GEOLOGICAL NOTES

LATENT FACIES MAPPING FROM BINARY GEOLOGICAL DATA[1]

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ABSTRACT

Many geological observation sets contain discrete-state data, which can be encoded as binary patterns. When there are conditional relationships between the variables, latent class analysis may be applied to subdivide the total sample into latent facies associations, which have local independence in the probability sense. Probabilities of latent facies assignments can be mapped areally as continuous surfaces of implied geological facies. Latent class analysis is rooted in simple probability theory and can be a useful technique in geological applications where observations are descriptive or weakly numerical. The method is illustrated by a latent facies mapping of the Morrison Formation (Upper Jurassic) in the subsurface of west Kansas.

INTRODUCTION

Geological observations are made on a variety of measurement scales, ranging in increasing information content from nominal to ratio. Although variables measured on a continuous scale are the most desirable for mathematical analysis, attributes characterized by simple presence or absence are common. Examples include the presence or absence of fossil types, mineralogies, lithologies, or bedding structures. Facies may be identified with certain associations of attribute occurrence, which reflect a common genesis. If several distinctive associations are discriminated, this character will be shown by conditional relationships in the joint occurrence of several attributes. When plotted as symbols on a map, the presence or absence of attributes can show regional patterns that pick out the geographic distribution of the underlying facies.

The use of binary presence-absence data considerably simplifies the decisions involved in codifying lithological descriptions. At the same time, the set of potential binary patterns to be mapped is two to the power of the number of variables, and so increase at an exponential rate. Even at low numbers, it is difficult to map the overlap of patterns so that its meaning can be assimilated easily. This complexity suggests however, that although the binary unit is the most simple representation, the combination of several binary variables as patterns can be rich in information. The binary combination set should be reduced analytically by methods sensitive to intrinsic associations that can both be mapped and interpreted. In this paper, we describe the use of a model based on simple probability concepts applied to binary lithological information from the Morrison Formation. The "latent class model" seeks to define hidden associations that collectively account for the joint occurrences of observation variables. For a geological application, these classes can be thought of as "latent facies." In the initial phase, three lithological variables are binary coded and analyzed to yield a unique solution for two latent facies. This provides a good introductory example where methodology can be related easily to probability concepts (and solved with a hand calculator). Model determinancy and other factors in higher-order models are then considered in conjunction with a three-class model based on four binary variables.

GEOLOGICAL SETTING

The Morrison Formation (Upper Jurassic) is restricted to the subsurface under much of western Kansas, where it ranges up to 350 feet in thickness. Merriam (1963) suggested

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that the upper part is correlative with the type Morrison in Colorado. A variety of late Jurassic stratigraphic equivalents in surrounding states have been suggested for the lower part, and these are documented by both Merriam (1963) and Zeller (1968). The informal usage of "Morrison" to describe Upper Jurassic sediments in the Kansas subsurface will be retained in this paper, although the implications of stratigraphic subdivision will be considered in the interpretation.

The major source of lithological information of this unit has been drawn from descriptions of drill-cuttings, supplemented by gamma-ray and resistivity logs. The section is dominated by sandy shales typically gray-green, but frequently varicolored in pastel shades. Limestone lenses occur locally (mostly in the upper part), while streaks of anhydrite and white-pink chalcedony chert are found in the lower part. Sandstone beds are most common in the east, often at the base of the section, but also within the upper division.

Systematic lithofacies mapping from drill cuttings data is hampered by the coarse sampling interval (conventionally 10 ft) and problems caused by infiltration of cavings and selective comminution of some mineral components by the drill bit. In addition, the generalized descriptions must be transformed from prose to numbers for quantitative mapping by interpolation between control wells. The Morrison Formation is particularly difficult to evaluate because of its very mixed character and, when present, components can range through "trace," "streaks," "stringers," to beds, so that consistent volumetric or thickness estimates are usually impractical. However, the crucial information content appears to be contained in the simple presence or absence of key lithologies at well locations, whose spatial distributions indicate patterns of stratigraphic and lateral lithofacies variations. This observation is suggested by maps prepared by Merriam (1955) in which he outlined areas where both chert and anhydrite were absent, chert-present/anhydrite absent, and both chert and anhydrite were present. He interpreted the distinctive geographic trends both in terms of localized environmental controls and stratigraphic overlap by younger Morrison sediments.

