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*A Glimpse into
Mathematical
Modelling*

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MAT

SERIE A: CONFERENCIAS, SEMINARIOS Y TRABAJOS DE MATEMÁTICA

No. 18

A GLIMPSE INTO MATHEMATICAL MODELLING

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Abstract. We consider some basic problems in mathematical modelling, such as formulation, mathematical setup, calibration of parameters, study of initial and boundary conditions and sensitivity assessment, through some simple mathematical models.

Resumen. Consideramos algunos problemas básicos en modelización matemática, tales como formulación, planteo matemático, ajuste de parámetros, estudio de condiciones iniciales y de contorno y evaluación de sensibilidad, por medio de algunos modelos matemáticos simples.

Keywords: Mathematical modelling; initial and boundary conditions; parameters; calibration; numerical experiments.

Palabras claves: Modelización matemática; condiciones iniciales y de contorno; parámetros; ajuste; experimentación numérica.

AMS Subject Classification: 00A69; 00A71; 00A72.

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A GLIMPSE INTO MATHEMATICAL MODELLING

P. M. Jacovkis¹

1. SYSTEMS AND MODELS

A system, for our purposes, is a (perhaps infinite) set of elements, with numerical or non numerical attributes, and such that some kind of relationships influence the elements. This definition is very general, in order to permit its application to almost all possible cases in which a mathematical model may be built. In fact, a mathematical model is the (usually simplified) representation of a system through the mathematical language. For instance, the mathematical model of the solar system (or, to be precise, one simple mathematical model of the solar system, because many other more complex mathematical models of the solar system may be constructed) has as its elements the sun and the planets (and perhaps the satellites of the planets, and the comets, etc.). The attributes of the elements are their diameters, their masses, their positions and their velocities, and the relationships are the differential equations that govern their movement. In this case the relationships are equations, but, in a linear program problem, for instance, the relationships are inequalities. The attributes do not need to be numerical, either: a fluvial model may include the transport and diffusion of suspended particles, and perhaps an important attribute of the particles is their classification as pollutant or non-pollutant.

The most primitive models are mental models. Each human being has mental models of the universe, of the place where he or she lives, of how things happen. Mental models may be inconsistent or incomplete, because to detect contradictions, for instance, a careful analysis (analysis that most human beings do not carry out) is necessary. But *homo sapiens* has the ability of communicating through language; so verbal models appear, that in general have less inconsistencies than mental models, and are more complete, because usually the verbal model is subject to some analysis, perhaps very intuitive. Anyway, a verbal model is not robust, in the sense that information verbally transmitted is usually changed, sometimes very much changed, from individual to individual.

When one of the most important technical advances of civilization appeared, namely writing, models began to be written. Usually a written model is more consistent and complete than a verbal one, because the writer has time to think about what he or she is going to write, and also is more robust, because, although a written document may be interpreted in different ways, this situation seldom occurs, at least until a long time has passed. But the real revolution in models happened when mathematical and physical models began to be formulated.

A mathematical model is a model that employs mathematical symbols and uses mathematical theories. A physical model is a physical construction that represents some physical process that we want to study. The elements of the physical construction may be exactly

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the elements of the process we are interested in, or they may be different, and some correspondence must be found between the behavior of our model and the behavior of the actual process.

When, more than sixty years ago, computers appeared, mathematical models began to be more and more complex, and more and more detailed. Because usually one creates a model to compute some result, that means that such and such element behave this or that way, and before the computers only very simple, mostly linear, models could be exploited (it was extremely tedious to solve a standard linear equation that includes a 10×10 matrix). Mathematical models are in general cheaper than physical models, and faster to implement: for instance, a mathematical model of a river such as, say, the Paraná River, can be easily prepared and easily changed into a mathematical model of the Uruguay River, whereas to prepare a physical model of the Paraná River at the INA (the Argentinean National Institute of Water Resources) a careful reproduction of the river bed (on a smaller scale) must be built, and in order to change this model into a model of the Uruguay River the first model must be almost completely destroyed and a new one must be built. Anyway, physical models continue being extremely important, for two main reasons: on the one hand, eventually all models (at least the first time they are used) should, if possible, be compared with what really happens in reality and, on the other hand, there are some physical phenomena that are not yet sufficiently known to be represented by mathematical equations and inequalities, unless one uses empirical relationships (which, of course, are extremely convenient, but not necessarily help when one is trying to understand the corresponding complex physical processes). For instance, turbulence is not completely understood, and there are no conceptual equations representing exactly the hydrological cycle, namely how rainfall in a basin transforms into discharge into a river.

2. MATHEMATICAL MODELS

Let us take a very simple model, namely a discrete model that simulates the growth of a population in absence of wars and natural constraints, such as lack of land or of food. Such a model may be written as

$$P_{n+1} = P_n(1 + \alpha), \quad (2.1)$$

where P_n indicates the population at the beginning of period n (for instance, at the beginning of year n) and α is the rate of growth of the population. Although we know the value of α , equation (2.1) is not enough for knowing completely the evolution of the population. And it is not enough because we need something more: we need the *initial conditions* (in this case, only one initial condition), that is, the value of the population at the initial period, that we may denote, without loss of generality, the period with $n = 0$. That is, we need also an equation

$$P_0 = a, \quad (2.2)$$

a being a (positive) real number that indicates the size of the population at the beginning of our computations. In fact, this is a model with only one variable, P , but the state of the system represented by the model at each period is indicated by the value of all its variables (in this case, one), and the initial state must be known, that is, the value of all its variables at the initial time must be prescribed.

This is a characteristic of all models that change with time, be it at a discrete number of instants, like this simple model, or at a continuum of instants². Models that change

²Anyway, from a practical point of view, the state of a continuum model must be computed only at a finite number of instants, so that some kind of “discretization” has to be adopted.

with time are called evolutionary models, or transient models, or dynamical models. In this kind of models, besides the equations - or, more generally, relationships - that govern their behavior, some data are *always* necessary: the initial conditions. For example, in a more complex model, the one-dimensional heat equation (the classical parabolic partial differential equations), that represents the conduction of heat in a one-dimensional infinite bar, namely

$$\frac{\partial u}{\partial t} = \sigma^2 \frac{\partial^2 u}{\partial x^2},$$

where $u = u(x, t)$ means the temperature at position x and time t , and σ^2 is the thermal diffusivity, the initial condition is

$$u(x, 0) = u_0(x),$$

where u_0 is a known function, that is, the necessary data are infinite, namely (theoretically) values for all x , $-\infty < x < \infty$ must be prescribed.

The problem with (deterministic) evolutionary models whose data are only the initial conditions (and the parameters, like σ^2 in the heat equation and the rate of growth α in the population model, but we delay the discussion on parameters to subsection 2.1) is that, if the model represents the physical process, all we can do is forecast the state of the model in the future, but we can not “modify” this future, in the sense that the future is completely determined by the equations and inequalities of the model and by the initial conditions³. But, when possible, we want not only to forecast but also to control, that is, to take measures in order that in some instant in the future the state of the system be a state that satisfies us, or at least a state that is as close as possible to a state that satisfies us. For that kind of “control” we need also other data. For instance, the evolution of population may be modified through immigration or emigration. If we represent with variable I_n the immigration or emigration (immigration will be a positive value, emigration a negative one) from time n to time $n + 1$, the equation (2.1) changes into

$$P_{n+1} = P_n(1 + \alpha) + I_n. \quad (2.3)$$

Of course, the existence of data I_n does not mean that in fact there is a “control”, that is, not always we can change the value of I in order to have, after a certain simulated period, the results we want. But sometimes we can.

In our parabolic partial differential example this “control” is available if instead of having an infinite bar we have a finite bar whose extremes are points a and b , that is, its points x satisfy $a \leq x \leq b$, and then the problem should be formulated as follows:

$$\frac{\partial u}{\partial t} = \sigma^2 \frac{\partial^2 u}{\partial x^2}, \quad (2.4)$$

$$u(x, 0) = u_0(x), \quad (2.5)$$

³In fact, this is exactly what Laplace had in mind when he wrote his famous phrase “We may regard the present state of the universe as the effect of its past and the cause of its future. An intellect which at a certain moment would know all forces that set nature in motion, and all positions of all items of which nature is composed, if this intellect were also vast enough to submit these data to analysis, it would embrace in a single formula the movements of the greatest bodies of the universe and those of the tiniest atom; for such an intellect nothing would be uncertain and the future just like the past would be present before its eyes.[10]” The equations of motion require as initial conditions the position and velocity of all elements of the system. As no boundary conditions are present, the initial positions and velocities determine the future positions and velocities. In fact, as classical mechanics is reversible, the time’s arrow is not important, and we are - theoretically - able to know not only the future but also the past.

$$u(a, t) = u_L(t), \quad u(b, t) = u_R(t). \quad (2.6)$$

In (2.6) u_L and u_R are the boundary conditions of the partial differential equation (2.4) with initial condition (2.5) (the theory of the heat equation shows that for a finite bar boundary conditions must be prescribed at both ends of the bar). So, using the terminology of partial differential equations, we could say that I_n is also a boundary condition. Perhaps we can control u_L and u_R , perhaps not. But it is obvious that, when boundary conditions are introduced, the results in the future are not completely determined by the state of the system at the initial time. In partial differential equations it is customary to call a problem with initial conditions, but not with boundary conditions, an initial-value problem, or a Cauchy problem, and a problem with both initial and boundary conditions a mixed initial-boundary problem⁴.

