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Modelling and prediction in a complex world

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Abstract

A complex system is an entity, coherent in some recognisable way but whose elements, interactions, and dynamics generate structures and admit surprise and novelty that cannot be defined a priori. Complex systems are more than the sum of their parts, and a consequence of this is that any model of their structure is necessarily incomplete and partial. Models thus represent simplifications in which salient parts and processes are simulated, and given this definition, many models will exist of any particular system. In this chapter, we explore the impact of this complexity on validating models of such systems. We begin with definitions and then identify key issues as being concerned with the characterisation of system equilibrium, system environment, and the way systems and their elements extend and scale. As our perspective on these issues changes, then so do our models with implications for their testing and validation. We argue that changes in the meaning of validity, posed by the use to which such models are to be put, are central to this debate, drawing these ideas together as conclusions about the limits posed to prediction in complex systems.

1. Defining complexity, modelling complexity

This inquiry is motivated by a long-standing concern for the most appropriate ways of testing and validating large scale models, specifically those designed to simulate and predict urban development. These types of model have always been characterised by their extensiveness but since their inception over 40 years ago, there has been a slow but inexorable rise in their complexity. This has been hastened by a sea change in the relation of science to knowledge, and the way we are able to use science in society. In many senses,

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our growing need for ever more complex models and the increasing difficulties in their validation mirrors the longer term shift from a certain to an uncertain world. The first 50 years of the last century, perhaps even the previous 200 years, was dominated by the notion that science would yield answers of the simplest kind to a wide range of applicable problems. But this certainty has gradually dissolved, and the reasons for this are diverse. At one level, this may be no more than one of those unfathomable psychological shifts in our awareness of the limits to our knowledge which occur periodically. At another level, it may be due to more experiences in using science in the quest for exact answers to socially important problems and the growing realization that such certainty is illusory. The recent history of social forecasting in this regard has been salutary. Both macro and micro events, from predictions of the stock market and the general performance of the economy to more local issues such as demographic change and traffic movements in cities seem beyond our understanding, not least our control, in that extraneous events now seem to dominate their behaviour. Although this may always have been the case, the models that were fashioned a generation or more ago now seem wholly inadequate.

None of this has daunted our curiosity in using science to explain and predict but it has changed it. Fifty years ago, the quest to build useful theories and models was dominated by the view that we could simplify and distil the essence of things so that we might capture sufficient of the social reality for rudimentary comprehension and decision. Despite recognition that the world was complex, it appeared simple enough to produce robust theory and models that might be employed in applications. With increasing uncertainty and the growing perception that the systems that we deal with are intrinsically complex, simplicity no longer seemed the watchword in the development of techniques and models. Prediction is now couched in qualification, and our science has become less orientated to forecasting, more of an aid to understanding and structuring debate. This is seen nowhere more clearly than in the shift to constructing ‘what if’ scenarios which now dominate most model-building.

The systems approach that was the foundation on which most operational urban development models were predicated [3], is strident in its advocation of three key principles of model-building. The first involves defining the system in its wider environment in such a way that the system has a crisp boundary with the outside world; in short, interactions of interest must be much denser within the system than outside. The second has become more controversial and this revolves around the idea that the system must manifest some equilibrium, that processes of change within it must imply some equilibrium and, if such processes are well behaved, then the equilibrium itself might be the focus of prediction. The third principle suggests the elements of the system that must be uniform or homogeneous in some sense, with the focus on explaining the order and regularity that such homogeneity implies. These principles did once appear to be implementable for urban systems but it is now easy to argue that none of these apply to even the simplest systems of interest to policy-makers. Such systems are impossible to close, their usual state is far-from-equilibrium, and often no such equilibrium ever exists. They are composed of heterogeneous agents and objects; indeed their very richness comes from such heterogeneity. The quest of science, it is now argued, should be to grapple with explanation and frameworks that attempt to contain, if not explain, such diversity. None of this bodes well for models in which traditional prediction is the goal.

During this period, systems theory has not remained still for complexity theory has gradually changed its form, some would say enriched it, but few are bold enough to define its current scope [7]. Most commentators define complexity implicitly through its various attributes and dimensions, and this is the path we will follow here. The very best way to characterise a complex system is by the states or conditions it can take on. If there are n elements describing a particular state, and each state is described by the (binary) existence or otherwise of a particular condition for each element, then there are 2^n distinct states. For example, there is a whole class of urban models built around cellular automata where the state of the system might be described by n cells with each cell being developed or not developed. In a system with say 10,000 cells or zones, then the number of possible states defies description. Add to this different ways or rules of generating these states, then the problem begins to scale in a manner that cannot be handled by conventional theorising. Of course, none of this is very new and this characterisation of complexity has been known for a long time. However, this change in worldview has transferred attention away from the more restrictive aspects of such models to their existence properties, with the consequence that the systems we deal with only now are perceived to have boundless complexity.

Most would agree that complex systems have an extensiveness in their elements or objects that make any fixed description incomplete. This immediately implies that all possible forms of the system are unrealisable, and their representation is rarely stable. In short, complex systems generate a dynamic which enables their elements to transform in ways that are surprising, through adaptation, mutation, transformation, and so on. This is sometimes described in terms of a system generating new designs often expressible as new forms. In any event, the hallmark of this kind of complexity is novelty and surprise which cannot be anticipated through any prior characterisation. All that can be said is that such systems have the potential for generating new behaviours. Holland [10], for example, describes complex (adaptive) systems as being systems that maintain their structure and coherence under all imaginable changes, in short through adaptation. Allen [1] goes much further and defines complexity in terms of the sources of unexpected change or 'unpredictability'. He says: "The simplest definition of a complex system is one that can respond in more than one way to its environment. The 'choice' in response arises from the fact that non-linear processes within the system can potentially amplify microscopic heterogeneity hidden within it". This, he argues, is the origin of that overworked term emergence, another way of describing behaviour that cannot be anticipated.

