ROBUST MODELING IN NATURAL SCIENCES *

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Abstract

We investigate here the notion of model robustness and its importance for modeling natural systems. In physics, robustness is related to several more specific notions like those of structural stability, normal forms and universality classes. A special attention has to be given to the scale of the description. In some cases, renormalization methods can be exploited to assess the robustness of the large-scale predictions of a model. We discuss in what respect robust minimal models, based on arguments of parsimony and typicality, fulfill the requirements for an operational and meaningful modeling approach in natural sciences.

Résumé

Nous envisageons avec un regard de physicien la notion de robustesse d'un modèle et son importance pour la modélisation des systèmes naturels. En physique, la robustesse est reliée à d'autres notions plus spécifiques comme la stabilité structurelle, les formes normales et les classes d'universalité. De façon essentielle, l'échelle de la description doit être prise en compte dans la construction d'un modèle et l'appréciation de sa validité. Des méthodes de renormalisation peuvent dans certains cas être exploitées pour tester la robustesse des prédictions à grande échelle d'un modèle. Nous discutons dans quelle mesure des modèles minimaux robustes, fondés sur des arguments de parcimonie et de typicalité, offrent une approche opératoire et pertinente des systèmes naturels.

1. Introduction. We investigate here the notion of model robustness and its importance for modeling natural systems. As early as 1966, Levins underlined, within the context of population biology, that any assessment on a (real) system based on a model requires a "robust representation" [18]. Robustness is a notion used within several scientific domains presenting each its specific notions of this property: analysis of sensitivity of the solution of an equation, rigidity of a numerical method in applied mathematics, robustness of an estimate in statistics. Here we will adopt a physicist's perspective: our aim is to devise operational guidelines for an understanding of real phenomena based on modeling. Two central concepts will be those of structural stability and universality. Note that defining and investigating the intrinsic robustness of a system, i.e. the persistence of its properties or behavior in response to various perturbations, is a different issue, not in the scope of the present paper (we refer e.g. to [15] for a review on this question).

2. Structural stability, normal forms, universality. *Structural stability* is a notion that originated in dynamical systems theory. It refers to the invariance of the topological

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type of the set of trajectories (the "phase portrait") for all dynamical systems sufficiently close to the considered one [9]. This ensures the persistence of asymptotic features, e.g. fixed points and their stability, in response to small changes in the evolution law. The exact and historical definition of structural stability is highly technical [1]. It requires defining a topology for measuring how similar two dynamical systems are. The similarity of their phase portraits is then expressed by the existence of a homeomorphism (a continuous mapping with a continuous inverse) between their respective sets of trajectories.

Structural stability of a dynamical system is equivalent to the robustness of any dynamic modeling involving it. However, it should be noted that the notion is relevant for a predefined set of features (large-scale properties, more precisely the topological type of the set of trajectories in the original definition) and not for all aspects of the behavior. For instance, the transient dynamics may be susceptible to small changes. The notion of robustness is thus relativistic: it refers to a predefined set of perturbations and to features that should be preserved upon perturbation. The larger the set of perturbations and the more stringent the invariance requirements, the stronger the robustness.

A second level of structural stability can be considered, that refers to the persistence of the behavior predicted by the model when one of its parameters is varied. The typical instance involves a parametrized family of dynamical systems. It then applies to the occurrence of a bifurcation, that is, a qualitative change in the fixed points and more complex attractors characterizing the stationary regime of the dynamics. What should here persist is the way in which the dynamics is qualitatively modified when the parameter is varied. This "higher-level" structural stability is related to the notion of *normal form*, defined as the simplest polynomial to which the parametrized family of dynamical systems can be reduced by a smooth transformation. The dynamics generated by the normal form displays the same kind of bifurcation as the original one when a coefficient of the polynomial is varied. For example, $dx/dt = x(a - x)$ is the normal form of the bifurcation corresponding to an exchange of stability between two fixed points ($x_1^* = 0$ is stable and $x_2^* = a$ is unstable for $a < 0$ whereas $x_2^* = a$ is stable and $x_1^* = 0$ is unstable for $a > 0$).