2.1. Parameters. We then always need as data (if the model evolves with time) the initial conditions; sometimes we need also some data that represent the external influences on the model along the time (the “boundary conditions” of partial differential equations) and finally we need a different kind of data: parameters, like α in equation (2.1) and σ^2 in equation (2.4). In general, parameters are constant, or they seldom change, during the simulation time, and often one of the most important problems in implementing a useful model is to have the right parameters⁵. Sometimes one can measure the parameters, and sometimes not. When one can not measure the parameters, it is necessary to *calibrate* them, that is, to obtain the values of the parameters as close as the actual (and unknown) data as possible. More about this subject will be said afterwards.

2.2. Stationary problems. Some models are not evolutionary problems, that is, time is not a variable. In these case we say that the models are stationary or steady-state. Many civil engineering models are steady-state, because engineers (and people in general) prefer steady-state bridges, tunnels, etc. Partial differential equations that govern steady-state phenomena are often elliptic. The simplest homogenous linear elliptic equation (in three dimensions) may be written

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0, \quad (2.7)$$

where $u = u(x, y, z)$ is a function of three variables in a three-dimensional domain Ω . In this case, data are provided by the boundary conditions (no initial condition is possible or necessary, given that the process does not change with time), for instance

$$u(x, y, z) = g(x, y, z) \text{ on the boundary } \partial\Omega \text{ of } \Omega. \quad (2.8)$$

Equation (2.7) is known as the Laplace equation. If instead of being homogeneous the right-hand-side is different from zero, namely

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(x, y, z), \quad (2.9)$$

⁴Let us remark at this point a difference between the heat equation (which is the simplest linear homogeneous parabolic partial differential equation) and the equations of motions about which Laplace was thinking: for the heat equation, the time’s arrow *matters*. We can predict the future, but not compute the past, and the interesting thing is that this is signalled by the fact that the parameter σ^2 *must* be positive.

⁵Sometimes, according to the value of a parameter a model behaves in completely different ways, and it is important to know what values of a parameter are the limits between one behavior and other. We shall not discuss this phenomenon in these notes.

the function $f(x, y, z)$ offers additional data, and equation (2.9) is called the Poisson equation. Of course, we can include coefficients multiplying each term, more terms, etc., and then these parameters must be measured or calibrated. Boundary condition (2.8) is called a Dirichlet condition, and of course there are other types of boundary conditions.

2.3. Deterministic and stochastic models. All these models, evolutionary or steady-state, are deterministic models, in the sense that assuming that the equations represent exactly the phenomenon under study, that we are able to perform all measurements with the required precision, and that if the errors originated in computing with a finite number of digits numbers that contain an infinite number of digits are satisfactorily bounded, we obtain the exact (that is, exact plus or minus some acceptable error) result: in an evolutionary model, for instance, we should obtain what will happen, under those parameters, those initial conditions and those boundary conditions, at the end T of the simulation time. But some (very important) models are stochastic models, in the sense that the model should reflect a reality where states change randomly. For instance, a queue model: the system consists of an employee who is busy with the first person in a queue, there are other people waiting in the queue, and the time of occupation of the employee with the attendee is random, as well as the time between the arrival of a client to the queue and the arrival of the following client. And we want to model this process.

Here there are two different problems: on the one hand, the computer is a deterministic machine: one hopes that, if one runs a program in his or her computer today, a rainy and chilly day, with some set of data, and tomorrow, a warm and dry day, the program is run with exactly the same set of data, the result will be the same. One could become extremely nervous if the result is different. How can we represent, with a deterministic machine, a situation that includes randomness? And, on the other hand, if the result is random, supposing that the first problem is solved, what does the result mean? The result could have been completely different, because random inputs are included in the model.

Focusing on stochastic models is not the scope of these notes, but we can say that the first problem is solved using *pseudorandom* numbers, that is, numbers deterministically generated but that statisticians can not detect as different from random, and the second problem is solved simulating many instances of the process under study, so that we can collect the relevant information necessary. By the way, stochastic models are usually evolutionary.

Let us now introduce some simple models.

3. POPULATION DYNAMICS

The simplest demographic model (or, if we are talking about living beings in general, not necessarily human, population dynamics model) is model (2.1), (2.2) or, if we include immigration/emigration, model (2.3), (2.2). Of course this model is not sustainable during a large period: eventually all the surface of the Earth would be occupied by human beings, without room for moving from one place to another. But for a short period the model may be perfectly realistic. We have mentioned that term I_n may be considered a “control”, in the sense that through this variable someone may try to obtain certain results after some years. Indeed it has been, or tried to be, a control. For instance, several countries (the immigration countries: United States, Canada, Argentina, Uruguay) during the 19st century had an active policy favorable to immigration (perhaps selective: the Argentinean Constitution, for instance, indicates someplace that Argentina is interested in *European* immigration) and other countries did not mind that some of its countrymen

leave the country (Italy, Spain) as a way to reduce social tensions. Not always the control worked exactly like planned: Britain was interested in emigration to its settlement colonies (Canada, Australia, New Zealand) but anyway many people from Britain emigrated to the United States.

Of course, the parameter α may be the control: a good health policy may increase its value, so that the population grows faster, and on the other hand a policy of birth control (like the Chinese one) may reduce α .

Finally, it is obvious that a continuous (exponential) version of this model may be built: if instead of a time step equal to one we have an arbitrary time step Δt , and α continues being the rate of growth for unit time, equation (2.1) becomes

$$\frac{P(t + \Delta t) - P(t)}{\Delta t} = \alpha P(t)$$

and with Δt tending to zero all becomes the ordinary differential equation

$$\frac{dP}{dt} = \alpha P(t)$$

with initial condition $P(0) = P_0$, whose solution is of course $P(t) = P_0 e^{\alpha t}$. The “boundary” condition would be the “instantaneous” immigration or emigration flux $I(t)$, if we take it into account, so that we could write

$$P(t) = P_0 e^{\alpha t} + I(t). \quad (3.1)$$

(3.1) is simply the continuous version, and (2.3) is the discrete version of this elementary population model.

Anyway, this model is often too simple. On the one hand, for long periods is unrealistic, given that the population can not grow indefinitely. On the other hand, we often need a more detailed model, that includes, for instance, how population is distributed according to age, geographic location or social class.

To take into account the first problem, the logistic model may be a good approximation. The idea is that the resources are sufficient only for a limited population, so that the rate of growth of population instead of being proportional to the population (like in an exponentially increasing population) is proportional to the population times a factor that decreases with the population. The simplest decreasing function is a linear function, so that the logistic continuous equation is

$$\frac{dP}{dt} = P(t)(a - bP(t)), \quad (3.2)$$

with, of course, the initial condition $P(0) = P_0$.

Analogously, the discrete logistic equation is

$$P_{n+1} = P_n \left(1 + aP_n \left(1 - \frac{P_n}{K} \right) \right) \quad (3.3)$$

or (if the time step is not unitary)

$$\frac{P_{t+\Delta t} - P_t}{\Delta t} = aP_t \left(1 - \frac{P_t}{K} \right), \quad (3.4)$$

and $b = \frac{a}{K}$.

We shall discuss equations (3.2) and (3.3) or (3.4) (for which of course we must also include the initial condition $P(0) = P_0$ separately). The continuous logistic equation was formulated for the first time by P.-F. Verhulst ([22])

3.1. The continuous logistic equation. The continuous logistic model is then governed by equation (3.2), which is a nonlinear first order ordinary differential equation, with initial condition $P(0) = P_0$. It can be proved that this equation has an explicit solution (see for instance [7]), namely

$$P(t) = \frac{a/b}{1 + \left(\frac{a-bP_0}{bP_0}\right)e^{-at}},$$

or

$$P(t) = \frac{K}{1 + \left(\frac{K-P_0}{P_0}\right)e^{-at}}$$

and then it is easy to see that

$$\lim_{t \rightarrow \infty} P(t) = \frac{a}{b} = K,$$

and that if $P(0) < K$ then $P(t)$ always increases, and is always less than K (if $P(t) > K$ then $P(t)$ always decreases and is always greater than a/b , although this case does not interest us). In fact, we can deduce this property analyzing equation (3.2) directly without knowing its explicit solution. Of course, we can introduce the immigration or emigration flux per unit time $I(t)$, but, taking into account that for physical or biological reasons the bound $a/b = K$ cannot be surpassed, we should write in this case

$$\frac{dP}{dt} = P(t)(a - bP(t)) + \min(I(t), K - P(t)).$$

Anyway, usually we are not interested in immigration or emigration flux when using the logistic equation, because the population is considered in a closed environment, or is a global population.

Here we have two parameters that need to be calibrated, namely a and b (or K). In cases as simple as governed by equation (2.1) or (3.2), which have few parameters, probably the best way to calibrate the parameters is applying directly, for instance, least squares: we have the recorded data for several times $t_{i_1}, t_{i_2}, \dots, t_{i_n}$, we know the initial population P_0 and then we search

$$\min_{\alpha} \sum_{j=1}^N (\ln P_{i_j} - \ln P_0 - \alpha t_{i_j})^2$$

for the exponential case⁶.

