

STATE-BASED RECONSTRUCTABILITY ANALYSIS

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ABSTRACT

Reconstructability analysis (RA) is a method for detecting and analyzing the structure of multivariate categorical data. While Jones and his colleagues extended the original variable-based formulation of RA to encompass models defined in terms of system states, their focus was the analysis and approximation of real-valued functions. In this paper, we separate two ideas that Jones had merged together: the “g to k” transformation and state-based modeling. We relate the idea of state-based modeling to established variable-based RA concepts and methods, including structure lattices, search strategies, metrics of model quality, and the statistical evaluation of model fit for analyses based on sample data. We also discuss the interpretation of state-based modeling results for both neutral and directed systems, and address the practical question of how state-based approaches can be used in conjunction with established variable-based methods.

I. INTRODUCTION

This focus of this paper is information-theoretic (probabilistic) state-based modeling of systems defined by categorical multivariate data. In this context, a “system” is what Klir terms a “behavior system” (Klir 1985) – a contingency table that assigns frequencies or probabilities to system states. In a “neutral” system, no distinction is made between “independent” variables (IVs) and “dependent” variables (DVs) or, equivalently, inputs and outputs. Such a distinction is made for “directed” systems, in which the IVs define the system state and the DVs depend upon this state. We consider both neutral and directed systems in this paper.

Restricting our scope to systems comprising only qualitative (categorical or ordinal) variables is not as limiting as it might seem since continuous (interval- or ratio-scale) variables can be made qualitative by discretizing (clustering, “binning”), although discretizing does sacrifice some of the information in the original values of the quantitative variable.

The concept of state-based modeling is central to Jones’ conception of “k-systems analysis” (Jones 1982; Jones 1985; Jones 1985; Jones 1986; Jones 1989). Jones, however, linked the state-based modeling idea to the concept of a “g to k” transformation. This transformation maps a real-valued function of the system state defined by the values of a collection of categorical or discretized variables (a “g-system”) into an isomorphic dimensionless function that has the properties of a probability distribution (the “k-system”). The k-system, which “has properties sufficiently parallel to a probabilistic system that RA (reconstructability analysis) can be invoked” (Jones 1985), is the starting point for Jones’s development of the state-based modeling approach. Since in this paper our starting point is a behavior system, we detach state-based modeling from the “g to k” transformation concept and demonstrate that state-based modeling applies to both neutral and directed systems, and for directed systems also to those which are stochastic. Thus Jones’ state-based modeling idea is an extension of the established variable-based RA framework (Klir 1985; Krippendorff 1986).

We define a model following Krippendorff: “A structural model consists of several components, each specified by a different parameter with respect to which it corresponds to the data to be modeled, and none is included or equivalent to another” (Krippendorff 1986). A structural model implies a joint probability distribution of the same dimensionality as the data. The model (“q” distribution) is constructed by maximizing its information-theoretic

33uncertainty (Shannon entropy) subject to the constraint that the explicit parameters in the model must match the corresponding values in the observed data ("p" distribution). There are many possible models of this sort for any given behavior system. The quality of a model can be assessed in terms of the degree to which the model accounts for the constraint in the data (fidelity) and the number of parameters (the degrees of freedom, df) required to specify the model (parsimony).

		B		
		b0	b1	
A	a0	0.120	0.090	0.210
	a1	0.070	0.720	0.790
		0.190	0.810	1.000

Figure 1. p(AB), a neutral behavior system

As an example, consider the very simple two-variable neutral behavior system shown in Figure 1, where the probabilities in the figure are derived from a contingency table with a sample size of N= 100. Three parameters are needed to specify **AB** since probabilities must sum to 1, hence $df(\mathbf{AB})=3$. The total constraint present in this system is the transmission

$$T = \sum p \cdot \log\left(\frac{p}{q}\right)$$

between the p distribution which is the **AB** data (Figure 1) and the q distribution of the **A:B** model that assumes that **A** and **B** are independent (Figure 2). In a "top-down" perspective (going down from **AB** to **A:B**), T is the constraint *lost* in the independence model relative to the data. In a "bottom up" perspective (going up from **A:B** to **AB**), T is the constraint *captured* in the data relative to the independence model. The two perspectives are equivalent, but have different emphases. Here, $T = 0.153$.