From this casual introduction, we can identify two key elements that define our view of complexity and complex systems models. The first is 'system extensiveness' along any spatial, temporal or topical dimension. Such systems cannot be simplified in the conventional way by reduction or aggregation, for in doing so, the richness of their structure would be lost. This, of course, is directly countered to the usual strategy in science, which involves distilling the essence of a phenomenon, the essence being defined in relation to some purpose, and thence using that essence as the basis for theorising and modelling. The second issue involves process. This can often be portrayed as the system's dynamics in space and time in which unexpected change takes place, new objects emerge, and existing objects transform. There are some logical difficulties in all of this, for once objects have emerged and once one has considered the logical limits to a system and its possible boundaries, to make any progress in terms of crisp and clear representations, then the system has to be bounded in space and time [5]. Much of complexity theory has, in fact, been concerned with demonstrating models of systems that were initially deemed inexplicable because they demonstrated surprising behaviour. Once understood, this behaviour is no longer surprising, but invariably it can only be explained by processes that exist at a micro level giving rise to phenomena at a macro level which, in turn, cannot be explained in traditional macro terms. In short, much of complexity theory and its modelling is rooted in explaining behaviours that have already been observed and in some sense, can thus be said to be no longer complex. As Gregory [8] has so eloquently noted: "Here 'emergence' does not mean mysteries popping out of the undergrowth; it means that with sufficient understanding of interactive processes, we should come to understand why a complex whole has properties its parts lack on their own, and how the parts are modified by the context in which they lie" (quoted in [2].

Interesting as these issues are, we will put them aside in this discussion. We are more concerned with demonstrating that a new generation of models alluding to complexity theory often, indeed usually, fall back on traditional strategies which have been conceived for a more certain, simpler world where the ambiguity characteristic of complexity is absent, or at least not to the fore. Our discussion, therefore, will focus on how we might model complexity in the face of infinite variety; or rather not about how to model it per se, but how to face it in terms of traditional ideas based on the validation of some structure against a well defined representation encoded in 'data'. This presupposes that even if a system is infinitely complex, then some simplification must take place. But how much? And more importantly, how do we deal with knowing that our models will always be 'inadequate' in a predictive sense? The issue of parsimony is under fire here, and there is little doubt that our own field has barely broached these issues. We persist in developing models that are intrinsically complex but which we attempt to validate against some reality which we represent as intrinsically simple. We do not seek to provide answers to this dilemma although we will identify strategies for dealing with it, which will invariably broaden the context.

We begin by exploring the traditional role of validation in modelling, in confronting models with data, and in replicating the traditional role of experiment in a social context. We will then discuss the problem of system definition—of bounding the system from its wider environment in time and space. This problem has been relaxed in various ways as we have learnt more about models and modelling and this has translated itself into ideas about simulation. Simulation differs from modelling in that simulations are dynamic and open-ended. We will chart this road to simulation which contains the essence of what Epstein [5] calls 'generative modelling', and we will discuss how this style of modelling has come to replace more traditional parsimonious approaches. We then broaden the context, examining the role of the model, the modelled, and the model user. It is in this context that changes in the emphasis given to the role of validation of a traditional kind can be legitimised. Finally we conclude by calling for this debate to become central to simulation and to the decisions used in constructing, testing, and using any kind of social systems model.

2. Traditional conceptions of theorising and modelling

The conventional process of model-building involves generating and testing theory through a cycle of induction and deduction. In this we follow Popper [15] who argues that science proceeds through a process of conjecture, thence refutation which is accomplished through a mixed process of induction and deduction. Models are theorised as hypotheses — inductively with respect to data or prior ideas — and are then tested and refined through confronting their predictions with new data both deductively and inductively. The process is confounded. Theories may come out of the blue insofar as they are the product of insights but they can usually be traced to assembling data, deriving relations, constructing hypotheses, testing these on new data, falsifying them, maybe refining or modifying them to make them more or less bolder, as the data and context suggests. In essence, the process is one in which testing and validation involves both theory and data with no privilege given to one or the other.

There are two rules which have been taken as central to the process of developing good models. The first is the rule of parsimony — Occam's razor — which suggests that a better model is one which can explain the same phenomena with a lesser number of intellectual constructs. This is often translated as lesser data or only as much data as is needed, and it is in this sense that theories and models simplify the real world. The second principle relates to independence in verification. A theory which is induced using one set of data needs to be validated against another independent set. In short, if a model is driven by data from one situation, being fine tuned or calibrated to that situation, the only valid test of the model is to then apply it to another situation independent of the first. As we shall see, parsimony and independence in validation are criteria that are rarely fulfilled in traditional modelling. In general, the essential difference between traditional systems and complex systems models is one where it is possible, in principle, to meet the criteria of parsimony and independence for the first set but not for the second.

We will illustrate the principle of parsimony first for its serves to show how data and model structure determine verification. The simplest model is one in which an dependent variable y measured over some range of values is explained in terms of some independent variable x measured over the same range. Often more than a single independent variable $x_1, x_2, \dots, x_n$ is used to explain variation in a single variable y with the implication that each independent variable accounts for some independent component of the variation in y. It could be argued that the more independent variables used in this way, the less parsimonious the model becomes and there is a natural tendency to think of these less parsimonious models as being over-determined. The simple graphical illustration in Fig. 1 makes the point when we compare (a) with (b). If we were to try to explain more dependent variables $y_1, y_2, \dots, y_m$ with less independent ones as we show in diagram (c), then there is a clear problem in that there can be no unique solution. Sometimes it is convenient to think of this kind of problem in terms of balanced equations which to be solvable, simultaneously say, must imply as many unknowns as knowns, as many dependent as independent variables. In fact, econometric models which replicate systems of equations sometimes partitioned into exogenous and endogenous variables invariably invoke such conditions of balance or simultaneity in effecting robust solutions. This is illustrated in model structure (d).

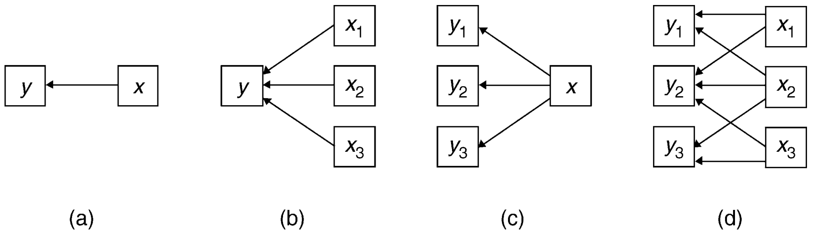

Fig. 1. Model structures linking dependent to independent variables.