The logistic case is more complicated: one may attack the problem from different angles. For instance, the curve obtained in the logistic case is a sigmoid, that is, has an S form; near the initial condition is similar to an exponential, and then we may try to use only values close to the initial time and obtain the coefficient a , and then approximate K for the rest of the values. Or we may “discretize” the equation, and use the discretization. Anyway, this example shows that calibrating a model is not necessarily easy, not only technically: in fact, a calibration consists in solving an inverse problem, that is, a problem in which, knowing the result, we want to obtain the data, or some

⁶By the way, although the time-honored least square method is the most used technique for calibrating models, it is not always necessarily the best: on the one hand, it has many “good” theoretical properties, and besides, we can obtain a minimum set of values using tools from mathematical analysis: the extremum value will be (if it exists at the interior of a domain) at a point where the derivative is zero; on the other hand, the method is not robust, in the sense that the existence of an outlier (or a bad measurement) may significantly change the result. Least squares is essentially a minimization in the space l^2 ; if we want to minimize in l^1 (that is, if we want to minimize the sum of absolute values, instead of sum of squares) the problem is one of least absolute deviations and a linear-programming approach can be applied, see for instance [1].

data, and inverse problems are often ill-conditioned in the sense of Hadamard⁷. Often the calibration (above all when many parameters exist) is empirically obtained (for instance, if one is trying to model a reach of a river with a hydrodynamic model, probably the calibration is performed through a “trial and error” approach, in which the experience of the modeler is fundamental; we shall comment on this point at section 5). Of course, theoretical mathematical approaches are possible, interesting and challenging; see for instance [6].

3.2. The discrete logistic equation. In this case, we have in general

$$\frac{P_{t+\Delta t} - P_t}{\Delta t} = aP_t\left(1 - \frac{P_t}{K}\right).$$

One can observe that in this case also the limit of the population is K , both for populations initially over or under K . If the time step is unitary, i. e., $\Delta t = 1$, we have

$$P_{t+1} - P_t = aP_t\left(1 - \frac{P_t}{K}\right),$$

that is,

$$P_{t+1} - P_t = P_t(a - bP_t),$$

with $b = \frac{a}{K}$, and then

$$P_{t+1} = P_t(1 + a - bP_t) = P_t(\gamma - bP_t),$$

with $\gamma = 1 + a$. Let now x_t be such that $P_t = \frac{\gamma}{b}x_t$. Then

$$\begin{aligned} \frac{\gamma}{b}x_{t+1} &= \frac{\gamma}{b}x_t(\gamma - \gamma x_t), \\ x_{t+1} &= \gamma x_t(1 - x_t). \end{aligned}$$

If $0 \leq x_0 \leq 1$, and $0 \leq \gamma \leq 4$, $x_t \in [0, 1]$ always. In a memorable paper ([18]; see also [14]), Robert M. May showed the surprising behavior of the equation, according to the value of the parameter γ . In fact, what one can prove is (we exclude from this analysis the initial values $x_0 = 0$ and $x_0 = 1 - \frac{1}{\gamma}$, for which $x_i = x_0$ always, and $x_0 = 1$, for which $x_t = 0$ if $t \geq 1$)

- (1) If $\gamma \leq 3$, the iteration converges (of course, if $\gamma \leq 1$ it converges to zero; if $1 < \gamma < 3$ the limit is $1 - \frac{1}{\gamma}$);
- (2) From 3 on, x_t will approach, oscillating, two values when t tends to ∞ until approximately 3.45 (3.44948...). Then - increasing γ - x_t will approach, oscillating, four values, then eight values, then sixteen values,... until around 3.57 (3.56994...).
- (3) Then chaos appears (except for some isolated ranges of λ with non-chaotic behavior), that is, slightly changing the initial value x_0 dramatically changes the behavior of the iteration. Besides, no oscillation of finite period can be observed.

The rate between two consecutive duplications tends to a constant (the Feigenbaum constant). So with the discrete logistic equation we may model situations in which a population has a chaotic behavior. As May says in his paper “... apparently erratic fluctuations in the census data for an animal population need not necessarily betoken

⁷Without formalizing too much, a well-conditioned problem is a problem in which

- (1) There exists a solution;
- (2) The solution is unique;
- (3) The solution depends continuously on the data of the problem.

An ill-conditioned problem is a problem that is not well-conditioned. Of course in order to formalize this definition we need a topology that gives meaning to the term “continuously”.

either the vagaries of an unpredictable environment or sampling errors: they may simple derive from a rigidly deterministic population growth relationship ... ”.

3.3. Delay. If the delay between the instant a descendant is conceived and it becomes fertile is significant (in the sense that the total population may have changed) both the exponential and logistic models (be they discrete or continuous) must be replaced by models with a time delay. The general continuous model should be now

$$\frac{dP(t)}{dt} = f(P(t - t_d)) \quad (3.5)$$

with t_d being the delay, and f a general function. For the exponential case (3.5) becomes

$$\frac{dP(t)}{dt} = \alpha P(t - t_d) \quad (3.6)$$

where α is a constant rate of growth. If the rate of growth $R(P)$ changes with the population, (3.6) becomes now

$$\frac{1}{P(t)} \frac{dP(t)}{dt} = R(P(t - t_d)). \quad (3.7)$$

In particular, the delay logistic equation is

$$\frac{dP(t)}{dt} = P(t)(a - bP(t - t_d)). \quad (3.8)$$

Equations like (3.5), (3.6), (3.7) or (3.8) are called delay-differential equations, and are often considerably more difficult to solve than ordinary differential equations. In fact, taking delay into account the solution can oscillate around the equilibrium point $P(t) = \frac{a}{b}$ or, what is worse, destabilize itself.

If we now analyze discrete equations with delay, that is, delay difference equations, we have for instance

$$P(t + \Delta t) - P(t) = \alpha \Delta t P(t - \Delta t), \quad (3.9)$$

(constant rate of growth),

$$\frac{P(t + \Delta t) - P(t)}{\Delta t P(t)} = R(P(t - \Delta t)), \quad (3.10)$$

(variable rate of growth) or

$$P(t + \Delta t) - P(t) = \Delta t P(t)(a - bP(t - \Delta t)). \quad (3.11)$$

(the discrete delayed logistic equation).

Remark that equations (3.9), (3.10) and (3.11) take into account automatically a delay Δt . When the time step Δt is different from the delay t_d the models are technically more complicated, for instance

$$P(t + \Delta t) - P(t) = \alpha \Delta t P(t - t_d) \quad (3.12)$$

or

$$P(t + \Delta t) - P(t) = \Delta t P(t)(a - bP(t - t_d)). \quad (3.13)$$

Let us now suppose that $t_d = \Delta t$. Then we use (3.11). We have now three different levels of time: $t + \Delta t$, t and $t - \Delta t$. If we now put $t = m\Delta t$, $P(t) = P(m\Delta t) = P_m$, what we get is

$$P_{m+1} - P_m = P_m(\alpha - \beta P_{m-1}), \quad (3.14)$$

where $\alpha = a\Delta t$ and $\beta = b\Delta t$. (3.14) is a (nonlinear) second order difference equation.

Let us analyze the stability of (3.14). We shall use the perturbation technique, namely, we shall suppose that the equation near the equilibrium point is a very small perturbation from it, that is,

$$P(t) = \frac{\alpha}{\beta} + \epsilon P_1(t),$$

where $\epsilon \ll 1$. Equivalently we may write

$$P_m = \frac{\alpha}{\beta} + \epsilon y_m,$$

with $t = m\Delta t$, such that $|\epsilon y_m| \ll \alpha/\beta$.

Replacing in (3.14) we obtain

$$\frac{\alpha}{\beta} + \epsilon y_{m+1} - \frac{\alpha}{\beta} - \epsilon y_m = \left(\frac{\alpha}{\beta} + \epsilon y_m\right)(\alpha - \alpha - \epsilon\beta y_{m-1})$$

and finally we get

$$y_{m+1} - y_m = -\beta y_{m-1} \left(\frac{\alpha}{\beta} + \epsilon y_m\right). \quad (3.15)$$

We neglect the nonlinear term $-\beta y_{m-1}(\epsilon y_m)$ and then we have

$$y_{m+1} - y_m = -\alpha y_{m-1}. \quad (3.16)$$

We may then remark that only $\alpha = a\Delta t$ determines the behavior of the population near the equilibrium.

Now, (3.16) being an homogeneous linear difference equation of second order, given two initial values y_0 and y_1 known the general solution has the form

$$y_m = c_1 r_1^m + c_2 r_2^m,$$

with coefficients c_1 and c_2 obtained thanks to the two initial conditions and r_1 and r_2 being the roots of the second order equation

$$y^2 - y + \alpha = 0,$$

that is

$$r_{1,2} = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \alpha}.$$

For this analysis we suppose that the roots r_1 and r_2 are different. If $\alpha \leq \frac{1}{4}$ both roots are real, and they have both a modulus lesser than 1, so that the stationary point is stable (the perturbation vanishes when m approaches infinity). If $\alpha > \frac{1}{4}$ the roots are complex and they have the form

$$r_{1,2} = \frac{1}{2} \pm i\sqrt{\alpha - \frac{1}{4}}$$

whose absolute values are given by the formula

$$|r_{1,2}| = \sqrt{\alpha},$$

so that the equilibrium point is stable provided that $\alpha < 1$, that is, $a\Delta t < 1$. The perturbation converges to the equilibrium point oscillating above and below it.

But if $\alpha > 1$, the perturbation oscillates diverging: the delay causes a destabilization of the population.

3.4. The Leslie matrix. Anyway, the exponential and logistic models, both in their continuous and discrete versions, are too simple for a more detailed analysis⁸. Often we want to know the evolution of different classes of a population. For example, we can divide the total population into individuals belonging to different geographic regions, or of different ages, or of different socioeconomic classes. Suppose a human population for which we want to know the evolution of its population pyramid, year after year. Let $P_n(E)$ the population that, at year n , has age E . We need of course decide from which day to compute the year, for instance, from January 1st. To age zero belong all individuals that are born during the year under analysis. And, supposing that there exists an age U such that the incorporation to this age of individuals older than U does not change significantly the size of class U , this age U will be the last one, and then, neglecting immigration and emigration, we can write the equations of a demographic model; firstly, the evolution from one year to the following of individuals that have already been born at year n :

$$P_{n+1}(E + 1) = P_n(E)(1 - T_m(E)). \tag{3.17}$$

Here $T_m(E)$ means the rate of mortality of individuals of age E . Equation (3.17) indicates the normal situation in which each year some people the same age of us die: we recognize this phenomenon when we participate in the annual party of our old schoolmates and at each party less and less individuals appear, because some of them died from party to party.

