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On aliases of differential equations

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Matematica. — *On aliases of differential equations.* Nota (*) di RUTHERFORD ARIS e GIANNI ASTARITA, presentata dal Socio Straniero C. TRUESDELL.

ABSTRACT. — Theory of chemical reactions in complex mixtures exhibits the following problem. Single reacting species follow an intrinsic kinetic law. However, the observable quantity, which is a mean of individual concentrations, follows a different law. This one is called «alias» of intrinsic kinetics. In this paper the phenomenon of alias of uniform families of differential equations is discussed in general terms.

KEY WORDS: Alias; Chemical reactions; Differential equations.

RIASSUNTO. — *Sulle alias delle equazioni differenziali.* La teoria delle reazioni chimiche in miscele complesse presenta il seguente problema. Le singole specie reagenti seguono una legge cinetica intrinseca, ma la quantità osservabile, che è una media delle concentrazioni individuali, segue una legge diversa. Quest'ultima è qui chiamata l'alias della cinetica intrinseca. Nella presente nota viene discusso in termini generali il fenomeno dell'alias di famiglie uniformi di equazioni differenziali.

INTRODUCTION

In the theory of chemical reaction in complex mixtures the following problem arises. The mixture is first represented as a continuous distribution with an index x in the interval $[0, \infty)$, such that, for example, $u(x, t)\,dx$ is the concentration of material of index in $(x, x+dx)$ at time t. The reactions of the indexed species are governed by a differential equation of some type of kinetics, but the observable quantity is a mean of the distribution

$$U(t) = \int_0^\infty h(x)\, u(x, d)\, dt$$

which is found to obey a different type of kinetics. This second type is said to be an alias of the first and depends on the initial distribution of the continuous mixture: for example, an exponential distribution of first order reactions can appear to react in the mean as if it were of the second order (Aris, 1968). Astarita and Ocone have recently introduced a type of kinetics, called by them uniform, whose aliases can be of almost any type (Astarita and Ocone, 1988). The purpose of this note is to draw attention to the phenomenon of the alias in the general context of differential equations.

UNIFORM FAMILIES OF DIFFERENTIAL EQUATIONS

Let $u(x, t)$ be a family of functions of t. The continuous parameter x may, without loss of generality, be taken to be in the interval. The family will be called uniformly pseudo-linear if it satisfies

$$u_t(x, t) = -\,k(x)\, u(x, t) f\left(\int_0^\infty K(z)\, u(x, t)\, dz \right) \tag{1}$$

(*) Nella seduta dell'11 febbraio 1989.

with

$$x(u, 0) = v(x) \,. \tag{2}$$

In this equation $k(x)$ is a positive monotonically increasing function with $k(0) = 0$, $k(x) \to \infty$ as $x \to \infty$ and no generality is lost if we take it to be x. The family is uniform because for all values of x the independent variable t (which we may regard as time) is locally distorted by the same factor f; it is pseudo-linear because, if this distortion is accommodated, the equations are linear in the distorted time. $K(x) \geq 0$, $v(x) \geq 0$ and its zeroth and first moments exist. By change of scales we can always take $v(x)$ to satisfy

$$\int_0^\infty v(x)\, dx = \int_0^\infty xv(x)\, dx = 1 \,. \tag{3}$$

The distortion of the time scale is effected by a solution of the form

$$u(x, t) = v(x) \exp\left[-xw(t)\right], \qquad w(0) = 0 \tag{4}$$

which clearly satisfies (2) and can be made to satisfy (1) by taking

$$w_t = f\left(\int_0^\infty K(z)\, v(z) \exp\left[-zw\right] dz\right) = F(w) \,. \tag{5}$$

This equation can be solved by quadrature giving w implicitly as

$$t = \int_0^{w(t)} dw/F(w) = \Phi(w(t)) \,. \tag{6}$$

Aliases of uniform families

Let

$$U(t) = \int_0^\infty h(x)\, u(x, t)\, dx = \int_0^\infty h(x)\, v(x) \exp\left[-xw(t)\right] dx = L(w(t)) \,, \tag{7}$$

where $L(w)$ is the Laplace transform of hv. If L is monotonic

$$w = L^{-1}(U) \tag{8}$$

is well-defined and

$$U_t = -w_t \int_0^\infty xh(x)\, v(x) \exp\left[-xw\right] dx = -F(w)\, M(w) = -G(U) \,, \tag{9}$$

where

$$M(x) = -L'(w) = \int_0^\infty xh(x)\, v(x) \exp\left[-xw\right] dx \tag{10}$$

and

$$G(U) = F(L^{-1}(U))\, M(L^{-1}(U)) \,. \tag{11}$$

G is called an alias of the family defined by f.

Examples

An elementary example is obtained if we take

$$(12)\quad v(x)=\frac{\alpha^{\alpha}x^{\alpha-1}}{\Gamma(\alpha)}\exp[\alpha x]\,,\qquad h(x)=\frac{\Gamma(\alpha)}{\Gamma(\alpha+\beta)}(\alpha x)^{\beta}\,,\qquad K(x)=\frac{\Gamma(\alpha)}{\Gamma(\alpha+\gamma)}(\alpha x)^{\gamma}\,,$$

Then

$$(13)\qquad \begin{cases} L(w)=(1+w/\alpha)^{(\alpha+\beta)}\,,\\ M(w)=(1+w/\alpha)^{-(\alpha+\beta+1)}(1+\beta/\alpha)\,,\\ F(w)=f((1+w/\alpha)^{-(\alpha+\gamma)})\,. \end{cases}$$

Thus

$$(14)\qquad G(U)=(1+\beta/\alpha)\,U^{\lambda}f(U^{\mu})$$

where

$$(15)\qquad \lambda=(\alpha+\beta+1)/(\alpha+\beta)\,,\qquad \mu=(\alpha+\gamma)/(\alpha+\beta)\,.$$

The restrictions on α, β are $\alpha>0$, $\alpha+\beta>0$, $\alpha+\gamma>0$, so $\lambda>1$, $\mu>0$.