A link to *catastrophe theory* [23] is apparent for a parametrized gradient dynamical system $dx/dt = -\nabla V(a, x)$, whose trajectories follow the steepest descent along the landscape $V(a, x)$ (the "horizontal" coordinates are a and x, and the "altitude" is $V(a, x)$). The bifurcations experienced by the dynamics when the parameter a varies correspond to singularities of this landscape (in mathematical terms a "surface" or "manifold") $V(a, x)$. The possible singularities are classified in seven types by catastrophe theory, each corresponding to a type of bifurcation (e.g. when two wells merge into a single one as is a varied, two stable fixed points and an unstable one merge into a single stable fixed points)

In theoretical physics, these developments led to the notion of *universality class*. A remarkable observation is that for some phenomena, typically second-order phase transitions (continuous change in the state of matter when temperature or some other control parameter varies), very different systems display the same behavior described by power laws in the neighborhood the transition point [12]. Models can be classified according to their scaling behavior at the phase transition, which defines their universality class. Here a qualitative observation (the features of the phase transition) leads to a quantitative prediction (the exponents of the power laws describing how thermodynamic quantities vary with the control parameter). For instance, the ferromagnetic-paramagnetic transition in a magnet (at which the magnet looses its spontaneous magnetization) and the critical liquid-gas transition in water are described by power laws of the form $(T - T_c)^\beta$, where T_c is the temperature of

the transition, involving exactly the same values for the exponents β. More generally, we can define a universality class as an ensemble of models sharing the same large-scale (i.e. collective or long-term) behavior. A model will be robust with respect to modifications that do not change its universality class; this sounds as a tautology but it is not, since multi-scale tools presented in § 4 have been developed to delineate universality classes and escape a case-by-case study of model robustness. A minimal model corresponds to the simplest element in the universality class: only the essential terms are kept. In the specific framework of dynamical systems, a normal form is the minimal model to describe a generic bifurcation, and the set of evolution laws related to the normal form through a smooth transformation corresponds to its universality class.

3. Models at several scales. A model is defined with respect to a scale of description. For real systems, consistent results should be obtained with models operating at different scales, hence possibly relevant within different theoretical frameworks. The paradigmatic example is that of diffusion. For instance, the diffusion of ink in water can be described in terms of deterministic microscopic equations describing molecular collisions, or using a Langevin equation describing the stochastic contribution of their thermal motion, or in terms of a Fokker-Planck equation describing the evolution of the probability distribution of the ink molecules, or in terms of a deterministic macroscopic diffusion equation describing the spatio-temporal evolution of the ink concentration. All these different descriptions of the Brownian motion of ink particles in water can be related one to the other, at the price of some approximations justified by their different description scales (e.g. the fast de-correlation of molecular motions to justify the noise term in the Langevin equation, or the large numbers of particles to justify a macroscopic description in terms of a continuous density) [12].

The above consistency requirement leads to articulate models of the same system at different scales. Depending on the specific setting, this can be achieved by passing from a discrete description at a microscopic scale to a continuous one for collective quantities at a macroscopic scale. Or conversely, by passing from a continuous description at a microscopic scale to binary features at a coarser resolution, mimicking an all-or-none behavior for the collective feature [14]. Controlled approximations are involved at each step from a microscopic description toward a more integrated one, which delineate its scope and validity [12]. Bottom-up derivation of macroscopic models amounts to dimensional reduction, accounting only for a small number of macroscopic quantities and systematic methods have been developed to address the question. They are typically based on scale separation between fast microscopic phenomena and slow large-scale trends [5, 7]. However, although the same system can be modeled at different scales, one description scale is in general most relevant for answering a specific question or for explaining the available data. Addressing questions relevant at different scales thus require different models of a given system.

We claim that an explanatory approach of a real system requires the use of *minimal models*, only based on the essential variables and parameters. A minimal model is sounder on epistemological grounds when only a limited knowledge of the system is available. It helps avoiding over-interpretation, e.g. giving a role to some details while ignoring other details that have similar impacts on the results, in strength and scope. A minimal model requires choosing the scale or level for representing the system at which the simplest model can be written. Indeed, because small-scale details are not fully known, often not even all identified, that the model should involve only a coarse description, allowing the precise knowledge of what is taken for granted in devising the model. This does not mean that reality is bound to be that simple, but that our description has to be unbiased and robust

with respect to an additional detail or to the intrinsic small-scale variability of the system.