For individuals who are in the group of age U , or go into this group from year n to year $n + 1$, a slightly different equation is necessary:

$$P_{n+1}(U) = P_n(U - 1)(1 - T_m(U - 1)) + P_n(U)(1 - T_m(U)). \tag{3.18}$$

Obviously, now the group of age U the following year consists of those who “arrived” at this group (from group of age $U - 1$) and those who were already U or more years old and survived.

Now we need to compute individuals born during year n :

$$P_{n+1}(0) = \sum_{E=E_1}^{E_2} P_n(E)T_f(E). \tag{3.19}$$

Equation (3.19) indicates that women can have children from age E_1 to age E_2 (we neglect the few cases of women who bear children too young or too old), and $T_f(E)$ means the rate of fertility of women of age E . Remark that it is important to know whether the rate of fertility is taken with regard of all individuals of age E (as is shown in equation (3.19)) or with regard only of women of age E . In this case, considering that more or less we can suppose that feminine population is one half of the total population, we have to take one half of $P_n(E)$, for each age.

This model may be written in vector form: if we consider the vector

$$\vec{P}_n = \begin{pmatrix} P_n(0) \\ P_n(1) \\ P_n(2) \\ \dots \\ P_n(U) \end{pmatrix}$$

then we have the equation

$$\vec{P}_{n+1} = \mathbf{A}\vec{P}_n \tag{3.20}$$

⁸In what follows we have used above all [3] and [7] as references.

where \mathbf{A} is the matrix

$$\begin{pmatrix} & & \dots & T_f(E_1) & \dots & T_f(E_2) & & \dots \\ 1 - T_m(0) & & & & & & & \\ & 1 - T_m(1) & & & & & & \\ & & & \dots & & & & \\ & & & & & & \dots & \\ & & & & & \dots & & 1 - T_m(U - 1) & 1 - T_m(U) \end{pmatrix}$$

Matrix \mathbf{A} has zeroes except where indicated and between the fertility rates $T_f(E_1)$ and $T_f(E_2)$. If class U is the class of all individuals of age U , and nobody is supposed to survive this age, and no assumption is made about the fertility ages, that is, individuals may be fertile since age zero (as in many species) matrix \mathbf{A} changes into matrix

$$\begin{pmatrix} T_f(0) & T_f(1) & \dots & & & & T_f(U) \\ 1 - T_m(0) & & \dots & & & & \\ & 1 - T_m(1) & \dots & & & & \\ & & & \dots & & & \\ & & & & \dots & & \\ & & & & & \dots & 1 - T_m(U - 1) & 0 \end{pmatrix}$$

This is a Leslie matrix, originally formulated by Patrick H. Leslie in the two fundamental papers [12], [13].

The parameters of the model given by equation (3.20) (with initial condition \vec{P}_0 given, of course) are the rates of fertility and mortality. Naturally, these parameters may also change with time; in fact, the parameters are “control” parameters, in the sense that with improvement in health conditions the rate of mortality may decrease, and for a richer and more educated society the rate of fertility decreases, because individuals begin bearing children at an older age, and less children die as infants (on the other hand, as less children die as infants the rate of fertility increases, so both phenomena should be analyzed). Typical numerical experiments should simulate the population of Argentina, for instance, under no variation of these rates, and under different kinds of variations, to see what could happen with the Argentine population in, say, fifty years. Anyway, when analyzing a country like Argentina, where many immigrants have influenced its population (during many years mostly European immigrants, now mostly Latin American immigrants), immigration must be taken into account, so that equations (3.17), (3.18), (3.19) should be replaced by

$$P_{n+1}(E + 1) = P_n(E)(1 - T_m(E)) + I_n(E), \quad (3.21)$$

$$P_{n+1}(U) = P_n(U - 1)(1 - T_m(U - 1)) + P_n(U)(1 - T_m(U)) + I_n(U), \quad (3.22)$$

$$P_{n+1}(0) = \sum_{E=E_1}^{E_2} P_n(E)T_f(E) + I_n(0). \quad (3.23)$$

In equations (3.21), (3.22) and (3.23) the corresponding immigration fluxes during year n have been included. We have written $I(U)$ meaning that we include in this flux the immigrants aged $U - 1$ and aged U or plus.

Of course we may have more complicated situations, that thanks to the current computing power may be approached, namely that there may be two (or more) different categories of classes, for instance by age E and by geographic section G . In this case the variables are $P_n(E, G)$, and the equations should be reformulated accordingly. They are cumbersome, but not difficult. We shall not continue in this direction, the readers can complete the equations.

3.5. Nonnegative matrices. Sometimes we need some general idea with regard to the behavior of the Leslie matrix, namely whether an equilibrium population is reached (not necessarily in the sense that an equilibrium population appears, but in the sense that the proportions in the population pyramid are stable). Therefore, some theory on *positive* and *nonnegative* matrices is convenient.

A positive matrix \mathbf{A} of order n is a matrix for which all its entries $a_{i,j}$ are strictly positive real numbers, that is, $a_{i,j} > 0$ for $a \leq i, j \leq n$. In 1907 Oskar Perron proved the theorem that carries his name, which is the following:

Theorem 1. *If \mathbf{A} is a positive square matrix, there exists a dominant eigenvalue $\lambda = \lambda(\mathbf{A})$ with the following properties:*

- (1) λ is positive and its associate eigenvector v has positive entries, namely,

$$Av = \lambda v,$$

with $\lambda > 0, v_i > 0 \forall i$,

$$v = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix};$$

- (2) λ is a simple eigenvalue (is a simple root of the characteristic polynomial);
 (3) The absolute values of all other eigenvalues μ are strictly less than λ , namely if μ is another eigenvalue, $|\mu| < \lambda$ (therefore, λ is the spectral radius);
 (4) Matrix \mathbf{A} has no other eigenvector with nonnegative coordinates.

The theorem is not difficult and its proof may be consulted in [11]. In fact, this theorem is only the beginning of the theory, because a more general result is needed. And a more general result is needed because the theorem has a restriction that significantly reduces its applicability: most matrices in the real world, for which this theorem could be applied, allow zero entries, that is, are nonnegative matrices (we define a nonnegative matrix \mathbf{A} as a matrix all whose entries $a_{i,j}$ are nonnegative, i. e. $a_{i,j} \geq 0$).

Nonnegative matrices are really important because they are extremely useful in many types of models. For instance, in the theory of Markov chains we have stochastic (square, finite or infinite) matrices, that is matrices \mathbf{P} with entries $p_{i,j}$ such that $p_{i,j} \geq 0 \quad \forall i, j$ and such that

$$\sum_j p_{i,j} = 1 \quad \forall i,$$

where there are, for instance, N possible outcomes (for finite Markov chains) or infinite possible outcomes, and $p_{i,j}$ is the probability of outcome j on this trial in a series of trials, provided that in the previous trial the outcome was j . (An excellent treatment of Markov chains may be consulted in [4].)

Other very useful application of nonnegative matrices is the Leontiev input/output theory in economics, where we have an economy (of a country, for instance) for which we have N different sectors of industries. Each sector produces a single kind of commodity. Let X_r be the production of sector r , $x_{r,s}$ the amount of good X_r whose destination is sector s and f_r the amount of X_r required for final demand. Then we have

$$X_r = f_r + \sum_{s=1}^N x_{r,s}. \quad (3.24)$$

Let us suppose that the economic model is *linear*, that is,, to obtain an unit of s we need $a_{r,s}$ units of r (where $a_{r,s} \geq 0$, naturally). Then

$$x_{r,s} = a_{r,s}X_s.$$

We call

$$\mathbf{A} = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,N} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,N} \\ & & \vdots & \\ a_{N,1} & a_{N,2} & \cdots & a_{N,N} \end{pmatrix}$$

the input/output matrix, or I-O matrix, or Leontiev matrix, and the $a_{r,s}$ are the technical coefficients, of the Leontiev coefficients. Obviously, \mathbf{A} is a nonnegative matrix. Furthermore, we have, from (3.24) and linearity,

$$X = f + \mathbf{A}X, \quad (3.25)$$

where, of course,

$$X = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{pmatrix}.$$

Now, two remarks are important regarding equation (3.25). On the one hand, the Leontiev coefficients are not completely determined by the current technology: if we do not include some parameter related to salaries, the level of salaries must influence the Leontiev coefficients, so that not necessarily two countries with the same level of development must have the same Leontiev coefficients (besides, some goods may be cheaper in one developed country than in other for geographical reasons, or for other reasons not related to the level of development). On the other hand, it seems extremely simple to solve a certain important control problem: we decide what will be the final demand f_s from all sectors, and, provided that matrix $\mathbf{I} - \mathbf{A}$ is invertible (\mathbf{I} is the identity matrix of order N), we only have to solve

$$X = (\mathbf{I} - \mathbf{A})^{-1}f \quad (3.26)$$

to know what should be the production that satisfies our requirements, and people would be very happy.

Of course, this is not true: on the one hand, the necessary production may be unfeasible, in the sense that we are not capable of producing the required units of some or all the sectors; on the other hand, there exist a subtler problem: the non singularity of matrix $\mathbf{I} - \mathbf{A}$ does not guarantee that the solution vector X has all its entries nonnegative. We shall return to this problem soon.

There are some extensions to the Perron theorem. The first one is the Frobenius theorem.