BASIC PROBABILISTIC ANALYSIS

The presence or absence of sandstone, limestone, and anhydrite in the Morrison Formation were coded as binary patterns for drill-cuttings descriptions from 313 wells in western Kansas. Maps of well locations for the occurrence of these lithologies are shown in figure 1. Distinctive geographical trends can be perceived suggestive of stratigraphic or facies controls. Frequencies of association between the variables are summarized graphically as the Venn diagram of figure 2. The numbers express the relative occurrences of all possible combinations. However, there is no immediate indication of which combinations occur more or less commonly than would be expected if there were no associations. A comparison can be made by calculating the expected frequency of each combination under the assumption of independent events. This is the product of the marginal probabilities times the total number,

$$\text{e.g.}, B_{ijk} = p_i p_j p_k * N$$

where $p_i = n_i/N$, and B_{ijk} is the expected number of occurrences of lithologies i, j, and k; p_i, p_j, p_k are the marginal probabilities of i, j, and k; N is the total number in the sample, and n_i is the number of occurrences of lithology i. The marginal probabilities of the absence of lithologies, i, j, and k, can be symbolized by p_{-i}, p_{-j} and p_{-k}, where $p_{-i} = (N - n_i)/N$. The six marginal probabilities of presence/absence are then used to generate the eight possible combination frequencies. A comparison of the frequencies of observed patterns and numbers expected as a result of independent events is shown in table 1. The potential significance of the differences between observed and expected totals was examined by a chi-square contingency test. The calculated test value clearly exceeds the critical chi-square at 5% significance, with a strong rejection of the null hypothesis of no association between the lithologies.

The conclusion from this is that the total sample cannot be characterized by independent lithologies. A possible alternative model is that the sample is the result of some mix of distinctive associations or lithofacies. Each lithofacies would be internally independent in the probability sense. This concept is the ba-

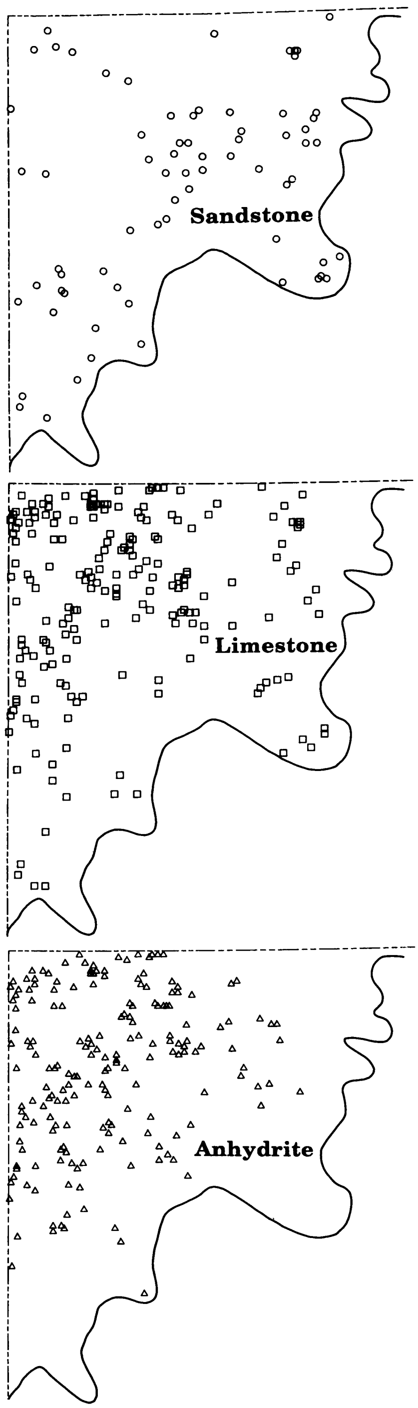

FIG. 1.—Distribution of occurrence of sandstone, limestone, and anhydrite reported in drill-cuttings from the Morrison Formation in Kansas.