All the model structures illustrated above imply some process of linking independent to dependent variables. This process in models which are statistically robust, is usually simple: it is additive, as in a linear model, or at best non-linear but in a tractable, mathematical way. Complications begin to arise when the processes involve rule-based systems which in practice cannot be reduced to tractable mathematical operations. Each of these model structures may best be thought of as one in which distinct processes determine the outcomes or predictions. For example, in Fig. 1(a), there is one and only one process determining *y*. In Fig. 1(b), there are three processes determining one output. In Fig. 1(c), there are three processes determining three outputs but the concern is that these three processes are determined as variants of only a single input. In Fig. 1(d), seven processes determine three outputs but these seven processes are determined by three inputs and thus the system is in a sense balanced. Strictly where there are more dependent than independent variables, then the processes involved must be further specified with independent data so that there is as much information to determine the outputs as there is input to the model.

Most models of urban development that were constructed for policy purposes from the 1960s on paid some homage to these principles. The best examples were those which mirrored model structures popularised in linear econometrics, the EMPIRIC model for Boston being the example par excellence [12]. The models built in the spatial interaction tradition (see Wilson [19]) also tended to meet these conditions, with distance playing a key determining role in predicting trip distributions, and enough independent data on location and trip distribution being assembled to provide robust calibrations. There is a sense in these models that you are not getting ‘something for nothing’, although they still suffer enormously from limits posed by the way the systems to which they have been applied were articulated and the inadequacies of theories that were assumed to be at work. Perhaps the clearest model which broke from this tradition and which illustrated distinctly the problems posed by the current generation of models based on complexity was Forrester’s [6] *Urban Dynamics* model. Apart from the fact that the model entirely defined away spatial variation by treating a hypothetical inner city disconnected from its wider environment, the model was not calibrated to data in any way. The model hypothesised countless dynamic relations involving the stocks and flows determining employment and residential activity volumes in the city which were culled from casual knowledge and observation. What validation there was involved superficial observations that the simulation appeared consistent with the characteristic features of US inner city areas at the time. More controversial were the longer term dynamics of the model which mirrored logistic growth and a vicious spiral of decline from which the city could not break free. It might be, as was argued at the time, that the purpose of this model was to raise the level of debate about the inner city, and not to provide an operational simulation. It was to foster discussion about possible policy issues. This is an argument we will return to as it is usually used to legitimate complex systems models which cannot be validated in the traditional sense. It is worth noting that Forrester's model, as one exemplar for the broader set of 'systems dynamics' techniques in management which Forrester himself developed, was one of the first to polarise the debate.

The second principle of good model-building involves testing the model in such a way that it can be validated in a context that is independent of that for which it has been initially developed. This is no more or less than the simple requirement in laboratory science that setting up an experiment, then validating the theory once is not a sufficient test; so much fine-tuning goes into setting up the experiment, that it is necessary to see how this transfers — generalises — to other situations. In terms of urban models, this is a strong requirement; it implies that the first true test of a model is not on the place where it is first developed and fine-tuned but in a second or subsequent place where it performs equally well or badly. Such dual applications have rarely been the case for reasons of happenstance rather than poor scientific practice. What usually happens is that some model structure is successively refined on different places and at different times, and in this way a little confidence is built up in the model's validity. The problem is often that the model is sufficiently different in each time and place to limit its generality. A formal study of different cross-sectional land use–transport models in the Lowry vintage which was designed to test the same model variants on different places was mired in data and computer software incompatibilities between these different places. Despite the heroic sentiments on which this project was established, the analysis was inconclusive [18].

There is, however, a rather special case where data-rich models containing homogeneous undifferentiated processes linking inputs to outputs do meet this requirement of independence. In situations where the observations are very extensive and homogenous, and where the system can be partitioned into distinct sets or regions without doing gross violence to its structure, then it is possible to develop the model on a sample of the data and validate it on the remaining full data set. This is a little like fitting a model to one part of a city and then validating it on the rest. Invariably this is not possible in cities for they are 'too complex'. Spatial variation is such that one would not expect a model of, say, the inner city to apply in quite the same way to a model of the suburbs. Nevertheless, where data sets are extensive and where the relations between inputs and outputs are assumed to be ubiquitous, then model fitting on a sample of the data followed by validation on the full set, less the sample, is quite widely practised. The best examples involve extracting pattern as in remote sensing data or in fitting neural nets to large data sets where the assumption is that everything influences everything else. However, although this is not usually possible for urban models, it is still possible to build structures which meet the conditions of parsimony and data balance and to validate these types of models in two places rather than one, which the principle of independence suggests. Such tight conditions require the model to be developed in more than one place by the same modeller working under the same conditions. Again for practical reasons, this is rarely possible.

So far, we have characterised models as being structures in which inputs are related to outputs in a simple causal manner; that is, where the relations between inputs and outputs are not usually the focus of inquiry, with assumptions being made that the way these relations are represented is robust. In the models sketched in the diagrams above, the focus is not on the nature of these relations but on whether or not the outputs are logically related to the input data. If they are not, then the usual strategy is to change the inputs, not the nature of the relations. In so far as the relations embody structure, these are determined from prior theory according to what seems to make sense. It is a straightforward matter to illustrate how these relations become ever more complex by simply adding intermediate outputs and stringing the relations together in the kind of chain that is illustrated in Fig. 2 below:

Successive relations convolute the original data series in such a way that there is little doubt that the causal processes invoked must be subject to detailed assessment and validation if the structure is to be meaningful. In fact, this strategy is often used in pragmatic model-building where the emphasis is on simply extracting some pattern in the initial data series x_1, x_2, x_3. Neural nets are of this nature but it is unlikely that they have any real meaning for the kinds of models that are now considered to be appropriate frameworks for understanding complex systems.