		B		
		b0	b1	
A	a0	0.040	0.170	0.210
	a1	0.150	0.640	0.790
		0.190	0.810	1.000

Figure 2. The q distribution of the A:B model

Only two parameters are needed to specify **A:B**, one from each margin; hence $df(\mathbf{A:B}) = 2$. The **A:B** model constrains the A and B marginal distributions to match those of the data, but is otherwise maximally uniform. As a result, $q(\mathbf{A:B})$ does not match $p(\mathbf{AB})$. T measures the difference between these distributions, and the statistical significance of T is assessed by Chi-square analysis. For the likelihood ratio Chi-square $L^2 = 2NT = 21.27$ and $\Delta df = 1$, and a significance level of $\alpha=0.05$,

an L^2 larger than 3.84 is required to reject the null hypothesis that the data **AB** and the independence model **A:B** are consistent with one another. In this example, clearly they are not. One cannot satisfactorily model the data with the independence model.

Within the framework of variable-based RA, there are no other models to consider. In the state-based perspective pioneered by Jones, however, there are many possible additional models. In the next section, we discuss the structure and specification of models for state-based RA. Then we assess how such models can address the competing objectives of fidelity and parsimony. Generally, we use the term "structure" to refer to a combination of parameters considered without reference to data, and the term "model" to refer to the actual parameter values of a structure when applied to specific data.

II. EXPLORING STATE-BASED STRUCTURES

In variable-based RA, parameters are values of complete marginal distributions (comprising one or more variables) that will, in the q distribution (the model), be constrained to match the corresponding marginal distributions derived from the p distribution (the data). In state-based RA, parameters do not specify *complete* marginal distributions (projections). Rather, they correspond to any linearly independent set of individual elements (cells) of the joint distribution or any of the marginal distributions. For the AB system shown in Figure 1, there are 8 candidate parameters: a0b0, a0b1, a1b0, a1b1, a0, a1, b0, and b1. The structure **a0b0:a1**, for example, constrains these elements in the joint distribution and the marginal A distribution to match their observed values.

Like variable-based RA structures, state-based structures can be categorized with respect to the degrees of freedom required for specification. For the AB system, as indicated above, there are 8 possible structures that utilize just a single df, one associated with each of the candidate parameters. There are 26 candidate structures that utilize two df, two less than the 28 possible two-parameter combinations ("8 choose 2"). Two combinations (a0:a1 and b0:b1) are excluded because they are degenerate in the sense that, since the marginal distributions must sum to unity, the second parameter adds no additional constraint. There are 36 candidate structures that utilize three df; 20 of the 56 possible three-parameter combinations are ruled out due to degeneracy. The non-degenerate

df	General Structure	Equivalence Class	Structures					70 structures total	
3	$\phi = \mathbf{AB}$	1	a0b0:a0b1:a1b0	a0b0:a0b1:a1b1	a0b0:a0b1:b0	a0b0:a0b1:b1	a0b0:a1b0:a1b1		
			a0b0:a1b0:a0	a0b0:a1b0:a1	a0b0:a1b1:a0	a0b0:a1b1:a1	a0b0:a1b1:b0		
			a0b0:a1b1:b1	a0b0:a0:b0	a0b0:a0:b1	a0b0:a1:b0	a0b0:a1:b1		
			a0b1:a1b0:a1b1	a0b1:a1b0:a0	a0b1:a1b0:a1	a0b1:a1b0:b0	a0b1:a1b0:b1		
			a0b1:a1b1:a0	a0b1:a1b1:a1	a0b1:a0:b0	a0b1:a0:b1	a0b1:a1:b0		
			a0b1:a1:b1	a1b0:a1b1:b0	a1b0:a1b1:b1	a1b0:a0:b0	a1b0:a0:b1		
			a1b0:a1:b0	a1b0:a1:b1	a1b1:a0:b0	a1b1:a0:b1	a1b1:a1:b0		
			a1b1:a1:b1						
							36 structures		
2	$\gamma = \mathbf{A:B}$	1	a0:b0	a0:b1	a1:b0	a1:b1			
			δ	2	a0b0:a0b1	a0b0:a0	a0b0:a1	a0b1:a0	a0b1:a1
			δ	3	a0b0:a1b0	a0b0:b0	a0b0:b1	a1b0:b0	a1b0:b1
			δ	4	a0b1:a1b1	a0b1:b0	a0b1:b1	a1b1:b0	a1b1:b1
			δ	5	a1b0:a1b1	a1b0:a0	a1b0:a1	a1b1:a0	a1b1:a1
			ϵ	6	a0b0:a1b1				
			ϵ	7	a0b1:a1b0				
						26 structures			
1	α	1	a0	a1					
			α	2	b0	b1			
			β	3	a0b0				
			β	4	a0b1				
			β	5	a1b0				
			β	6	a1b1				
						8 structures			