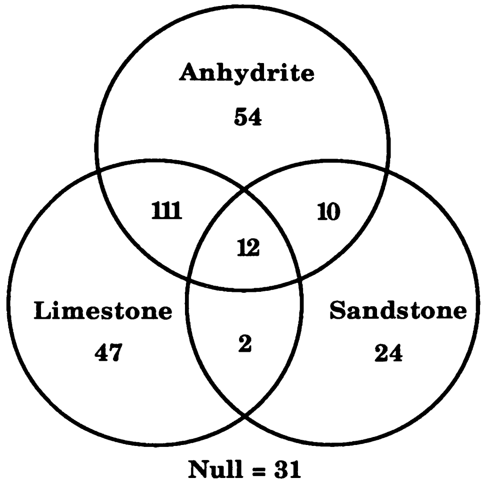

FIG. 2.—Venn diagram of frequencies of mutual occurrences of sandstone, limestone, and anhydrite reported in drill-cuttings from the Morrison Formation in Kansas.

sis for "latent class analysis" initiated in the early fifties, primarily by Lazarsfeld (1950) and his students. Their model postulated a few distinct latent classes of attitude to "explain" the observed variety of response patterns made by subjects to a series of discrete-state questions. They equated their method with the diagnostic procedure of medicine, where the collective presence or absence of symptoms reflects the operation of causative diseases. By analogy, observed associations of rock types can be considered to be diagnostic of ancient controls of sedi-

TABLE 1

FREQUENCIES OF BINARY PATTERNS FOR THE PRESENCE (1) OR ABSENCE (0) OF SANDSTONE (S), LIMESTONE (L) AND ANHYDRITE (A) OBSERVED IN MORRISON FORMATION SECTIONS (O) AND EXPECTED BASED ON AN INDEPENDENT-EVENTS MODEL (E)

S L A	O	E
0 0 0	31	37.2
0 0 1	54	55.2
0 1 0	47	60.6
0 1 1	111	90.0
1 0 0	24	10.7
1 0 1	10	15.9
1 1 0	24	17.5
1 1 1	12	25.9

NOTE.—Chi-square value is 37.61, significant at the 5% level and 4 degrees of freedom.

mentation. Latent class analysis uses some simple ideas of probability, which are explained below in connection with a three-variable, dual latent class model.

Let x_i, x_j, x_k be three binary variables that have the values of either 1 or zero as responses to items i, j, and k. Their mean values will be p_i, p_j, p_k, the probabilities that an individual response will take the value 1. The joint probabilities of paired items are p_{ij}, p_{ik}, p_{jk}. The covariances of the binary variables are:

$$c_{ij} = p_{ij} - p_i p_j$$

$$c_{ik} = p_{ik} - p_i p_k$$

$$\text{and } c_{jk} = p_{jk} - p_j p_k$$

Notice that these covariances will be zero in cases where the two variables are independent. They are central moments of second order, while the central moment of third order is given by:

$$c_{ijk} = p_{ijk} - p_i c_{jk} - p_j c_{ik} - p_k c_{ij} - p_i p_j p_k$$

If there are no associations between the variables, then the pair- and triple-joint probabilities are the same as the product of their component marginal probabilities, e.g., $p_{ijk} = p_i p_j p_k$. In this situation, the sample can be thought of as a single set consisting of independent variables. Alternatively, non-zero values of the central moments indicate systematic associations between the variables. In this case, the sample might better be modeled as consisting of several subsets, or "latent classes," each of which consists of independent variables.