As we have implied, one focus of complexity theory is on ways in which processes generate patterns. In terms of the structure illustrated above, a typical model in the urban domain might be illustrated as follows. Imagine that each independent variable involves an attribute or attributes of some location — represented by a cell or spatial agent. This cell has some state which might be land use. The process of changing land use, which is the dynamic that the model needs to capture, might thus be construed as following a number of stages, as for example, through the process of land conversion. It will depend of course on other locations or cells in the system and land might go through several processes of change before it becomes fully developed: it might be purchased, assembled, remain idle, be used for temporary facilities and so on. The causal chain above might represent this process. In principle, each of its elements should be explicit and capable of being validated with observed data. In practice, this is rarely if ever the case. The data set would be too large, it would be impossible to collect in its entirety, it may even be impossible to observe and measure. Yet the processes are known to be important. Other criteria must thus be used. If the model is broadened and the input elements are no longer confined simply to cells but become heterogeneous with respect to type — x_1 might be cells, x_2 agents, x_3 institutional constraints and so on, then the processes implied by the chain are even more

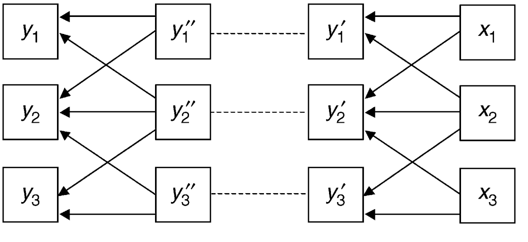

Fig. 2. A model structure incorporating multiple processes.

complex; the system diagram above simply shows what might be related to what without any implication that there is a standard way of fitting dependent variables to the independent. Add to this sets of parameters, themselves unknown in strength and value, then the problem begins to explode and very soon there is no way that all elements of the model can validated. This is even before any consideration that the model structure contains processes that generate unknown or emergent objects or patterns. In such cases, it is impossible to sweep across the parameter space in an effort to calibrate the structure, even though this time-honoured method is the usual strategy for confronting the model with data.

In the face of these difficulties, the model-builder often resorts to what we will call here the ‘Forrester strategy’ — not testing the implied causal structure at all, but relying on a simple correspondence between inputs and outputs, and also working up the model from discussions with politicians and decision-makers who do not evaluate their system of interest in the reflective, somewhat detached manner of science. We do not mean to denigrate this strategy because it is often useful and in certain circumstances inevitable. Forrester [6] himself, in developing his model, said: "I approached these discussions knowing the conceptual nature of the structure being sought, but not the specific details of the structure or the institutional components and behaviour to be fitted into it. The others brought the knowledge of the pressures, motivations, relationships, reactions, and historical incidents needed to shape the theory…" (p. ix). And he continued by saying: "Actually the book comes from a different body of knowledge, from the insights of those who know the urban scene first hand…" (p. x).

Moreover in very complex systems, the notion of seeing if a model produces plausible patterns which look right in a superficial way has been lauded as a much more appropriate way than the mindless statistical testing that has taken place with many modelling ventures in the past. It was Mandelbrot [13: 21] who said in the context of fractal geometry: "… to see is to believe …". The critical issue in complex systems models is that this is not the only strategy. There are many qualitative tests that are possible with respect to how plausible structures are which generate believable predictions, and these should be mapped out. In fact, there has been hardly any work whatsoever on strategies for validating models which deal with intrinsically complex systems, and one purpose of this paper is to raise awareness and encourage debate in this domain.

To summarise before we begin to sketch out the key elements of intrinsically complex systems and their models, it is clear that the difference between traditional models and the new generation that we are appealing to here is one which relates to how causal structures are treated. In traditional urban models, the focus is on simple causes. Insofar as these are convoluted, it is through making the system extensive, through repeating these simple causes over many categories but not by elaborating the causal chains that link inputs to outputs. The most extreme variants of this style simply assume that the causal structure is a homogeneous nexus of additive factors as in multiple regression or in neural nets. The emphasis is largely on validating these kinds of models using data which drives these simple causes. In contrast, complex systems models have multiple causes which display a heterogeneity of processes that are impossible to observe in their entirety. The focus is on more qualitative evaluation of a model’s plausibility in ways that relate to prior analysis of the model’s structure. In both styles of model, the wider context is important in validating the model too. What the model is to be used for—its purpose—is all important, particularly so where a degree of belief in its predictions may have to be suspended because of its complexity. Criteria for developing such models are not well-worked out and in urban systems theory this has become an important challenge.

3. The problem of closure

A key concept in general system theory involves the notion of the system and its environment. Systems are usually defined as existing in a wider environment with the system containing all the quantities and qualities of direct interest but with a recognition that for the system to function, it must import and export energy into and from its wider environment. Good system design assumes that the interactions within the system are much denser in strength and connectivity than those between the system or its environment and in this way, a system is assumed to be relatively independent of its environment. In short, although it may not be possible for a system to function without considering the relations to its environment, the central focus of interest is on the interactions within the system. Whether or not such criteria can be applied to the systems of interest here is a moot question. Much work has assumed that systems can be defined in this way but there is plenty of anecdotal evidence that suggests that only the most trivial systems strictly meet these requirements. Indeed some of the most powerful critiques of contemporary urban modelling have been based on the artificiality of closure. Again the example par excellence is the Forrester [6] model of the inner city, which entirely ignored the dependence of the inner on the outer city and vice versa, through obvious links such as the journey to work and industrial dependence.

Complexity theory relaxes this criterion somewhat. In particular, the focus is on systems that scale—from the local to the global. Cities and economies are structured in this fashion as all studies of world cities in the modern economy demonstrate. One of the most intriguing features of complex systems is their ability to simulate the way local action generates some global order, and this in itself is often taken as the very definition of complexity. The ability of systems to handle local action that generates global pattern implies emergence in that there is nothing in the local actions that implies the global pattern. Usually it is the interactions that take place locally that generate the higher order pattern, and it follows that for such systems to be simulated, this kind of link cannot be broken through artificial closure. The archetypal example of local action leading to global order is in the phenomenon of segregation in residential neighbourhoods due originally to Schelling [16], in which a mild preference for living adjacent to one's own group leads to very strict homogeneous spatial segregation. In such cases, it is clearly impossible to simulate neighbourhood dynamics without recourse to the entire city as the effect would not be captured without considering all neighbourhoods.

In a wider context, it is hard to know how to simulate the development of the financial core in a world city, for example, without some dynamics of the more global economy of cities being present within the model, and it is easy to see how this argument might ultimately imply that all cities everywhere need to be modelled simultaneously for the essential features of interest to be captured. This problem also appears to have become more intense as cities have become more interconnected through the development of technologies that aid interaction. Moreover, the very notion of a system of interest being one that is a cluster within a wider system is questionable. Systems function because of local and global connectivity as, for example, in social networks which are held together by weak ties, rather than strong clusters. In short, the idea of partitioning a system and fixing a level of inquiry at a particular layer in the hierarchy of connections can be problematic. Recent research into the phenomena of 'small worlds' is revealing, where the very notion of a 'small world' implies such local-global linkage [17].