Table 1. Equivalence classes and general structures of state-based structures for the 2x2 AB system. The variable-based **A:B** independence model is shown in bold (equivalence class 1 for df=2, general structure γ). One could add to the bottom of this table the uniform distribution which has df=0.

structures are summarized in Table 1 which also indicates the four state-based models equivalent to the variable-based model **A:B**. Clearly in this case and in general there are very many more state-based than variable-based models.

For any particular df, structures can be further organized into *equivalence classes* where, for any given p distribution, all structures within the same equivalence class generate identical q distributions. Equivalence classes can in turn be grouped into *general structures*, which can be arrayed in a lattice; this is discussed below after the equivalence class idea has been explained.

For the **AB** system shown in Figure 1, there are 6 equivalence classes in the df=1 category, and 7 equivalence classes in the df=2 category (Table 1). One of these equivalence classes corresponds to the **A:B** variable-based structure. All 36 non-degenerate three-parameter structures belong to the same equivalence class, since any df=3 structure will generate a q distribution that matches perfectly the p distribution (the data).

Since marginal distributions are simply projections of the full joint distribution, any parameter of a state-based structure can be characterized as the sum of one or more elements

of the p distribution. Specifically, any state-based structure can be described by an (df+1) x n matrix, S, where n is the number of elements in the p distribution and (df+1) ≤ n. For a 2x2 (n=4) **AB** system such as Figure 1, the structure **a0b0:a1** (for which df+1=3) can be described by

$$S = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

where the columns of the matrix correspond to the elements of the p distribution: a0b0, a0b1, a1b0, and a1b1, respectively. The constraint imposed by a structure can then be summarized by the matrix equation

$$S \cdot q = S \cdot p \quad (1)$$

For any given p distribution, the right-hand side of this equation is a known constant vector with cardinality df+1. The last row in the S matrix is the same for all structures -- it enforces the constraint that the elements of the q distribution must sum to one. The last element of the right-hand side vector of Equation (1) is thus always one. For further discussion of this matrix formalism, see (Anderson 1966).

The structure matrix S can represent any state-based structure. In particular, if S is an $n \times n$ matrix and all rows of S other than the last row are drawn without duplication from the $n \times n$ identity matrix, then S will constrain the q distribution to match the p distribution exactly. (This is called the "saturated" model.) While it provides a framework for specifying state-based structures, the structure matrix representation is actually more general, since it allows arbitrary combinations of cells that may not correspond to elements of any marginal distribution.

The concept of structure degeneracy can also be formalized in terms of the structure matrix. If the rank of S is less than the number of rows in S , then the structure characterized by S is degenerate. The structure matrix also provides a mechanism for determining equivalence classes. A necessary condition for two state-based structures to be in the same equivalence class is that their structure matrices have the same rank. Given two state-based structures defined by the structure matrices S_1 and S_2 , both having rank r , we can determine if the structures are in the same equivalence class by forming a combined structure matrix S_{12} that includes all the rows from both S_1 and S_2 . If the rank of S_{12} also equals r , then the structures represented by S_1 and S_2 are in the same equivalence class.

