(t) + \ldots + c_{in}\cdot e_n(t),$$

where we denoted $c_{ij} \stackrel{\text{def}}{=} C'_{ij}(1)$. In this case,

$$\frac{dt}{t} = dT,$$

where we denoted $T \stackrel{\text{def}}{=} \ln(t)$. Thus, for the new variable T, we get the same system as before

$$e'_i(T) = c_{i1} \cdot e_1(T) + \ldots + C_{in} \cdot e_n(T).$$

So, its solution is a linear combination of functions

$$T^m \cdot \exp(k \cdot T) = (\ln(t))^m \cdot \exp(k \cdot \ln(t)) = (\ln(t))^m \cdot t^k.$$

What is a family is both shift- and scale-invaraint? The only functions that can be represented in both forms $t^m \cdot \exp(k \cdot t)$ and $(\ln(t))^m \cdot t^k$ are polynomials. Thus, every element of a scale- and shift-invariant family is indeed a polynomial.