The solution of the latent class variables follows from the model axiom that the classes are locally independent in the probability sense. A set of "accounting equations" can be written that are the logical outcome of local independence. These equations are described for three observational variables and a postulated two-class structure, but can be generalized to higher-order models. The proportions of the sample, v_1 and v_2, to be assigned to the two classes must sum to unity:

$$v_1 + v_2 = 1$$

The "manifest" marginal probability, p_i for item i, is linked with the "latent probabilities" in each class, θ_{1i} and θ_{2i}, by:

$$p_i = v_1\theta_{1i} + v_2\theta_{2i}$$

Two additional equations of this form related the manifest probabilities for items j and k with their latent probabilities. The manifest joint probability, p_{ij}, is given by:

$$p_{ij} = v_1\theta_{1i}\theta_{1j} + v_2\theta_{2i}\theta_{2j}$$

while similar equations apply to the other probabilities, p_{ik} and p_{jk}. Finally, the manifest triple joint probability, p_{ijk}, is related to the latent probabilities by:

$$p_{ijk} = v_1\theta_{1i}\theta_{1j}\theta_{1k} + v_2\theta_{2i}\theta_{2j}\theta_{2k}$$

The unknowns in this equation set are the proportions of the two classes and the six latent probabilities. The solution is uniquely determined by the eight accounting equations for the three-variable/two-class model. Although it is not a linear simultaneous set, in this special limiting case, the equations can be solved by the following quick method. Lazarsfeld and Henry (1968) p. 41–43 demonstrate that:

$$c^2_{ijk}/(c_{ij}c_{ik}c_{jk}) = (v_2 - v_1)^2/v_1v_2 = (1/v_1v_2) - 4$$

where the c-terms are the central moments of the second and third order described earlier. The two latent class proportions can then be solved, because their summation to unity provides a second equation. The latent probabilities are solved next by using the accounting equation:

$$p_i = v_1\theta_{1i} + v_2\theta_{2i}$$

and the relationship:

$$(\theta_{1i} - \theta_{2i})^2 = c_{ij}c_{ik}/c_{jk}v_1v_2$$

for each of the three item variables.

Returning to the Morrison Formation data, the presence or absence of sandstone, limestone, and anhydrite are three binary items that can be analyzed in terms of two latent classes, as described above. The manifest marginal and joint probabilities, together with central moments, were derived from the oc-

TABLE 2

MORRISON FORMATION TWO-CLASS LATENT STRUCTURE

Class	Size	Sandstone	Limestone	Anhydrite
1	.345	.578	.493	.258
2	.655	.037	.687	.776

currence frequencies shown on the Venn diagram in figure 2. Estimates of class proportions and latent probabilities were calculated using the latent class procedure and are listed in table 2. The facies aspect of each class is apparent from comparisons between the values of these latent probabilities. The first class can be characterized as a "clastic facies," with moderate probability of sandstone, a similar probability for limestone, and a low probability for anhydrite. By contrast, the second class is marked by a vanishingly small probability of sandstone, an increased probability of limestone, and a threefold increase in anhydrite. In the discussion of this paper, we will refer to this second class as the "chemical facies."

In order to map the distribution of these implicit facies, the lithology response pattern from each well must first be classified in terms of the two latent classes. The conditional probabilities of the identification of any pattern with one or other of the classes can be calculated by Bayes' rule:

$$Pr(1|ijk) = v_1\theta_{1i}\theta_{1j}\theta_{1k}/p_{ijk}$$

$$\text{and } Pr(2|ijk) = v_2\theta_{2i}\theta_{2j}\theta_{2k}/p_{ijk}$$

The conditional probabilities for the various lithology patterns are listed in table 3. Each well location in the Morrison data set was assigned the probability of classification with the clastic facies class associated with its lithology pattern. A map of these probabilities (fig. 3) shows striking distinctive regional elements rather than a complex mosaic. The contours are based on values interpolated between well control, so that the mapped classification is a grouped aggregate of neighboring wells. By the same token, errors in lithological description will show up at wells whose probabilities are at marked variance with those of their neighbors. Since geographic coordinates are not used in the latent class computations, the map provides useful feedback information to check original cuttings descriptions. Although the probability map is keyed explicitly with clastic facies class classification, the map simultaneously displays the complementary probability of assignment to the chemical facies class. The clastic facies occupies a belt adjacent to the subcrop, broken by a major northwest trending lobe which projects across a platform area dominated by chemical facies patterns.

The three-variable/two-class case is the simplest latent class model, but is easy both to understand and compute, and also provides useful results. In the next section, we consider more generalized latent class models which are extensions of the same concepts, but involve higher numbers of classes and differing numbers of binary variables. In particular, we apply a four-variable/three-class model to the Morrison Formation. This allows the comprehensive use of all lithological information concerning sandstone, limestone, anhydrite, and chert. Shale can be ignored as a variable, since it is ubiquitous throughout the Kansas Morrison.

HIGHER-ORDER LATENT CLASS MODELS

Higher-order models can be considered which postulate m latent classes, based on n

TABLE 3

MORRISON FORMATION TWO-CLASS LATENT CONDITIONAL PROBABILITIES

Pattern	Conditional Probability	
S L A	Class 1	Class 2
0 0 0	.55	.45
0 0 1	.12	.88
0 1 0	.35	.65
0 1 1	.05	.95
1 0 0	.97	.03
1 0 1	.82	.18
1 1 0	.95	.05
1 1 1	.66	.34