A way to derive a minimal model is to introduce *effective parameters*, encapsulating in a single coefficient a wealth of underlying features and mechanisms, with no need for their explicit description nor even for their exhaustive identification. They were named "sufficient parameters" by Levins [18], by analogy with sufficient statistics. Let us cite a few examples: the elastic coefficients involved in the mesoscopic description of a long heterogeneous molecule, e.g. DNA, as a continuous and homogeneous elastic filament; the relative dielectric constant multiplying the bare one in order to describe how the presence of water modifies electrostatic interactions between molecules; the kinetic constants involved in the description of a chemical reaction in terms of mass action law and accounting for several intermediary steps and transient species; the growth and death rates involved in the demographic study of a population averaging the individual specificities and peculiar life history; the effective diffusivity involved in the homogenized description of diffusion in a porous medium, in terms of a simple diffusion equation with no need to describe the complicated and disordered geometry of the medium; the eddy diffusivity involved in the similarly reduced description of passive scalar transport (e.g. pollutant or marked particles) in a turbulent flow [5]. These examples illustrate that effective parameters depend on the microscopic level in a complicated way, which one does not intend to describe nor even unravel. An important advantage of effective descriptions is thus their robustness with respect to the detailed knowledge of the underlying phenomena. A change in the value of an effective parameter can accommodate an additional mechanism or some errors in the available experimental knowledge. The use of effective models enlightens that the nature of the models should not be confused with the nature of the system. For instance, a statistical description is not necessarily associated with a random evolution law or spatial disorder. It can be chosen as the most efficient way to account for the system features in case of a high-dimensional or chaotic underlying dynamics [21].

In a similar spirit, analyzing an experimental time series may benefit from encoding the data using a finite alphabet, that is, distinguishing only a finite (small) number of classes of states, e.g. active/inactive in case of a behavioral sequence [20]. A theoretical support is provided by symbolic dynamics, according to which the main features of an evolution can be reconstructed based simply on the knowledge of the phase space regions that are successively visited by the system (for a suitable partition of the phase space). Here again, a qualitative knowledge is enough to derive quantitative features of the dynamics [6].

4. Renormalization methods. Systematic approaches, known as *renormalization methods*, have been developed in theoretical physics for determining universality classes with respect to large-scale behaviors, more specifically scaling behaviors [5, 12, 13]. Their implementation is technically sophisticated but their principle can be stated in a simple way. They proceed in recursive steps, termed renormalization transformation. Each achieves an integration of the smallest scales and associated degrees of freedom into an effective, "renormalized" model, describing the *same system* with a coarser resolution. An acknowledged example is the renormalization of the Ising model describing a magnet as a system of spins, placed at the nodes of a lattice and each interacting with its nearest neighbors. The renormalized model considers blocks of spins (e.g. four on a square lattice) as units. It involves an effective coupling constant describing the interaction between adjacent blocks, such that the macroscopic behavior is unchanged. Renormalization thus defines a transformation in a space of models, and its iteration generates "trajectories". A trajectory relates models describing the same system at different scales. Convergent trajectories reflect the convergence

of the large-scale predictions of the initial models. A fixed point of the transformation corresponds to a model displaying self-similar features (in the above example, a model describing the ferromagnetic-paramagnetic transition point). At a fixed point of the renormalization transformation, unstable directions correspond to essential terms in the model, influencing their large-scale predictions. Stable directions correspond to irrelevant terms, with respect to which the model is structurally stable. Universality classes are thus associated to the different fixed points of the renormalization flow and their basins of attraction.

Initially devised for computing exponents of scaling laws, renormalization methods can be extended into a method for assessing the structural stability of a model with respect to its large-scale predictions. Specifically, a term in the initial model is irrelevant for the large-scale behavior if it is damped by renormalization, meaning that its effective influence is decreased at higher scales. Conversely, amplification of a term by renormalization means that its influence is determinant in the large-scale behavior. Renormalization transformation defines a flow in the space of models. We refer to [5, 12, 13] for a detailed account of this conceptually powerful methodology. Basically, it underlines the relativity of a model. Instead of investigating the features of a single model, it leads to change the level of the study and to work in a *space of models*, discussing whether they may, or may not, reflect the same reality. This is precisely the notion of robustness of a model.

5. Arguments of parsimony and typicality. The issue of model selection has been largely addressed throughout the history of statistics [4]. It relates to the very notion of robustness in statistics [11], a vast domain with a large literature. A complete and fair account of this topic is beyond the scope of this contribution. We will only mention two general criteria, parsimony and typicality.