Theorem 2. *Every nonnegative square matrix \mathbf{A} of order n has an eigenvalue $\lambda = \lambda(\mathbf{A})$ with the following properties:*

- (1) λ is nonnegative, and its associated eigenvector w has nonnegative entries:

$$\mathbf{A}w = \lambda w,$$

with

$$w = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix}, w_j \geq 0 \quad \forall j;$$

- (2) If μ is another eigenvalue of \mathbf{A} , then $|\mu| \leq \lambda$;
 (3) If $|\mu| = \lambda$ then μ is of the form $\mu = e^{2\pi ik/m} \lambda$, with k and m positive integers, $m \leq n$.

Except for the third property, which is more complicated, the other properties are easily deduced supposing \mathbf{A} is the limit of positive matrices. The proof can also be consulted in [11].

We need two other definitions to arrive at the main Perron-Frobenius theorem.

A nonnegative square matrix \mathbf{A} is reducible when, transposing conveniently its rows and columns, we are able to obtain a matrix of the form

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}_1 & \mathbf{B}_2 \\ \mathbf{0} & \mathbf{B}_3 \end{pmatrix}$$

where \mathbf{B}_1 and \mathbf{B}_3 are square submatrices, $\mathbf{0}$ is a submatrix composed exclusively of zeroes, and \mathbf{B}_2 is other submatrix.

The adjective *reducible* comes from the fact that, taking into consideration changes of the x and b entries, solving $\mathbf{A}x = b$ is the same as solving $\mathbf{B}x' = b'$ (where x' and b' are x and b , respectively, with conveniently changed subindices), and we have reduced the problem, because, partitioning conveniently b' and x' as

$$b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}, x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

we have

$$\mathbf{B}x = \begin{pmatrix} \mathbf{B}_1 & \mathbf{B}_2 \\ \mathbf{0} & \mathbf{B}_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$

and this equation may be decomposed into

$$\mathbf{B}_3 x_2 = b_2,$$

$$\mathbf{B}_1 x_1 = b_1 - \mathbf{B}_2 x_2,$$

where we have first obtained x_2 (solving a lower order equation) and then solving the other equation, also simpler. Of course the best situation is when \mathbf{B}_1 and \mathbf{B}_2 have the same order (if the order of \mathbf{A} is even).

An irreducible matrix is a square matrix that is not reducible.

Now we can formulate the Perron-Frobenius theorem.

Theorem 3. *If a nonnegative matrix \mathbf{A} is irreducible, then its spectral radius is a simple eigenvalue $\rho(\mathbf{A})$, all eigenvalues of \mathbf{A} with the same modulus are also simple, \mathbf{A} has an eigenvector x all whose entries are strictly positive corresponding to $\rho(\mathbf{A})$, and all other eigenvectors of \mathbf{A} with nonnegative entries are multiple of x .*

For its proof, see [5] or [2].

A nonnegative square matrix \mathbf{A} is *primitive* if there exists a natural number m such that \mathbf{A}^m is a positive matrix.

If the irreducible square matrix A is primitive, we can “almost” arrive at the result of Perron:

Theorem 4. *The following conditions are equivalent for a nonnegative square matrix \mathbf{A} :*

- (1) \mathbf{A} is irreducible and $\rho(\mathbf{A})$ is greater than the modulus of any other eigenvalue;
- (2) \mathbf{A} is primitive.

For a proof, see [2].

These theorems are extremely useful when treating with nonnegative matrices. For instance, let us analyze for a moment a typical stochastic matrix \mathbf{P} . It is easy to see that 1 is an eigenvalue of \mathbf{P} (in fact, if we take the vector

$$\vec{\mathbf{1}} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix},$$

as \mathbf{P} is stochastic we have $\mathbf{P}\vec{\mathbf{1}} = \vec{\mathbf{1}}$, so that 1 is an eigenvalue and $\vec{\mathbf{1}}$ is an eigenvector). If \mathbf{P} is strictly positive, Perron's theorem indicates that, as $\vec{\mathbf{1}}$ has all its entries positive, 1 is the spectral radius.

Let us now analyze the nonnegative matrix \mathbf{A} of (3.20). If \mathbf{A} is irreducible and primitive we have the following theorem (see [3] for a complete proof):

Theorem 5. *(The fundamental theorem of demography.) If the nonnegative matrix \mathbf{A} is irreducible and primitive, let λ be the strictly dominant eigenvalue of \mathbf{A} and v its associate vector (with all entries positive). If \vec{P}_n is the solution of*

$$\vec{P}_{n+1} = \mathbf{A}\vec{P}_n,$$

with an initial state \vec{P}_0 with some nonzero entry, then

(1)

$$\lim_{n \rightarrow \infty} \frac{\vec{P}_n}{|P_n|} = \frac{v}{|v|},$$

where for any vector v , $|v| = \sum_i |v_i|$ is the norm l^1 of v ; as in our case all entries are nonnegative, for \vec{P}_n this mean the total population at time n ;

(2) If $\lambda < 1$ $\lim_{n \rightarrow \infty} |P_n| = 0$ and if $\lambda > 1$ $\lim_{n \rightarrow \infty} |P_n| = \infty$.

That is, the dominant eigenvalue is the *growth rate* of the population. After many iterations, when we are "close" to the limit, the proportion of the different ages with respect to the total population is more or less constant: if the dominant eigenvalue is 1, then the population tends to an equilibrium.

Let us now investigate the Leontiev matrix. We can be sure that (3.26) has a reasonable solution (from the economic point of view) if the spectral radius of \mathbf{A} is less than one, because in this case the series

$$(\mathbf{I} - \mathbf{A})^{-1} = \mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \mathbf{A}^3 + \dots \quad (3.27)$$

converges (because if the spectral radius is less than one, as the spectral radius is the infimum of the norms of matrix \mathbf{A} , we have

$$\|\mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \mathbf{A}^3 + \dots\| \leq \|\mathbf{I}\| + \|\mathbf{A}\| + \|\mathbf{A}\|^2 + \|\mathbf{A}\|^3 + \dots = \frac{1}{1 - \|\mathbf{A}\|},$$

$\|\cdot\|$ being a norm such that $\|\mathbf{A}\| < 1$). And in that case obviously the solution will have nonnegative entries, because is obtained with sums and products of positive terms. If \mathbf{A} is irreducible, often the Perron-Frobenius allows as to estimate the value of the eigenvalue

corresponding to the spectral radius, and see whether (3.26) has a feasible solution. But many times we are almost sure that \mathbf{A} is irreducible. Let us analyze why.

In general, for a square matrix A of order N (not necessarily a Leontiev matrix, or a nonnegative matrix) with entries $a_{i,j}$ there is naturally a graph associated to the matrix, namely a graph whose vertices are the points $1, 2, \dots, N$ and there is an edge between vertex i and vertex j if and only if $a_{i,j} \neq 0$. Naturally, if the matrix A is symmetric, the graph is not directed, else it is directed. A graph is strongly connected if from each vertex a path exists to any other vertex, and it can be proved without too much difficulty the following theorem:

Theorem 6. *A matrix is irreducible if and only if its associated graph is strongly connected.*

The proof may be consulted in [2].

The economic meaning of this theorem is the following: if Leontiev matrix \mathbf{A} is irreducible, the strong connectivity of its associated graph shows that each sector is necessary for each other sector, directly or indirectly. So in general we may assume that when a Leontiev matrix of the economy of a developed country is prepared, the matrix is irreducible: except for very small isolated areas with an economy of subsistence (usually neglected in the preparation of the Leontiev matrix) the economy of a developed country is integrated, and that means exactly that the associated graph is strongly connected.

3.6. The Usher matrix. Let us return to the Leslie model, but suppose now that the simulation time step instead of being equal to the time step during which an individual belongs to a class (as is the case with the Leslie matrices) is *less* than it. For instance, the simulation time may be, as before, one year, but the classes include individuals from age 0 to age 9, from age 9 to age 19, \dots , etc. The at each time step a proportion of individuals jump from class h to class $h + 1$, and the remaining individuals of class h continue belonging to class h . We can easily deduce that, if classes are $1, 2, \dots, K$, so that at time n the population vector \vec{P}_n is

$$\vec{P}_n = \begin{pmatrix} P_n(1) \\ P_n(2) \\ \vdots \\ P_n(K) \end{pmatrix},$$

then we represent the dynamic behavior of the model through the vector equation

$$\vec{P}_{n+1} = \mathbf{B}\vec{P}_n,$$

where now \mathbf{B} is called the Usher matrix, and has the form

$$\mathbf{B} = \begin{pmatrix} t_{1,1} + f_1 & f_2 & \dots & f_{K-1} & f_K \\ t_{2,1} & t_{2,2} & \dots & 0 & 0 \\ & & \ddots & & \\ 0 & 0 & \dots & t_{K,K-1} & t_{K,K} \end{pmatrix},$$

where now we have written f_i for the rate of fertility of individuals of group i , $t_{i,i-1} = 1 - T_m(i)$, with $T_m(i)$ the rate of mortality of group i , and $t_{i,i}$ denotes the proportion of individuals of group i that remain in that group after the time step. It is easy to see that an Usher matrix is irreducible if $f_{1,K} > 0$ and all $t_{i,i-1} > 0$; besides, if two successive groups are fertile (that is, if it exists an i such that f_i and f_{i+1} are greater than zero) the matrix is primitive.