Closure is a generic issue in defining systems although we can distinguish between temporal and spatial ways of separating the system from its wider environment. In terms of modelling time, many systems have been closed entirely. Time is defined away and the system studied as though it were in equilibrium. In most systems, equilibrium is an assumption based on convenience. For living systems, there can be no intrinsic equilibrium although there may be steady-state activity in which the system renews itself in a balanced manner. For a time in the middle of the 20th century, it did seem as though cities and economies were in some sense stable but with the passing of the industrial era, it is all too clear that the structure of any city cannot be explained at a single point in time. Equilibrium is a concept that is also inconsistent with interactions between the local and the global. Systems become ever more volatile as we disaggregate to basic units, or rather, systems become ever more homogeneous as we scale them up by averaging activities. In one sense, what is to be explained is how this scaling and averaging takes place—how cities appear stable and equilibrium-like at higher spatial and temporal scales than at the finer scale. Moreover if we separate their dynamics into coarse and finer spatial scales, then we would miss the fact that policies designed for one scale often have an impact at a different scale; in dealing with one level of the hierarchy only, true consequences are missed.

In fact, if the focus is broadened a little, cities must be seen as being far-from-equilibrium in that their order is a consequence of continual change. What this implies is that the dynamics of cities is unlikely to be very smooth. Although volatile bubbling change at the low level gets averaged out as we aggregate, this does not appear to lead to radical changes in the trajectories of systems such as those formed through phase transitions and similar discontinuities. Much of course depends on how the system is articulated but the message of complexity theory is that to understand significant urban change, then the system must not be closed in such a way that its dynamics are reduced to only one variety when several different varieties are clearly present. This is not simply an issue of spatial closure for it also relates to the time interval over which the dynamics are captured. Averaging time intervals also reduces variation but an equally significant issue involves the position at which the dynamics are first recorded. Inevitably there has to be some temporal closure in that the system must be started at some point in time. This is equivalent to choosing initial conditions and if these are selected in such as way as to destroy critical processes, then the entire dynamics can be confounded.

In urban systems, closure with respect to the range of activities, land uses, agents, or objects which represent the focus of inquiry, is similarly problematic. However, it is when classes or attributes interact with dynamic and/or spatial patterns that significant concerns arise. For example, by aggregating two or more activities together, critical dynamics might be collapsed or spatial variation cancelled out. In one sense, this kind of issue is related to scaling which in turn relates to how different levels of hierarchy relate to one another. Effects that occur similarly between levels, which can sometimes act as the basis for partition but in a different vein, might require explicit representation, thus mitigating against any partition. We could continue our discussion of system closure almost indefinitely but the key point that we have made several times is that complex systems are difficult to close from external influences. Indeed the very definition of complexity presupposes that systems have infinite extent and variety and that their unique and novel behaviour comes from the interaction of diverse effects that must somehow be accounted for within the system definition and representation. This implies a contradiction: systems that cannot be bounded and separated from their wider environment must be inherently unpredictable.

4. The road to simulation: artificial systems as virtual laboratories

Models are, by definition, a simplification of some reality which involves distilling the essence of that reality to some lesser representation. Such simplification is usually for some purpose although in science that purpose may be entirely justified in terms of satisfying our intellectual curiosity. Usually it is more than this although intellectual inquiry is generally a prerequisite. Nevertheless, any model will always contain more assumptions about the reality than are testable in that the very act of defining the system of interest involves contextual assumptions that remain implicit, hence not testable without a radical change in perspective. The difference between complex systems models and those that appeal to the principles of strict parsimony—those that we have been referring to here as traditional models—is one that revolves around the explicitness of assumptions. In essence, traditional models are those in which all relations defining the model are testable while complex systems models have chains of relations that are explicit but untestable in principle and/or untestable because data and observations of their processes are not available.

We appreciate that some might argue with our suggestion that complex systems models are not usually parsimonious. There are clearly examples of models of complex systems, such as the Schelling [16] models of spatial segregation, which articulate local action that leads to global pattern in the simplest terms. However, even in that case, although the model is simple in its rules, observations of how individuals exercise their preferences to segregate are rarely available and the data to test such models is never complete. A clearer way of signifying the difference between traditional and complex models involves the way they are parameterised. Traditional models are those in which all processes linking their inputs to their outputs can be fine tuned by parameters that enable their outputs to be matched to data. In contrast, although all the processes within a complex system model might be capable of parameterisation, many of these are not parameterised; there is no intention of fine tuning these values to match observations for such observations are not likely to be available.

A good example of the difference between these two types of model can be elaborated through traffic models of pedestrian movement. A spatial interaction model based on principles of gravitation would assume that travel densities would vary according to some function of travel time or distance or cost between any origin and destination. That function could be parameterised in such a way that the predicted traffic densities would be matched against observed volumes. If the functional form is varied within the overall bounds of the problem, finding the best fit of some relevant function to data is usually possible. However, if the model were conceived of as one in which the actual paths of the pedestrians according to the local geometry of the system were to be modelled—and it might be assumed that for a good prediction of the traffic densities of pedestrians the local geometry is important—then various processes relating pedestrians to local geometries through their cognitive and visual abilities could then be linked to more aggregate origin and destination behaviour. The number of degrees of freedom of the problem thus explodes enormously in that various algorithms for obstacle avoidance and congestion would have to feature. Usually only very general data is available for such obstacle avoidance and it is unlikely, in this latter case, that the model could be fitted to data in its entirety. Moreover the number of different but equally plausible causal structures enabling the agents to proceed through the local environment make testing all model types against data quite impossible.

To summarise, in traditional models we can divide the set of assumptions into those that are explicit, hence testable, and those that are implicit. The parsimony of these models resides in the fact that all the explicit assumptions must be testable. In complex systems models, explicit assumptions can be divided into those that are testable and those that are not. This immediately presents a dilemma in that these two sets of assumptions often interfere with one another, and it is usually impossible to test one set and not the other. In short, the fact that such models can only be tested partially means that they cannot be validated at all, and even though it is possible to associate some data to some subset of these models' outputs, this is rarely done as such a test is seen as arbitrary. Complex systems models are, however, constructed in the full knowledge of these difficulties. Difficulties arise, however, when their assumptions are not laid bare and remain hidden. Such models are usually justified on the following premise: that the processes that underpin them are too important to leave out and that it is preferable to include such processes even though it is not possible to validate them against data. The trouble with this view is that it is difficult to justify and its rationale usually depends on intuition. Moreover, the choice of whether to develop a complex systems approach or its simpler antecedent often depends on wider issues involving the purpose of the model, the policy-user context in which it resides, and sometimes the 'cultural' context in which we find ourselves which affects the degree of acceptance of the problems involved.