Two or more equivalence classes which are identical under swaps of (a) variable names and/or (b) variable state names constitute a general structure. The general structures shown in Table 1 can be arrayed in the following lattice.

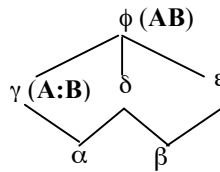


Figure 3. Lattice of general structures from Table 1. The uniform distribution (not shown) would be a child of both α and β .

III. EVALUATING STATE-BASED MODELS

A state-based model of a behavior system encompasses two related ideas: given a p distribution and a candidate structure S , the q distribution is constrained to satisfy (1), and otherwise relaxed so to maximize information-theoretic uncertainty. This can be achieved either through iterative proportional fitting or by using gradient-based optimization methods to maximize $H(q) = -\sum q \cdot \log q$ subject to the

constraint (1) and the requirement that all elements of the q distribution be greater than or equal to zero.

Because state-based structures exist that are less constrained than the variable-based independence structure $A:B$, this structure should not be taken as the bottom of the Lattice of Structures. Since it maximizes uncertainty for any specified degrees of freedom, the *uniform distribution* is a more appropriate bottom model. Returning to this example of Figure 1, and using the uniform distribution as a reference model for calculations of information, the variable-based $A:B$ independence model captures 78% of the information, I , in the data (Table 2), where $I(\text{model}) = (T(\text{uniform}) - T(\text{model})) / T(\text{uniform})$.

	T	%I	df	L ²	p
AB (data)	---	100%	3	---	1.000
A:B	0.153	78%	2	21.27	0.000
a1b1	0.010	99%	1	1.35	0.509
uniform	0.710	0%	0	98.50	0.000

Table 2. Summary results for variable- and state-based models

Although its specification requires fewer parameters, the $df=1$ state-based model **a1b1** does much *better* than the variable-based $df=2$ **A:B** with respect to information capture. The **a1b1** model generates the q distribution shown in Figure 4.

		B		
		b0	b1	
A	a0	0.093	0.093	0.187
	a1	0.093	0.720	0.813
		0.187	0.813	1.000

Figure 4. The q distribution implied by the state-based a1b1 model

As indicated in Table 2, the **a1b1** model captures 99% of the information in the data, relative to the uniform reference model. Furthermore, $L^2 = 1.35$ for this model, indicating no basis for rejecting the null hypothesis that the model is consistent with the data ($p = 0.509$). p is the probability of making an error by rejecting the null hypothesis that q is the same as p .

This example demonstrates that state-based models can, in principle, represent behavior systems more accurately and more parsimoniously than the best variable-based models. This example also illustrates some differences between our approach to state-based modeling and Jones' k -system analysis. The original system (Figure 1) is a neutral system, with no quantitative system function. The g -to- k

normalization of k-systems analysis cannot be applied to it, but the state-based idea *can* be applied. Also, the above analysis uses a top-down perspective that compares progressively simpler models to the data, while Jones' k-systems analysis is cast in a strictly bottom-up framework. Finally, and critically, the statistical significance of a model is here assessed; this is not done for (and not appropriate to) k-systems approximations of real-valued functions.

Of course, state-based analysis is also applicable to directed systems, in which one or more variables are designated as "dependent" in that their values depend on other (independent) variables. Consider, for example, the directed – and stochastic -- system of Figure 5 (N=1247), in which variables A and B are the independent variables and Z is the dependent variable. Note that this system is not deterministic (k-systems analysis is restricted to deterministic systems).