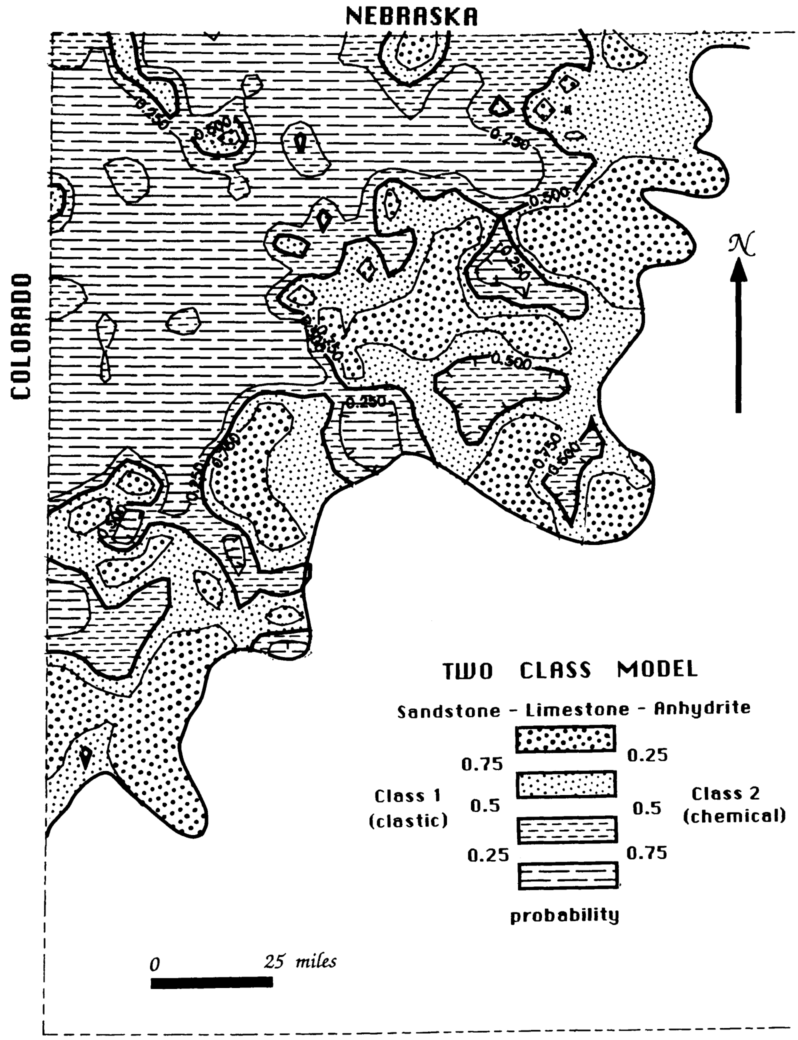

FIG. 3.—Two-class latent lithofacies map of the Morrison Formation in Kansas, based on conditional probabilities of class assignment.

binary variables. There are practical limitations on the feasibility of models with a large number of classes, since the number of response patterns increases as two powered by the model order, and doubles again with each new variable. Consequently, the higher orders can require inordinately large sample sizes if the probabilities of most combinations will be estimated as anything else than zero. Even in simple models, a small sample size and/or weakly heterogeneous probability structure can result in latent probabilities which are either slighly negative or exceed unity. These "impossible" estimates simply reflect that the samples provide *estimates* of population parameters and that the latent classes define a *model* of associations. Nevertheless, computed latent probabilities must be constrained within the conventional range to yield rational pattern frequencies.

The number of unknown latent parameters will match the number of accounting equations when:

$$m(n+1) = 2^n.$$

With an insufficient number of binary variables, there can be no unique solution, and the model is not identifiable. Otherwise, either a solution or, more commonly a "best-fit" set of parameters, can be located by a generalized technique of latent class analysis. The generalized method fits a specified order of latent class model to the input variables by maximum likelihood and rational latent probability constraint (Everitt 1984, p. 76–86). The optimum solution provides the best possible match between the frequencies of binary patterns predicted by the latent class model and those actually observed in the sample. In the partition of the Morrison Formation data into two latent classes, there was a unique solution, since this was determined by the use of three variables. The solution was rational because of the strong conditional character in manifest probabilities and the moderately large sample size. In other applications, one or more of these properties may not hold and the solution is one of best-fit. Where the joint probabilities of the total sample are closely matched by products of marginal probabilities, realistic partitions become impossible.

The Morrison Formation data set was expanded to include the occurrence of chert, in addition to the presence or absence of sandstone, limestone, and anhydrite, used earlier. The possible binary pattern combinations now number sixteen and their frequencies in the Morrison are shown in the Venn diagram of figure 4. The four variables were then analyzed in terms of a three-class latent model. The results were examined to see whether a tripartite division was an improvement on a two-class model, or if the bipartite division was a more reasonable representation of the data structure. A solution based on three classes and four variables will not in general fit the data precisely and hence a best fitting model must necessarily be chosen using some criterion of misfit. Everitt (1984) described an iterative algorithm to find a maximum likelihood solution. His algorithm converges to a point at which all the partial derivatives of the log-likelihood are zero. Unfortunately, the log-likelihood often has a large number of critical points, most of which do not represent maxima. The Everitt technique is extremely sensitive to choice of initial estimates and can easily converge to a critical point which does not represent a maximum. Furthermore because the parameters are subject

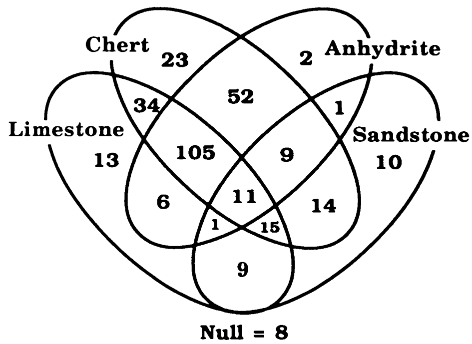

FIG. 4.—Venn diagram of frequencies of mutual occurrences of sandstone, limestone, anhydrite and chert reported in drill-cuttings from the Morrison Formation in Kansas.

to the constraints that all probabilities must lie between zero and one, a global maximum for the log-likelihood may occur at a boundary point at which not all of the partial derivatives are zero.