Although there is no one-to-one correspondence between complex systems and simulation models, we will loosely refer to the methods of complex systems models as simulation. Simulation usually implies some form of computational process which in urban systems is often mapped onto a temporal dynamics in some explicit way. Simulation in time involves recursion if only because the same model structures are repeated through time (with one set of outputs becoming the next time period's inputs). Such models often generate more than one outcome. Indeed the possibilities for generating an entire range of scenarios always exists in time for slight changes from time period to time period might be amplified or dampened or both. Moreover, different model structures might converge on the same type of prediction, implying some kind of equifinality that is yet another hallmark of complexity. In talking of simulation, however, we must digress slightly and note that microsimulation models of the kind developed originally by Orcutt et al. [14], and in an urban context by the Leeds group [4] are not really in the tradition of complexity theory. These are in the spirit of traditional models where simulation refers to the sampling of events from known distributions and thence scaling up to entire populations for predictive purposes.

Prediction involves generating unknown events and in traditional models, such events usually pertain to the future. The ability to calibrate the model by fine-tuning the parameter values in such a way as to replicate a known—present or past—situation provides some confidence in using the model to predict the future. If the model is replicated in a different but known situation and performs well in that it survives such a test, there is even greater confidence in its ability to predict the future. Traditional models thus get the present right and are then used to predict the future. In contrast, complex systems models can never predict the present definitively and thus the focus changes on exploring a variety of presents—where the actual present and its variants are just different versions of some unknown future. Simulation enables such models to generate different outcomes, which under some circumstances might appear to be different futures but really define a space of different model outcomes. The way this space is generated is not simply through systematic variations in parameter values, which is the time-honoured method of model calibration in the case of traditional models, but through varying the model structures within some limits, that is usually varying the rules that encode different processes into the model, thus simulating different experiments within a kind of 'virtual laboratory'.

This notion of exploring the space of all model outcomes and all model types is central to the simulation of complex systems in that it has become the main way of model testing. This is hardly model validation although it could be regarded as a way to check plausibility and to test the robustness of model structures to changes in causal structures. This space of model structures might be likened to a phase space which defines various model outcomes in terms of model variables. In calibration, the phase space is defined by dimensions associated with the model's parameters and their range of values. In complex systems modelling, the phase space is more qualitative in form, consisting of some mapping of different causal structures onto various dimensions and then some measurement of the model's outcomes under these different structures. Sometimes the various rule sets which mirror these causal structures are parameterised so that the model can be evaluated quantitatively in terms of its performance against standard measures. This is a little like setting up different experiments within the virtual laboratory where not only the variables defining the experiments are varied but the experimental apparatus is modified from experiment to experiment. In a sense, what constitutes the phase space depends upon how rich the model is. In parsimonious, traditional models such as the spatial interaction type we noted before, it is the space defined by the parameters and their values (associated with distance functions); in complex systems models, it might consist of several different spaces relating to different rules and structures, in a wider hierarchy of types. This broadens the problem as it is possible to produce different types and levels of assumption which are capable of being varied although are not capable of being parameterised. In fact, it is even possible to begin to change the very object of study and its representation in this way although in practice such experiments and explorations have rarely been developed.

There are many examples we can review which illustrate these points and we will examine some of these in more detail in the next sections. Suffice it to say that the most instructive in the urban domain are those which allude to complexity and the generation of emergence such as those based around ideas of cellular automata (CA). For example, CA models are organised around processes of change in local neighbourhoods where action-at-a-distance is espoused. Physical change in cities clearly depends on some local function as is the case of the growth of any structure which must remain connected for its very existence, but it is also clear that activities and people do not only locate according to local actions restricted to a limited neighbourhood space. The rule sets which are used to condition development are also rich and the prospect for testing such models directly is problematic. For example, there are many neighbourhood configurations and many rules sets and the space which is set up by this range of possibilities is enormous. It is not possible to chart such a space and strategies for doing so are quite limited. This problem is best seen in the basic theory of cellular automata as promulgated by Wolfram [20]. Although Wolfram [20] is able to exhaustively illustrate the possible system outcomes for systems such as the two state (a cell is on or off, developed or not developed), three cell regular neighbourhood in one-dimensional form where the all possible rules for switching the cells on or off are enumerated, this breaks down for nine cell neighbourhoods in two dimensions and all higher orders. Even with these limited possibilities, a bewildering range of behaviour is possible and one is forced to conclude that most models that we are working with are arbitrary in this respect, based on a loose consensus of what seems plausible but not on any definitive evaluation of the appropriateness of model structures. Until we are able to move beyond this, then all complex systems models will remain contestable and inconclusive.

Finally it is worth noting that Epstein [5], amongst others, has argued that complex systems modelling is generative by definition, more a strategy for generating possible model structures and showing their consequences than a technique for developing fully-fledged definitive models with strong predictive capability. It is arguable in any case whether strong predictive capability is what is required in social systems (because it is probably not attainable) but generative modelling can be equally problematic. In essence, exploring different model types in the absence of data might be useful if equally, but very different, plausible structures are possible, but this is not likely. More likely is the case where there is some agreement about the main elements that can condition or determine some sequence of events but where the operation of these elements is unknown and where different sequences of these can generate very different consequences. In these situations, there is really no alternative but better data and observations so that it is possible to discriminate between these model types. In turn, this pushes the argument back towards traditional modelling where calibration against unique data is the only option.