A	B	Z	p(ABZ)	p(Z AB)
a0	b0	z0	0.030	0.128
a0	b0	z1	0.203	0.872
a0	b1	z0	0.156	0.816
a0	b1	z1	0.035	0.184
a1	b0	z0	0.205	0.480
a1	b0	z1	0.222	0.520
a1	b1	z0	0.037	0.249
a1	b1	z1	0.111	0.751
			1.000	

Figure 5. p(ABZ), a directed behavior system

For such systems, both variable- and state-based RA have natural interpretations in terms of the conditional probability distribution for the dependent variable, Z. At one extreme, the saturated model **ABZ** (the data) allows a different Z distribution for each of the four system states defined by A and B. Since we are interested only in the relationship between Z and the independent variables A and B, and not in any relationship among the independent variables, the appropriate bottom reference model is not the uniform distribution but the independence model, **AB:Z**, which asserts that the independent variables provide no information at all about Z. For this model, a single marginal Z distribution is assumed for all the system states defined by A and B.

The degree to which **AB:Z** (or any other model) is consistent with the data **ABZ** can be assessed statistically, as described in Section III above. In the variable-based framework, between the extremes of **ABZ** and **AB:Z**, there are three other candidate models: **AB:AZ**,

AB:BZ, and **AB:AZ:BZ**. The model **AB:AZ** asserts that Z is related only to variable A; model **AB:BZ** has a similar interpretation. Model **AB:AZ:BZ** assumes that A and B both influence Z, but that there is no interaction between A and B with respect to their influence on Z.

Table 3 gives results for all variable-based models and some state-based models for Figure 5, sorted by information, where

$$I(\text{model}) = (T(\mathbf{AB:Z}) - T(\text{model})) / T(\mathbf{AB:Z})$$

Although **AB:BZ** is the best variable-based model simpler than the data, it captures only about 17% of the information in the data while utilizing nearly as many degrees of freedom (df=5) as exist in the data (df=7). Moreover, the **AB:BZ** model is not statistically consistent with the observed data (p = 0.000, i.e. - there is no chance of error if we assert that the model differs from the data).

Model	T	%I	df	L ²	p
ABZ	---	100%	7	--	1.000
AB:Z:a0BZ	0.0002	100%	6	0.3	0.603
AB:Z:a0b1Z	0.0696	61%	5	120.3	0.000
AB:Z:a0b0Z	0.0876	51%	5	151.4	0.000
AB:AZ:BZ	0.1478	17%	6	255.5	0.000
AB:BZ	0.1482	17%	5	256.2	0.000
AB:Z:a1b1Z	0.1610	10%	5	278.4	0.000
AB:Z:a1b0Z	0.1720	3%	5	297.4	0.000
AB:AZ	0.1777	0%	5	307.2	0.000
AB:Z	0.1780	0%	4	307.6	0.000

Table 3. Summary results for directed system models

As was the case for the neutral system described above, state-based models for this directed system can capture more of the information in the data using the same or fewer degrees of freedom. The model **AB:Z:a0b1Z**, for example, specifies that the conditional distribution for Z must match the observed distribution for the a0b1 system state, and that a single Z distribution will be used for all other system states. This model has df=5 just as the variable-based **AB:BZ** model does, but the **AB:Z:a0b1Z** model captures 61% of the information in the data. It is still, however, inconsistent with the observed data (p = 0.000).

The **AB:Z:a0BZ** state-based model, however, is simpler than the data (df = 6, Δdf = 1), captures essentially all of the information in the data, and is statistically indistinguishable from the data (p = 0.6029) given the sample size (N = 1,247). The **AB:Z:a0BZ** model specifies

that, when the system is in state a_0 , the joint BZ distribution will match the observed data. Otherwise, the probabilities for the model distribution (q) will be maximally relaxed, consistent with the AB and Z margins.

It is worth noting that state-based models for directed systems also can specify *partial* agreement with conditional distributions for dependent variables. For instance, the model **AB:Z:a0b1z0** would require that the calculated probability $q(a_0b_1z_0)$ and conditional probability $q(z_0 | a_0b_1)$ match their observed values. Of course, models of this sort are applicable only when the associated dependent variable has more than two states.

The statistical analyses of Figures 1 and 5 used a top-down approach. L^2 and Δdf could also be calculated relative to the independence model, rather than the data. In this case, a very low p would mean that ascent to the model is statistically justified. This bottom-up approach is especially natural for directed systems.