Parsimony promotes the use of a model based on a minimal number of parameters. Much work has been devoted to devise quantitative guidelines to achieve this goal, for instance Akaike's information criterion [4] or the minimum description length principle [8, 22]. A celebrated joke wondered about the minimal number of parameters required to fit an elephant [24]. It is often completed with a bit of criticism by mentioning that adding one parameter allows the elephant to move its ears, indicating that with enough parameters, one is able to fit anything, with no certainty that the model captures reality in any way. The use of minimal models has been promoted to avoid this flaw, deliberately choosing to sacrifice precision to realism and generality [18]. Construction of a minimal model could besides proceed in several steps: starting from a complicated model, taking into account all identified mechanisms and parameters, then performing sensitivity and structural stability analyses to gradually prune the model and keep only the essential terms.

Typicality is a probabilistic argument, prescribing that the model has to capture the most probable behavior. It is supported by concentration theorems and statistical laws, describing the emergence of an overwhelmingly probable collective behavior in many-body systems [16]. Looking for typical models meets the prescription of avoiding biases in the description, what has been promoted by Laplace as the *principle of indifference*: a probability distribution should account only for the known constraints (yielding an equiprobable distribution in the absence of any knowledge). This idea has been formalized in statistical physics and information theory: in devising a model for a probability distribution, minimizing the bias amounts to maximize the entropy of the distribution under the constraints imposed by the setting [2, 10, 16]).

6. Modeling as an explanatory strategy. A model is nothing but the formal expression of a set of working hypotheses. In particular, it is a means for reasoning, beyond verbal formulation. It is also a way to rigorously generate predictions to be confronted to experiments and data. We recall the celebrated statement by Box: "All models are wrong, some are useful" [3]. What is true in a model is the relationship between the ingredients and their outcomes. These predictions are more likely to reflect actual processes if they are robust with respect to the details of the model. This is the reason for our strong support for the use of minimal models. A set of working hypotheses currently defines what is termed a *statistical ensemble* in theoretical physics, or a *null model* in statistics. Modeling helps to rigorously derive all the consequences and predictions of the considered hypotheses, for instance under the form of the probability distribution of some observable or index. It is then straightforward to confront experimental data to these predictions, and to quantitatively assess whether they significantly differ or not. In the first case, it means that reality escapes the explanatory scenario underlying the null model, and that additional ingredients or mechanisms have to be added [19]. Modeling is thus *a way of hypothesis checking*. An inspiring discussion in the context of seed dispersal modeling can be found in [17].

This points to an apparent limitation of minimal models. They are powerful tools to explain classes of behaviors. This can also be seen as a weakness. An explanatory scenario basically aims at a qualitative agreement. Applications and engineering purposes require quantitative predictions. However, in a second step, once the dominant mechanisms have been delineated by means of minimal models, additional details have to be taken into account. Starting from a robust minimal basis makes a gradual increase of the number of variables and parameters tractable, while limiting the risks of missing the main phenomenon or being misled by false alternatives.

The recommended approach is thus to proceed in several steps, especially for complicated systems involving numerous mechanisms, variables and parameters with no obvious hierarchy in their importance. First, starting from a raw modeling including all what can be described, introduce effective terms and effective parameters to recursively short-cut microscopic details, and prune the inessential terms regarding the behavior of interest. This yield a minimal model. The identification of dominant mechanisms achieved in devising this minimal model has then to be validated by confronting the predictions of the model with the observations. Then, a quantitatively more accurate agreement can be looked for by refining the minimal model.

7. Conclusion. Modeling relies on the choice of a representation and a framework. It can be deterministic or stochastic [21], discrete or continuous [14] according to the scale of the description and the type of predictions one intends to obtain. Basically, one has to devise a specific model for each specific question. Accordingly, a cluster of complementary models will be necessary to account for a complex system. Robustness in physics is related (although involving a different terminology) to the notions encountered in statistics, e.g. the robustness of an estimate or the issue of model selection.

A deep issue is the link between the robustness of a system and the robustness of its modeling. As a rule, the more sensitive to parameter values the behavior is, the easier will be the estimation of these parameters. This has been quantified in statistics with Cramer-Rao bounds. In parallel, the more sensitive to parameter values the behavior is, the more dramatic the estimation errors are for predictions. Roughly, the idea is that a robust real system will be more difficult to model faithfully. For instance, it is difficult to gain knowledge by probing the system's response to various perturbations. In counterpart,

capturing its main features by means of a minimal model will be enough to capture the core of its behavior. Minimal modeling helps to unravel general principles ruling the system's behavior, typically statistical laws for physical systems, regulation for living systems and control for artificial systems. In this regard, modeling gives insights on the robustness of real systems and its origin. However, this final discussion is rather pertinent to epistemology rather than to theoretical physics, and lead to a more general reflection on the link between a model and the underlying reality.

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