5. Modellers, the modelled, and users: purposes and roles

Our entire discussion so far has been without reference to any purpose for studying complex systems or for building appropriate models thereof. Purpose is clearly important, some would say central to what is done, for this conditions how we think about what is modelled and how the system of interest is to be modelled. In a sense, everything follows from this. But in principle, every kind of model can be used for every purpose. Whether this is so will depend on users, not on the models per se, although there is a tendency for certain types of models to be used for certain groups of users. We can structure models along many different continuums but one which is central to usage depends on the degree to which their predictions, whether or not they pertain to the past or the future, are believable. Many models may be useful even though their outputs might not be believable in that the way they point up and focus events and issues serves a much more important purpose than the generation of hard predictions. We will refer to this spectrum of believability as one which begins with discursive models whose predictions can only be treated in qualitative terms, through to models which generate hard numbers which are as believable as any model might be. There is a strong sense in which complex systems models are less believable than traditional models as we have implicitly argued in the preceding discussion and although such models were rarely used in policy contexts in the past, their use is changing. It is no longer possible to relegate complex systems models to non-policy contexts. In fact as our contemporary view of the usefulness of science has become more uncertain and confused, groups of users have emerged—enlightened one might argue—who are comfortable with engaging in policy discussions using qualitative forms of modelling, or models whose believability rests on their plausibility and not their ability to replicate known situations.

We need to unpack this spectrum in much more detail but it is usually only fruitful with particular applications in mind and these we will introduce briefly in the next section. A particularly useful way of defusing the role of modelling is to consider the process of use as one of 'story telling'. The extent to which the story told is believable of course is always at issue but no matter what the model says about the past or the future, it tells a story [9]. The story may not be very good, just as the model may not be good either but the notion that models provide just another way of examining a situation is a good starting point in any application. In fact, this is always the case anyway as the notion of learning about any problem involves different and contrasting viewpoints, some of which may be dismissed, others which will gain ground, and in this, quantitative systems model can have a central role to play. In short, there is always an educational role for modelling and if this role is construed as broadly as possible, then any model can, in principle, be used for any purpose. Pedagogy is important in all contexts, for in solving problems directly or indirectly, individually or in group discussion, models which polarise and focus on the key issues are essential. Most models are designed to do this through their role in simplification.

Perhaps the most obvious use of complex systems models which generate unexpected change is for learning, education, and in the broadest sense for entertainment. Models for these purposes do not have to meet strict requirements of validation, unless the purpose is to educate and learn about those specific types of models. More usually such models are designed to stress specific issues, to highlight and to focus, rather than to predict for purposes of problem solving and policy. In fact, models with emergent properties based on evolutionary principles such as those which have been developed in artificial intelligence and artificial life, are increasingly being adopted in game simulations, in web site design, and in digital transactions processing. These kinds of system are strongly influenced by the design of new methods for automated reasoning, rather than any concern for testing how such models might replicate the past or the present. However, it is now clear that the considerable effort which has already gone into the development of computer games at all levels from pure entertainment to formalised education, has already had a major impact on simulation. There is evidence that what is state-of-the-art game design today is often incorporated into the e-science of tomorrow. Computer graphics interfaces are a classic example but so is algorithm design and perhaps more importantly, the ability of game designers to think 'out of the box', reveals possibilities for scientific modelling that ordinarily would not be attempted in normal science [11].

In one sense, thinking about complexity in the way we have been sketching is so new in terms of a science of cities, that it is not surprising that the traditional norms of theory development and hypothesis testing have been relegated to the background. For example, most urban models based on analogies to cellular automata have been more concerned with simply getting such models constructed and demonstrating that a rich dynamics can be generated, rather than with any strict methods for their validation. This was perhaps the case 30 years or more ago with Forrester's [6] *Urban Dynamics* model which was one of the first attempts to demonstrate the kind of digital richness that was possible with modern computer systems. Although we clearly need much more explicit principles for complex systems model development which broach directly the question of validation from all perspectives, there is a parallel problem which has become significant. The systems of interest—in our case cities—have themselves changed during this period when digital science has become possible. The traditional attempts to classify and describe cities in coherent terms, which have dominated urban science for the last 100 years or more, have increasingly come under scrutiny. The very systems that we have been concerned with have become more complex as much through the development of digital technologies as through changing life styles and economic conditions of the urban population. In other words, there is now a strong debate about how we should classify cities—how we should describe them—that takes us back to an earlier stage of science. The difficulties in validating complex systems models may be as much to do with the fact that the categories and classes, the objects and elements that we consider significant, have also changed. These new models are as much for engendering the debate about classification as for developing new robust theory which can be validated in the traditional way.

Let it be clear that in this paper, we are not arguing at all that complex systems models should be abandoned and that we should return to more traditional strategies of developing parsimonious models. Nor are we arguing that parsimony is not relevant to complex systems models for some of the best models are parsimonious in a way that illustrates the principles of emergence and surprise. What we are calling for is a new strategy for dealing with these models. We need to be explicit about the purpose for modelling and we need to consider the extent to which a complex systems model contains hypotheses that should be validated numerically against observable data. We need to be clear about the line between explicit and implicit assumptions, about the role of prediction and exploration. In fact, a tentative suggestion would be that all models—traditional or complex—should mix calibration with exploration. In the last analysis, it is hard to see the value of a model that does not touch reality at some point in which that reality can be replicated 'unambiguously'. In this way, we consider exploration of model structures as well as more detailed methods for calibration to be essential in any process of model validation. It is in those models—and there are currently many of them—where such validation is not invoked whatsoever except perhaps at the most casual level, that we feel that a much more explicit process of modelling should be invoked. We also feel that all modelling should be paralleled with extensive debate, with the construction of alternative models—through counter modelling as in the debate over national economic futures in some western countries—and with alternative conceptions of data and observations. Where these ambiguities remain, there should be extensive questioning of model structures and purposes.

A contrasting focus for urban modelling is policy-making. Traditional models were largely built from the middle of the last century with urban problems and policy responses in mind. It is worth noting that this genre of models were often called ‘operational’ models in contrast to theoretical models, although in urban studies there was a strong correspondence between operationality and theory; operational modellers invariably invoked the macro theory of the city that had been crudely fashioned in urban geography and economics during the previous half century. In short, the notion that models for policy-making must replicate the past, in some measure, was widely assumed. The idea that systems theory and analysis which appeared so useful for military and logistical problems at that time could be used for solving social problems also reinforced this assumption. At the same time, this suggested that a good model for policy-making would be one in which that same model could be used for managing and controlling the city through some optimisation of its structure. The concept of a system and its control was thus central to this consensus.

Furthermore, the idea that the systems of interest were stable in some way was also essential to this quest. The concept that static models could be developed which replicated the situation at a point in time—an equilibrium—and that these models could be used to predict a future point in time which in turn would also be an equilibrium, was basic to this philosophy. This, as we have seen, has become untenable, leading to an unravelling of the basic idea that we are dealing with systems that are a simple enough to describe and predict in this way. There has been a loss of faith in this style of modelling, although the view still persists that, for models to be operationally useful, they should replicate the past and the present in a sufficiently robust way to give confidence in their use for prediction. Models which cannot be validated are thus no different from qualitative reasoning, from intuition, or even dictat which were the usual schemes used to develop policy prior to the computer era.