IV. SEARCHING THE STATE-BASED STRUCTURE LATTICE

Unfortunately, the benefits of state-based modeling are coupled with an enormous increase in the number of models that must be considered. As indicated above, an **AB** system has just one alternative variable-based model (**A:B**) but, if the variables are binary, there are 70 nondegenerate state-based models. Even after models have been grouped into equivalence classes, and a canonical model from each class chosen, there are 14 models whose distributions need to be generated.

For variable-based modeling, variable cardinalities do not affect the lattice of structures, but for state-based modeling, the number of state-based structures increases not only with the number of variables in the system, but also with the cardinality of the variables. For example, a two-variable **AB** system in which just *one* of the variables has *three* states rather than two still has only one other variable-based model (**A:B**), but this system has 11 candidate state-based parameters and 1,023 possible parameter combinations that utilize 5 or fewer df. Even after rejecting degenerate structures, 568 distinct structures that can be grouped into 129 equivalence classes remain to be evaluated. While an exhaustive search might be feasible for very simple systems involving only a few variables and a small number of states per variable, a different approach is clearly required for more complex behavior systems.

Jones (1985) proposed a "greedy algorithm" that determined the best one-parameter model, then used that as the starting point for evaluating two-parameter models, and so on. The algorithm works well in practice but does not guarantee the optimality of the final model. An obvious extension of Jones' greedy algorithm is to prune less heavily at each step, retaining two or more candidate models as a starting point for searching at the next level of complexity (i.e., utilizing more df). A very different approach to searching the state-based Lattice of Structures using Fourier transforms is sketched in (Zwick, 2002).

When the state-based modeling approach is viewed as an extension to variable-based modeling, an obvious search strategy is to identify the best variable-based model and use that as a starting point for evaluating candidate state-based models. Since every variable-based model can be specified from the state-based perspective, it should be possible, in principle, to start with the best variable-based model and determine if adding an additional state-based parameter can efficiently improve the model's conformance with the data. Alternatively, it may be possible to remove a parameter and reduce the model's complexity without sacrificing too much fidelity.

V. CONCLUSIONS AND FUTURE DIRECTIONS

The investigations described in this paper build on the work of Jones and his colleagues in order to establish state-based RA as a natural extension of accepted variable-based RA methods. Results to date have demonstrated that:

- State-based RA can be used even where the k-systems framework is inapplicable, e.g., to analyze distributions (1) where there are *multiple* interrelated quantitative dependent variables, (2) where dependent variables are categorical, (3) where systems are neutral, or (4) where systems are stochastic.
- The reference model for state-based RA is not limited to the uniform distribution. For directed systems, the variable-based independence model may provide a more appropriate reference. Also, the bottom up approach using either of these reference models can be replaced by a top-down approach using the saturated model as the reference model (this might be especially appropriate for neutral systems).
- The lattice of structures for state-based models is related closely to the variable-

based lattice. Equivalence classes can be established with matrix methods.

- Searching the state-based lattice of structures can be used to further improve the results of searching the variable-based lattice.
- Methods previously applied in variable-based RA for evaluating the statistical significance of differences between models apply equally to state-based RA. g-to-k-normalization, which converts a quantitative system function to a probability distribution, does not provide for (or require) such statistical assessment.
- State-based modeling can be used to enhance decision analysis. This is not discussed in this paper, but see (Johnson and Zwick 2000)

Explorations reported in this paper were done mostly with spreadsheets, but the Discrete Multivariate Modeling (DMM) group (Zwick, 2001b) at Portland State University is developing a comprehensive software platform (OCCAM) for reconstructability analysis (Willett and Zwick, 2002) which will support state-based analysis. For a review of RA including state- and latent variable-based modeling, see (Zwick 2000a). RA overlaps very considerably with log-linear (LL) modeling, which is widely used in the social sciences (Bishop et al 1978; Knoke and Burke 1980), so state-based modeling is an important extension of LL modeling as well. For recent work in RA which makes extensive use of Jones' k-systems framework, see (Klir 2000).

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