In particular if

$$(16)\qquad f(V)=V^{m-1},\qquad G(U)=(1+\beta/\alpha)\,U^{n},\qquad n=\lambda+(m-1)\mu$$

and if $m>0$, n can have any value (Astarita, 1989). Another important case is

$$(17)\qquad f(V)=V^{p}/(1+V^{q})^{r}\ \text{giving}\ G(U)=(1+\beta/\alpha)\,U^{\sigma}(1+U^{\kappa})^{\rho}$$

where $\sigma=\lambda+p\mu$, $\kappa=q\mu$, $\rho=r$.

Devising aliases

We clearly have a number of elements at our disposal and we might ask how far we can go in choosing them arbitrarily. If, for example, we seek the f that will yield a given G with v, h and K given by (12),

$$(18)\qquad f(V)=(1+\beta/\alpha)^{-1}\,V^{-\lambda/\mu}\,G(V^{1/\mu})\,.$$

If f, G are specified and v and h are given by (12), K must be such that

$$(19)\qquad \int_0^{\infty}K(x)\,v(x)\exp[-wx]\,dx=f^{-1}[G(L(w))/M(w)]\,.$$

In particular, if we let $\alpha=1$, $\beta=0$ this gives

$$(20)\qquad \int_0^{\infty}K(x)\exp[-xs]\,dx=f^{-1}[G(s^{-1})\,s^{2}]\,,$$

where f^{-1} is the inverse function of f and $s=1+w$.

For example, if $f(V)=1/(1+V)$ and $G(U)=U$ we find $K(x)=1-\delta(x)$, where $\delta(x)$ is Dirac's delta fuction. Thus the family obeying

$$(21)\qquad u_t(x,t)=-\,xu(x,t)\Big/\left\{1-u(0,t)+\int_0^{\infty}u(x,t)\,dz\right\},\qquad u(x,0)=\exp[-x]$$

appears, in the aggregate $U(t) = \int_0^\infty u(x,t)\,dx$, to disappear exponentially, for $\dot{U} = -U$ and $U(t) = \exp[-t]$. A $K(x)$ so derived may, or may not, have meaning in the motivating kinetic model. In this example, $u(0,t) = 1$ since it satisfies $u_t(0,t) = 0$, $u(0,0) = 1$. Thus

$$u_t(x,t) = -xu(x,t) \Big/ \left\{ \int_0^\infty u(z,t)\,dz \right\} \tag{22}$$

which represents reaction on a totally covered surface. Clearly $F(w) = 1 + w$, $M(w) = 1/(1+w)^2$ so $G = 1/(1+w) = U$. If we ask what K gives an alias of $G(U) = U^2$, $G(s^{-1}) = 1$ and, since $f^{-1}(G(s^{-1})\,s^2) = 0$ giving $K \equiv 0$ and recovering the ancient result cited in the introduction. If $G(U) = U^n$, $n > 2$, derivatives of the distribution $u(x,t)$ with respect to x begin to appear and these cannot be justified kinetically. For example $n = 3$ leads to $\overline{K}(s) = s - 1$ or

$$1 + \int_0^\infty K(z)\,v(z) \exp[-zw]\,dz = 1 - u(0,t) - \{(d/dx)[v(x)\exp[-xw(t)]]\}_{x=0} = (1+w)$$

and hence $F(w) = U$, $G(U) = U^3$, but $u_t = -xu/u_x$ is not sensible kinetically. On the other hand we know that the choice of $f \equiv 1$, $\alpha = 1/2$, $\beta = \gamma = 0$ also has the alias $G(U) = U^3$ and is kinetically acceptable.

It appears therefore that what we would like to be able to do is to choose f and K to be kinetically acceptable and to find the initial distribution $V(x)$ and weighting function $h(x)$ that will lead to a prescribed alias G. Some progress toward this end may be made as follows. Let

$$U = \int_0^\infty h(x)\,v(x) \exp[-xw]\,dx\,, \qquad V = \int_0^\infty K(x)\,v(x) \exp[-xw]\,dx \tag{23}$$

be the Laplace transforms of hv and Kv with w as transform variable. Further let

$$\Phi(w) = \int_0^w dw'/F(w')\,, \qquad \Gamma(U) = \int_U^1 \frac{dU'}{G(U')}\,. \tag{24}$$

Then integration of the relation $FM = G$ gives

$$\Gamma(U) = \Phi(w) \qquad \text{or} \qquad U = \Gamma^{-1}\Phi(w) \tag{25}$$

thus if f and K are specified and G is the desired alias, v can be chosen and V, F and U can be found in this order. By inversion of U, the product hv can then be calculated and hence h, the weighting function.

Conclusions

It would appear that within this class of differential equation there is considerable freedom in choosing a distribution so that its «lumped» behaviour is of a different stamp. There are some limitations however and it may not be possible to get a group of Montagues to behave, as a crowd, like a given Capulet. For example if $G(U) = U^n$, $0 \leq n < 1$, $U(t)$ falls to zero in a finite time. It follows from (6), that F, and hence f and K, must be such that the integral $\int_0^\infty dw/F(w)$ is finite. This is why the purely linear case, $f \equiv 1$, cannot have an alias $G(U) = U^n$ with $n < 1$.

Whether results of this kind can be extended to higher order equations is an open question. There is some incentive to do this from the kinetics of diffusion and reaction in porous catalysts (cf. Luss and Golikeri, 1971). The results for first-order differential equations have proved useful and merit further mathematical investigation.

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