There is a sense in some policy-making that models which cannot predict the present and are unlikely to be able to predict any kind of future might still be useful. This forces the argument back to education and learning, to ‘modelling as story telling’, and to the use of models to engender and structure discussion and debate. There is a limit to how far this perspective can be justified. Much depends upon the specifics of the situation where such models are found useful, on the nature of the problem and the relative values and disposition of the users and decision-makers. In these cases, then the use of models to generate ‘what if?’ scenarios is the main basis for application where such scenarios define bounds to the solution space within which possibilities for the future might be discussed and debated.

Before we conclude, we should note two related issues. First models are increasingly being used to communicate other kinds of idea/as vehicles on which other less controversial issues might be conveyed. The use of models to help in visualisation is a classic example where visualisation often requires a more specific focus which only predictions from models can enable. Scenario building is the classic case in point, as are all kinds of urban design which require visualisation. Our second digression is no less significant. The lines between the modeller, the modelled, and the user are increasingly blurred. This is a question of cognition in that the kinds of actions and interactions which form the substance of the new generation of complex systems models mirror processes of decision which in turn are those that are employed by model users in policy-making. This is no more or less than the idea that the user is part of the system to be modelled and is often no different in behaviour from the rest of the system that is being modelled. In less charitable terms, complex problems have been described as those in which the solution is part of the problem—the plan or planner is part of the problem—and this is an issue that is taxing us in how we might represent decision processes in the city whilst using those same models to engage in similar decision-making.

6. The limits to prediction

As we have explained, the time-honoured principle used in testing theory against data involves specifying causal structures or chains in which independent variables are used to explain an equivalent number of dependent variables. This occurs in such a way that the predictions are useful and interesting, thus adding to our knowledge of how the world works. This is the principle of parsimony, or requisite variety. Invariably theories contain more than can be tested in that there are basic, often implicit, assumptions which might be testable against data but are not, while many theories imply relationships which cannot be tested against data for observational reasons or simply for lack of data. Such theories may well be plausible but they cannot be regarded as parsimonious in the sense we have portrayed here. However, there remains a basic problem with theories and models that meet our criterion of parsimony. We may well be able to rigorously test a theory by setting up a model which can be uniquely calibrated, hence testable against data but the causal explanation implied by the theory may not be unique in itself. For example, by changing the independent data driving the explanation, we may be able to build equally good models which predict the same outputs but we are still left with choosing between one model and the other. One might argue that if there are equally good reasons for choosing either set of independent data, then we are still unable to choose. One can push the argument back and say that if there are two or more different sets of independent data which explain the same phenomena equally well, then there must be correlation between these sets of data and thus they are not in and of themselves independent from one another. This, however, may not be the case or at least we may not be able to decide that it is.

A good example relates to city growth. It is often argued that cities grow around their central cores and that more wealthy income groups can afford to commute longer distances to work in these cores, thus exercising their preference for more space at the edge of the city. This is a crude paraphrasing of the way urban economic theory explains the organization of land use around the core of the industrial city. In short, land use organization is based on the trade-off between travel cost, rent, and space required which are a function of income. However, an equally good explanation of urban growth is that cities have grown outwards around their cores because this is the only way they could do and still function with their work at the centre. As technology has progressed during this period, densities of development get lower and the size of sites get larger as the city grows in that we can generally afford more. Higher income groups are thus forced to live in these more distant areas even if they do not want to due to the fact that there is no place else they can reside and consume the space even if they could afford it. Of course, one might argue that these two competing explanations might be merged in some way but it is entirely possible that each may explain actual development in the monocentric city to the same (numerically) high level.

Thus parsimonious models are not all that they might seem and there is a strong case for building models which contain plausible mechanisms even if we cannot test these mechanisms. The problem is that short of statistical or numerical criteria, good rules for choosing models based on a combination of discursive and reflective analysis as well as standard quantitative evidence are not well-developed. In the case of CA-like models, there are so many assumptions about the representation of space and the nature of the transition rules that are used to determine development that it is not possible to definitively use such a model to make predictions that we can act upon. In such instances, we are always forced back to the argument that such models are pedagogic, that they are demonstrations of what is possible, and in the last analysis, provide vehicles for discussion, for counter modelling, and for argumentative discourse. This may, of course, be said for all science and its application to human affairs.

There are two issues that we should draw together which further illustrate the limits to prediction posed by models of complex systems. The first is the issue of emergence which strongly relates to scale and space in urban systems in that models of local action can be demonstrated to give rise to global order. These we would submit are invariably pedagogic in that once understood, then the phenomena of global order explicable in terms of local action is no longer surprising or mysterious. What is more to the point is that models that can give rise to specific objects or places that emerge from local and other actions are still worth exploring. For example, models that generate growth poles where none existed before are important in that although we might know the generic reasons for such growth, the precise conditions for their emergence may not be known. Such models can be used to explore these conditions, again in a pedagogic way.

This leads to the second issue which limits our predictive powers. Most of the models that we are alluding to here contain mechanisms which involve choosing the drivers of growth using some sort of random processes. For example, choosing cells to be developed is often a process of determining the probability that they might be developed and then choosing actual allocations to these cells, based on these values using Monte Carlo methods. It is entirely possible to structure these types of model in a deterministic frame but most would agree that the certainty implied in this is problematic. If the usual course involving random simulation is adopted, then there is the problem of knowing what actual simulations mean when they can vary from run to run. The notion of taking some central limiting simulation is problematic too when decisions within these structures are invariably determined by applying discrete thresh-holding. There are important issues too in knowing how to deal with predictions that emanate from such models. One feature that we have not addressed here is that because all models are now digital and can be communicated across networks, it is possible to set up effective interfaces to their use in many different situations. Such digital dissemination is now possible and this we urgently need ways of illustrating how these models work so that we can assemble teams to improve such simulations and to learn about their limits in the widest possible domains. Where we are dealing with systems that are intrinsically uncertain and infinitely complex, then the only way forward is to learn the limits to such systems and in this way, to fashion our models to account for such limits.

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