4. TRAFFIC MODELS

Now, we change from discrete algebraic models to models governed by partial differential equations. In a brilliant approach, two well-known specialist in fluid mechanics, Lighthill and Whitham, formulated the traffic model as, in a sense, a fluid dynamics model, where the vehicles (cars, buses, vans) were assimilated to particles of a fluid [16]⁹. Independently of Lighthill and Whitham, Richards [19] also modelled the traffic flow through a fluid dynamics approach; he published his result in a journal specialized in this type of problems. Thereafter, an abundant bibliography has appeared; here we follow above all the book by Haberman [7]. It is not strange that the theory appeared in the '50 of the past century: after the Second World War the access of the western European middle classes to car's ownership (until then restricted to American middle classes) originated often traffic problems that ought to be solved.

The model we shall present is very simple: we consider a highway with one lane, and we do not allow overtaking (the model will probably hold reasonably well for bridges and tunnels, where in many countries it is not allowed to overtake another vehicle). Besides, we shall consider a mean length L of the vehicle (when we eliminate these restrictions the models are more complex and challenging, of course, but in general it is useful to begin with a simple theory and then to increase its complexity - if feasible). Taking vehicles individually, we say that the position of vehicle i at time t is $x_i(t)$, its velocity is $dx_i(t)/dt$ and its acceleration is $d^2x_i(t)/dt^2$.

We consider a short time step Δt between times t and $t + \Delta t$, and count the vehicles that pass an observer located at a point x . The quantity measured is the *traffic flow* $q(x, t)$ during the interval $[t, t + \Delta t]$. We suppose a continuum of vehicles, and fix a very small unit of time, changing conveniently the time step (of course now the quantity q is not necessarily an integer). Analogously, we consider a "picture" at time t of the vehicles between points x and $x + \Delta x$. This quantity we call the *density* of vehicles $\rho(x, t)$ in the interval $[x, x + \Delta x]$; again, we suppose a very small space unit, and ρ does not need to be an integer. In certain simple cases we can compute ρ directly, for instance if we consider vehicles of same length equally spaced with distance d between them. If Δx is, say, one kilometer, then the density (vehicles per kilometer) is

$$\rho = \frac{1}{L + d},$$

(of course L and d should also be measured in kilometers). Now, if all vehicles have constant velocity u , in Δt units of time each vehicle will cover $u\Delta t$ kilometers, say (with the corresponding units of u), and then it is easy to see that $q = u \times \rho$. It may be shown (and it is very intuitive) that if we accept that a *velocity field* exists, namely that at each point x at instant t we suppose that a "point" vehicle through x has velocity $u(x, t)$, then

$$q(x, t) = u(x, t)\rho(x, t),$$

and of course

$$u(x, t) = \frac{dx}{dt}.$$

Individualizing the vehicle located at x at time t as $x(t)$, we may write

$$u(x(t), t) = \frac{dx}{dt},$$

⁹This paper is the second part of a very important paper [15] devoted to a simplified model in one-dimensional fluid dynamics; the comparison of both papers allows us to observe where the differences exist between the "original" fluid dynamics approach and the "adapted" traffic one.

and knowing the position of the “particle” at initial time 0, namely

$$x(0) = x_0,$$

we have a first order differential equation.

4.1. A conservation equation. We must now obtain a conservation equation. Let us take a spacial interval $[x, x + \Delta x]$, and a time interval $[t, t + \Delta t]$. We have that the quantity of vehicles that enter the interval $[x, x + \Delta x]$, namely (approximately) $q(x, t)\Delta t$, minus the quantity of vehicles that leave this interval, namely (approximately) $q(x + \Delta x, t)\Delta t$, must be equal to the variation of the quantity of vehicles that are into this interval at time $t + \Delta t$ with regard to time t , namely (approximately) $(\rho(x, t + \Delta t) - \rho(x, t))\Delta x$, that is,

$$(q(x, t) - q(x + \Delta x, t))\Delta t = (\rho(x, t + \Delta t) - \rho(x, t))\Delta x.$$

We now divide by Δx and Δt , let both Δt and Δx tend conveniently to zero, and obtain

$$-\frac{\partial q(x, t)}{\partial x} = \frac{\partial \rho(x, t)}{\partial t},$$

that is,

$$\frac{\partial \rho(x, t)}{\partial t} + \frac{\partial q(x, t)}{\partial x} = 0,$$

or, taking into account that $q = u\rho$,

$$\frac{\partial \rho(x, t)}{\partial t} + \frac{\partial}{\partial x}(u(x, t)\rho(x, t)) = 0 \quad (4.1)$$

The conservation law says simply that something that “enters” (if there is no creation or destruction of this “something”) either goes out or is accumulated (supposing that what “enters” is greater than what “leaves”).

We have here the partial differential equation (4.1), and two unknown functions ρ and q , or ρ and u . We need some kind of “equation of state” that relates both functions. If we make the assumption that $u = u(\rho)$ (that, is, the velocity depends on the density of the flow, what seems (at least in many cases) plausible¹⁰), we get then

$$\frac{\partial \rho(x, t)}{\partial t} + \frac{\partial}{\partial x}(u(\rho(x, t))\rho(x, t)) = 0$$

or, more generally

$$\frac{\partial \rho(x, t)}{\partial t} + \frac{\partial}{\partial x}q(\rho(x, t)) = 0. \quad (4.2)$$

If q is a linear function of ρ , equation (4.2) is the simplest hyperbolic partial differential equation, namely

$$\frac{\partial \rho(x, t)}{\partial t} + c \frac{\partial \rho(x, t)}{\partial x} = 0, \quad (4.3)$$

where $c = dq/d\rho$. In this case, let us then search for a solution over the line $dx/dt = c$ of the total derivative

$$\frac{D\rho(x(t), t)}{Dt}. \quad (4.4)$$

¹⁰For instance, if there is no other vehicle in the highway, $\rho = 0$, and then the maximum velocity u_{max} may be attained: $u(0) = u_{max}$, where u_{max} is a technical or legal bound. On the other hand, if $\rho = \rho_{max}$, we have bumper-to-bumper vehicles, and the velocity is zero, $u(\rho_{max}) = 0$. A decreasing function may be constructed between these values.

We have

$$\frac{D\rho(x(t), t)}{Dt} = \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial x} \frac{dx}{dt} = \frac{\partial\rho}{\partial t} + c \frac{\partial\rho}{\partial x} = \frac{\partial\rho}{\partial t} + \frac{dq}{d\rho} \frac{\partial\rho}{\partial x} = 0.$$

That means that, over the line $dx/dt = c$, the total derivative (4.4) is zero. That is, over that line ρ is constant, and therefore, if $x = ct + x_0$, then $\rho(x, t) = \rho(x - ct, 0) = \rho(x_0, 0) = \rho_0(x_0)$, which we know because it is the initial condition. So equation (4.3), the simplest homogeneous linear hyperbolic equation, is easily solved: the solution is exactly the initial condition transported, at time t , a distance ct .

What happens if q is a nonlinear function of ρ , namely

$$\frac{dq}{d\rho} = c(\rho)?$$

In this case let us again try the solution over the curve $dx/dt = dq/d\rho = c(\rho(x(t), t))$. Thanks to the fundamental theorem of ordinary differential equations, we know that, under plausible initial conditions (that we assume) a solution, at least until a certain time T is reached, exists. We take again the total differential $D\rho(x(t), t)/Dt$ over dx/dt and again we find that the total derivative is zero, so that the solution is a constant, like before, so that dx/dt is a line like before. But we know that for nonlinear functions things are different from what they are for linear functions, so what is wrong with our argument?

Nothing. There *is* a difference. Before, all curves $x = ct + x_0$ differed only in the initial point x_0 , they were parallel, and now they may have different slopes, namely, the curves are $dx/dt = c(\rho)t + x_0$. But that means that two lines, beginning at x_1 and x_2 , may move away from each other, or they may intersect, depending on the values of their respective slopes. If they move away, everything is all right. But if they intersect, then the solution of (4.3)¹¹ has a discontinuity, because at the intersection point different values coming from different points cannot give the same solution. In these cases what we have is called a *shock*, and represents exactly that: a crash between a vehicle that reaches another vehicle forward but at a slower speed.

What we have obtained is a *shock wave*. The theory of hyperbolic equations as conservation laws and shock waves is - apart from its extreme usefulness in many situations, for instance in the examples above - fascinating from the mathematical point of view, and may be consulted in many textbooks, for instance in the excellent text ([20]).

We have seen that we may begin with a legitimate and very “good” (in the sense that it is as continuous and derivable as we want) initial condition and in spite of it we arrive at a discontinuity. Anyway, the world does not finish after this discontinuity: we may continue working with the equation, under the definition of *weak* solution, a concept which is extremely useful in many instances. What is exactly a weak solution? The idea is, in general, that a weak solution is a solution that not necessarily has all the properties that an “authentic” solution has, and that if a problem has an “authentic” solution, this solution is also a weak solution. The simplest idea is analyzing derivatives: suppose that in an interval $[a, b]$ we have a function $f(x)$, with a derivative $f'(x)$. Let us take an arbitrary function $g(x)$ with a continuous derivative such that its support (the closure of the points where $g(x)$ is not zero) is strictly contained in (a, b) , the interior of $[a, b]$ (that is, $g \in C_0^1[a, b]$). Then let us look at the integral

$$\int_a^b f(x)g'(x)dx.$$

¹¹Remark that now $c = c(\rho)$ is not constant anymore, so that now (4.3) is *not* linear.

