Aquatic Ecotoxicology: Explanation of Empirical Formulas

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Formulation of the Problem. 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. Several semi-empirical equations $\frac{dC}{dt} = f(C)$ describe this decreases. In most cases, $f(C)$ is a polynomial (mostly quadratic). In other cases, the formula is fractional-linear: $f(C) = \frac{a + b\cdot C}{1 + d\cdot C}$. In this talk, we use invariance ideas to provide a theoretical explanation for these empirical formulas.

Invariance Ideas. The numerical value of each physical quantity depends on the selection of the measuring unit, and on the selection of the starting point. 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.

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. 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: $t_F = 1.8\cdot t_C + 32$.

We want to find out how the reaction rate $r \stackrel{\text{def}}{=} \frac{dC}{dt}$ depends on the concentration C. 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. The simplest type of family if when we fix several functions $e_1(t)$, …, $e_n(t)$, and consider all possible linear combinations $C_1\cdot e_1(t) + \ldots + C_n\cdot e_n(t)$. For example, if we take $e_1(t) = 1$, $e_2(t) = t$, etc., we get polynomials. If we select sines and cosines, we get what is called trigonometric polynomials, etc.

Which family should we select? For time, there is no preferred measuring unit and no preferred starting point. So, it makes sense to select a family which is invariant with respect to scalings and shifts. It is known that in all such invariant families, all the functions are polynomials. This explains why in most cases, the empirical dependence $r = f(C)$ is polynomial.

Beyond Linear Transformations. In some cases, we can also have non-linear transformations between different scales. For example, there are two natural scales for describing earthquakes: energy scale and logarithmic (Richter) scale. What are natural nonlinear transformation? As we have mentioned, linear transformations are natural. 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.* 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. It is known that every element of such a group is a fractional-linear function. This explains why the dependence $r = f(C)$ is fractional-linear.