Integrating by parts we have

$$\int_a^b f(x)g'(x)dx = [f(x)g(x)]_a^b - \int_a^b g(x)f'(x)dx,$$

where the value between the brackets is the difference between the values at b and the values at a . But, as $g(x)$ is zero at both points, we in fact have

$$\int_a^b f(x)g'(x)dx = - \int_a^b g(x)f'(x)dx,$$

and this happens for all functions $g \in C_0^1[a, b]$. Now, if it exists a function $h(x)$ such that for each $g(x)$ differentiable that is zero at the extremes we have

$$\int_a^b f(x)g'(x)dx = - \int_a^b g(x)h(x)dx,$$

we call $h(x)$ a weak derivative of $f(x)$. It has some of the properties of a derivative, but not all, but the properties it has are enough for many problems. Moreover, as we shall see in the following footnote, a weak derivative sometimes is not even a “proper” function, the concept is key in theory of distributions, and “extending” the concept of derivative we can use it for a derivative of any order. Of course, when $f(x)$ actually has a derivative, this derivative coincides with $h(x)$ (this is of course a necessary condition for having a reasonable definition using the word “derivative”)¹².

In the same sense, forgetting traffic problems, we can define a weak solution for a scalar conservation law. Strictly speaking, consider the general conservation law in $t > 0$

$$u_t + f(u)_x = 0, \quad u(x, 0) = u_0(x). \quad (4.5)$$

A bounded measurable function $u(x, t)$ is called a weak solution of the initial value problem (4.5) with bounded and measurable initial data u_0 , when the equation

$$\iint_{t \geq 0} (ug_t + f(u)g_x)dxdt + \int_{t=0} u_0gdx = 0 \quad (4.6)$$

¹²This notion of “weakness” has generalizations. Disregarding technicalities, let us take the Heaviside function $H(x)$, namely

$$H(x) = \begin{cases} 0 & \text{if } x < 0, \\ 1 & \text{if } x \geq 0. \end{cases}$$

Let us now take the Dirac delta “function”, namely $\delta(x)$ such that for all convenient functions $g(x)$ we have

$$\int g(x)\delta(x)dx = g(0).$$

The Dirac delta (which, in fact of course is *not* a proper function), is, according to our previous definition, the weak derivative of the Heaviside function, because, for any convenient function $g \in C_0^1[a, b]$, where $a < 0 < b$,

$$\int_a^b H(x)g'(x)dx = \int_0^b g'(x)dx = [g(x)]_0^b = -g(0) = - \int g(x)\delta(x)dx.$$

holds for all functions $g \in C_0^1$. Of course it is not too difficult to prove that (4.6) holds when u is an “authentic” solution of (4.5).

There is more to say about shocks. When a shock exists at a point x and time t , and (4.6) holds, the discontinuity is a “jump”: the values

$$u(x_l) \quad \text{and} \quad u(x_r),$$

where x_l and x_r mean the limits from the left and from the right, respectively, are different. The discontinuities form smooth curves Γ (in the sense that, apart from the right and left limits on both sides of Γ , the function u is smooth away from Γ), and, if we call $[u]$ the jump $u_l - u_r$, and analogously $[f(u)] = f(u_l) - f(u_r)$, we have the following

Theorem 7. $s[u] = [f(u)]$, where $s = dx/dt$ is the speed of the discontinuity.

The proof may be consulted in [20].

Relation $s[u] = [f(u)]$ is called the *jump condition*, or *Rankine-Hugoniot condition* in gas dynamics.

4.2. The Riemann problem in traffic. There is a famous problem in gas dynamics, called the Riemann problem, in which (for a one-dimensional situation) the initial conditions are constant at the left and at the right of a certain point, say, $x = 0$, but there is a discontinuity at 0. That is, using the notation of equation (4.5) we have, as initial condition

$$u(x, t) = \begin{cases} u_l & x < 0 \\ u_r & x > 0 \end{cases} .$$

The Riemann problem is enormously important in the theoretical and numerical research of hyperbolic partial differential equations, see for instance the text [20] already mentioned. It can easily be adapted to traffic situations that we suppose are governed by the conservation law (4.2), namely, suppose

- (1) Vehicles move uniformly along a road with density ρ_0 , and suddenly a traffic light turns red at time $t = 0$.
- (2) The same situation, but now the vehicles are all waiting (with density ρ_{max}) that the traffic light turns green, and the traffic light turns to green a time $t = 0$.

It can be proved (see [7]) or, for the general approach in gas dynamics, [20], that in the first situation there is a shock, namely each vehicle “crashes” against the vehicle that is already halted (in fact, of course this is only an approximation, because normally there are slowing downs phenomena included in the process, and no crash). In fact, we have a kind of Riemann problem with

$$\rho(x, 0) = \begin{cases} \rho_0 & x < 0 \\ \rho_{max} & x > 0 \end{cases} .$$

The shock propagates “backwardly”; the path of the shock must satisfy the shock condition

$$\frac{dx_s}{dt} = \frac{[q]}{[\rho]} .$$

We know the initial condition of this ordinary differential equations, namely $x_s(0) = 0$; besides, at time 0 and at the position $x = 0$ of the traffic light we shall have maximum density $\rho = \rho_{max}$ (because the first vehicle has stopped and the following vehicles will stop bumper-to-bumper). Therefore,

$$\frac{dx_s}{dt} = \frac{\rho_{max}u(\rho_{max}) - \rho_0u(\rho_0)}{\rho_{max} - \rho_0},$$

but as $u(\rho_{max}) = 0$ (no movement is possible in a bumper-to-bumper situation) we have finally

$$\frac{dx_s}{dt} = \frac{-\rho_0 u(\rho_0)}{\rho_{max} - \rho_0} < 0.$$

As we had said, the shock moves backwardly. Using the initial conditions, we may write

$$x_s = \frac{-\rho_0 u(\rho_0)}{\rho_{max} - \rho_0} t.$$

So we may remark that the shock moves through a line, with constant velocity x_s , and at time t the shock will be at position $x_s t$. Behind the shock, vehicles move forward with a constant density ρ_0 ; ahead of the shock, vehicles are standing still. In this simplified model, vehicles must decelerate from $u(\rho_0)$ to zero “instantaneously”; a more accurate model should take into account that usually vehicles decrease their velocity, perhaps very quickly, but without crashing. Anyway, very often the model coincides, to a reasonable approximation, with what really happens.

In the second situation all is smoother. The density is maximum for the vehicles waiting that the light turns green and when it turns green the vehicles begin to move rightwards. The Riemann conditions are

$$\rho(x, 0) = \begin{cases} \rho_{max} & x < 0 \\ 0 & x > 0 \end{cases}.$$

In this case the first vehicle may go (and we suppose that it goes) with maximum velocity u_{max} (because there is no vehicle ahead, that is, density is zero ahead of it) but the following cars must wait until they are able to move (an experienced situation for all drivers); If the distance between vehicles is L , the n^{th} vehicle should wait until time

$$t = \frac{(n - 1)L}{-u_{max} \rho'(\rho_{max})}$$

to move.

Interesting and useful experiments have been performed with this model, for instance at the Lincoln tunnel, in New York.

Incidentally, the Riemann problem may also be applied to a sudden dam break situation. Without analyzing the equations (we shall say something thereabout in the next section) we can suppose that upstream the dam a reservoir exists with a constant water level h_{const} , and downstream the dam the water level (that we may suppose constant too, for simplicity) is $h_{downstream} < h_{const}$. Analyzing carefully the variables and the equations, a similar phenomenon happens.

5. SHALLOW WATERS

Suppose now that we have a “not too deep” watercourse, that is, intuitively speaking, a watercourse shallow along all its course, and we assume that the lateral velocity is negligible, as well as the vertical velocity. We then have a one dimensional system of quasilinear hyperbolic partial differential equations: it may be proved (see for instance [21]), under reasonable physical assumptions, that the equations that govern the one-dimensional shallow water open channel flow are

$$\frac{\partial S}{\partial t} + \frac{\partial Q}{\partial x} = 0, \tag{5.1}$$

$$\frac{\partial}{\partial t} \left(\frac{Q}{S} \right) + \frac{1}{2} \frac{\partial}{\partial x} \left(\frac{Q}{S} \right)^2 + g \frac{\partial Z}{\partial x} + g \frac{Q^2}{D^2} = 0, \tag{5.2}$$

where x is the spacial coordinate along the longitudinal axis of the watercourse, t is the time, $Q = Q(x, t)$ is the discharge at point x and instant t , $Z = Z(x, t)$ is the surface level measured from a fixed plane of reference, $S = S(Z(x, t), x)$ is the wetted cross sectional surface at point x when the level is $Z(x, t)$, g is the acceleration of gravity, and $D(Z(x, t), x)$ is the conveyance at point x and level $Z(x, t)$, conveniently related to the frictional resistance to the flow. The conveyance is a parameter that indicates the influence of the geometry of the watercourse, its bed, the vegetation, etc., on the flow: it is intuitive that water flows very differently in a rectangular glass channel than in a watercourse where the cross sections have a very complicated geometry and, besides, there exists a significant vegetation on the bed. Equations (5.1) and (5.2) are usually called the Saint Venant equations of fluvial hydraulics (the conservation of mass and conservation of momentum equations, respectively), for the rôle the great French engineer of the 19th century had in their formulation. Technically speaking, we have a one-dimensional gradually varied unsteady water flow in open channels or rivers with arbitrary cross-sections and fixed bed, governed by the Saint-Venant hydrodynamic equations. Naturally, as there are two equations, there must be two independent functions whose existence (and unicity) should be guaranteed under certain assumptions. The functions are Z and Q , generally, although Q sometimes (above all in channels with a very simple geometry, and in two dimensions) may be replaced by the velocity $V = Q/S$, and Z can be replaced by S , if a one-to-one relationship exists between Z and S at each point x . Let us remark that if a relationship can be established between the discharge Q and the level Z , we can neglect the equation (5.2) and equation(5.1) becomes a scalar conservation law, as we saw previously. In fact, this is the kinematic equation, that Lighthill and Whitham treated in their article [15]. Sometimes, when few data are available, a complete hydrodynamic (fluvial) model must be replaced by a simpler one, a kinematic model.

Of course we need initial conditions, say, $Q(x, 0) = Q_0(x)$, $Z(x, 0) = Z_0(x)$, and, as the reach of river we are analyzing is not infinite, boundary conditions that, for watercourses with a certain type of flow called *subcritical*¹³ are one at the upstream boundary a and the other at the downstream boundary b . For instance, $Q(a, t) = f_1(t)$, $Z(b, t) = f_2(t)$. Boundary conditions, as well as initial conditions, must satisfy certain physical constraints that do not interest us now. If we use a simplified kinematic model, as we have only one equation in this case, only one boundary condition is necessary, namely the discharge upstream. A description of the problems that can be treated with the hydrodynamic or kinematic equations in fluvial basins may be consulted in [8].

The Saint Venant equations cannot be analytically solved except in very special cases, so that they must be numerically solved. This is not a problem nowadays. A vast amount of very efficient numerical methods exist to solve the equations, see for instance [23]. The technical problem is not solving the Saint Venant equations, the technical problem is (sometimes) to find the conveyances D . In fact, we have a lot of parameters: at each point of the river the cross sectional geometry may vary, the type of bed may also vary, and the conveyances depend also on the water level. So often we must have values of D , for instance, 100 points that represent significant points in a river, and at each point for, say, 20 different heights. So we need to calibrate 2000 parameters, and, although theoretically to find the values of parameters that minimize the differences between the results of a model run with historical records and the real records is an inverse problem, usually it is

¹³A subcritical flow is a flow where the (dimensionless) Froude number Fr is less than 1, $Fr = V/\sqrt{gh}$, where V is the velocity of the fluid and h the hydraulic radius, that is, wetted cross-sectional area divided by surface width. If the Froude number is greater than one, we have supercritical flow, and both boundary conditions must be prescribed upstream.

simpler and more efficient to have an experienced modeler that, by a carefully designed trial and error method, perhaps automatically running the model several times, obtains the required values. Of course, the modeler will begin with educated guesses, that is, if the river is similar to other rivers on which he or she had worked (in the sense that the type of bed is similar, and/or the geometry is similar, and/or the discharges are similar, etc.), it is reasonable to think that it is possible to begin the calibration using values of conveyances already used in the other river. It is possible also that the modeler will need several historical records (for instance, the records of water levels for a dry year, for a year neither particularly dry nor particularly wet, and for a wet year), in order that many different situations may be simulated and compared with actual data recorded.

Other problem that may exist modelling rivers (and in many other situations) is what is called the “warming-up” of the model. To carry on a run we need boundary conditions and initial conditions. Boundary conditions are in general known: for a calibration run, for instance, one may use as upstream boundary condition the water levels recorded at the upstream point during a certain period, and as downstream boundary condition the corresponding water levels. But not necessarily one knows what is the initial state of the river, that is, the heights and discharges at all discretization points¹⁴. Then a process is necessary by which, beginning with sound initial conditions (sound in the sense that are physically reasonable: for instance, the surface slope corresponding to a steady state situation), and slowly carrying the boundary conditions until they have the initial values they should have (and then sometimes maintaining these values during a certain period, in order to begin the “real” run with a steady state situation), one can begin the run: the model is already “warmed-up”. This is one of the fundamental differences between problems in partial differential equations (and sometimes other types of equations) with only initial conditions prescribed, that is, Cauchy problems, and mixed initial-boundary problems like this one: in Cauchy problems once the initial conditions are given, if the problem is well posed in Hadamard’s sense the results in the future are (neglecting numerical errors) completely determined, and can not be changed by any means: if we have not the real initial conditions (or initial conditions sufficiently close to the real conditions) we shall never obtain satisfying results. But in mixed initial-boundary problems often the boundary conditions “force” the problem to approach convenient conditions, and then we use them.

By the way, the “warming-up” problem helped Edward Lorenz detect the phenomenon of chaos: with his very ancient (for our standards) computer (a Royal McBee LGP-30) Lorenz was working in weather prediction, via a very simple (and now very famous) model (a “toy” model) consisting of three ordinary differential equations slightly nonlinear¹⁵. He had “good” initial conditions for a certain simulated time, but to go from this state of

¹⁴Here we suppose that the problem is numerically solved by finite differences, that is, by conveniently replacing derivatives by incremental quotients at certain points, the discretization points. If other type of numerical method is used, there will be perhaps slight modifications in this approach, but essentially the idea is the same. This remark holds also for the analysis of conveyances above mentioned.

¹⁵For the sake of completeness we write here his equations:

$$\begin{aligned} dx/dt &= \sigma(y - x), \\ dy/dt &= x(\rho - z) - y, \\ dz/dt &= xy - \beta z. \end{aligned}$$

Here σ is the Prandtl number and ρ the Rayleigh number. The three parameters σ , ρ and β must be positive, and the system is chaotic for certain values of ρ . Remark that chaos is not associated with complexity of the equations: there are only three equations, and the “nonlinearity” is weak (only the product of two functions).

the system to the state he was really interested in, and then perform the experiments he wanted, he ought to spend a lot of machine-time (the computer was very slow). So he used a (printed) description of the state of his system at the appropriate simulated time; the printed numbers were rounded to less decimal points than the actual numbers, as represented in the computer memory, but as he believed that his problem was well posed he did not care for the slight difference. The surprising result (the trajectories were completely different) opened the path to the theory of chaos, and was published in [17], becoming a very famous and profound paper.

6. BUILDING AND OPERATING A MODEL

Now, both in discrete and continuous models, there are some general rules which, if possible, we follow: we formulate the problem, and try to “translate” the problem into a mathematical model. The mathematical model should not be more complex than necessary: it makes no sense to prepare a very detailed model that requires many different kinds of data when we are not able to collect (or to collect in a near future) or imagine the data. The model should also take into account the computer resources available: although nowadays we can use extremely powerful computers and clusters, some problems are really “big”, for instance some 3D meteorological models; never prepare a model that you can not find a computer to run it in. Sometimes the programming of the model forces us to re-analyze the equations, or even to re-analyze the assumptions. Anyway, with the model programmed and implemented, after many runs with artificial or special data, we are able to calibrate the model. After calibration, it is necessary to validate the calibration: how do we know that the calibrated parameters are (more or less) the *actual* parameters, and not parameters that “force” the model to approximate the real situations we have used for calibration, but not other situations? If possible¹⁶, it is necessary to validate the model with other real situations not used for calibration: for the model to be considered well-calibrated, the differences (in the chosen norm) between the simulated results and the real values must be reasonably similar to the differences obtained in the runs used for calibration. When the model has many parameters, it is possible that according to the input data some parameters are or are not involved in the calculations; therefore, it is convenient that the validation runs assure that all parameters take part in the calculations (of course that means that it is important that the calibration runs allow the calibration of all parameters). But only after the model has been sufficiently calibrated¹⁷ can we really take advantage of it.

If the model is ready for the numerical experiments we want to perform with it, then it may be a powerful tool to assess the feasibility or the consequences of different alternatives. For instance, with a demographic model we can evaluate, for different rates of fertility or mortality, what will the population pyramid be taking a horizon of, say, 50 years¹⁸. Then we can, for children and teenagers who should be in school, compute how many teachers we need, how many buildings, and then the necessary budget. Of course, some policies may be unfeasible, perhaps for physical or technical reasons (it will be impossible

¹⁶Sometimes we have no time, or no other historical record, to validate the model.

¹⁷Of course not always are we totally satisfied with the calibration. Anyway, when using a model it is important to know how well it represents the phenomenon modelled, so as to avoid conclusions not sufficiently backed.

¹⁸How distant the horizon can be depends, of course, on the type of model. For a Leslie-type demographic model the horizon may be reasonably distant, because it is a linear model, and linear models are stable. But a meteorologist predicting the weather must be satisfied with an horizon only some days in the future, because, as Lorenz showed, the problem is ill-posed.

to get that number of teachers in those years, or the political cost of assigning too much money to education - and, for instance, not enough money for the old - is too high, etc.). Naturally, what the model offers us is a menu of scenarios: it would be very dangerous to believe that one, and only one, is the outcome associated with an alternative, because always there are “boundary conditions” that we do not control. For the traffic model it is possible to evaluate how convenient could be the construction of a new tunnel or bridge in a city. For the fluvial model, many runs may be performed, to experimentally detect what happens when downstream, for instance, we have a dam, and several alternatives of water release (that is, discharge as downstream boundary condition) are tested.

It is always important to know what the model can *not* do: for instance, a fluvial model using a finite difference implicit method for numerically solving the Saint-Venant equations is not apt to model the sudden breaking of a dam, because in this case we must surely analyze a shock wave, and finite difference implicit methods usually smear out the shock wave.

Sometimes the modeler is one person, experienced in the problem, in its mathematics, and in programming. But usually (above all if the problem to be modelled is complex) an interdisciplinary group works in the modelling. Depending on the problem, perhaps an engineer (or a demographer, in one of our examples) with an applied mathematician, and a computer scientist, and assistants. Each scientist or professional must be able to understand the language and the type of approach of the others; this is not only important and useful for the success of the modelling, but also is incredibly enriching for all participants.

Finally, it is interesting to remark that, as a tool in modelling, applied mathematics may sometimes become an experimental science, in the sense that its criteria begin to look like the criteria of physicists or engineers. Sometimes a careful and good strategy for the design of experiments is extremely convenient. An analysis of this kind of approach in applied mathematics may be seen in [9].

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