The authors have further found that the likelihood function has a great many local maxima. Alternative models to the maximum likelihood solution, which degrade the maximum likelihood fit almost imperceptibly, often exist with fitted parameters widely different from those found by the maximum likelihood solution. The authors believe that these alternative models should be examined.

A common approach to find the global maximum of a function over a constrained set is to use a transformation to convert all the local maxima to critical points (Box 1986), then choose systematically a large number of possible initial points (Aird and Rice 1977) and iterate each to find a variety of possible local maxima. This procedure was applied to the Morrison Formation data using the IMSL (International Mathematical and Statistical Library) routine ZSRCH to systematically locate initial points, and the subroutine of ZXMIN to iterate these points a small number of times for the location of possible critical points. ZSRCH is described in Aird and Rice. ZXMIN is based upon the Davidson-Fletcher-Powell quasi-Newton algorithm and is succinctly described in Press et al. 1986. The candidates for critical points were ordered in terms of log-likelihood. High value locations were further iterated until convergence. Essentially equivalent, but lower value, locations were eliminated. ZXMIN produces an estimate of the Hessian of the log-likelihood that was used to determine if the identified critical points represent maxima or not. All identified independent local maxima were printed for consideration. Except for the production of alternative models, this is the approach used by the IMSL routine ZXMWD to find a global maximum of a function over a constrained set.

As a final evaluation, the predicted binary pattern frequencies can be compared with the observed frequencies using the chi-square statistic. For the Morrison Formation data set, the optimal solution judged by both the maximum likelihood and the chi-square criterion results in the pattern frequencies listed in table 4. The chi-square statistic is 0.726 with one degree of freedom, indicating an excellent fit with observational data.

The proportions of the three latent classes and their latent probabilities of sandstone, limestone, anhydrite, and chert (table 5) are easily interpreted, especially when compared with the two-class structure (table 2). The first class is extremely similar to the "clastic facies" of the two-class division with respect to the proportional size and latent probabilities of sandstone and limestone. This latent clastic facies is marked by moderate probability of sandstone as contrasted with the other classes, where sandstone has a low or zero probability of occurrence. By implication, the second and third classes are equivalent to a subdivision of the "chemical facies" of the two-class model. The chert component clearly has a higher association with these two chemical facies than the clastic facies. The chemical facies probabilities of sandstone are low, probabilities of anhydrite and chert are high, and probability of limestone ranges from moderate to high. These two classes are distinguished almost entirely by a strong association of limestone with the third class, as compared with the second, whose limestone probability is similar to that in the clastic facies. In summary, the three classes can be identified as a sandstone facies, an anhydrite-chert facies, and a limestone-anhydrite-chert facies. The strong polarization of limestone between the two chemical facies suggests that the subdivision is real, although the basic structure of the data seems determined by a simple differentiation between clastics and chemical rocks. A map of assignations of well patterns to these latent facies provides valuable additional information for model verification and interpretation.

The three conditional probabilities for each lithology pattern were calculated using the equations cited earlier. These express the relative probability of membership in the three latent classes given the responses in the pattern. In the case of the two-class model, the conditional probabilities of the well control

TABLE 4

Observed and Three-Class Model Predictions of Sandstone (S), Limestone (L), Anhydrite (A), and Chert (C) in the Morrison Formation

Pattern S L A C	Obs. freq.	3-Class Model prediction
0 0 0 0	8	9.6
0 0 0 1	23	22.6
0 0 1 0	2	1.9
0 0 1 1	52	52.2
0 1 0 0	13	11.4
0 1 0 1	34	34.5
0 1 1 0	6	6.2
0 1 1 1	105	104.7
1 0 0 0	10	9.0
1 0 0 1	14	13.7
1 0 1 0	1	1.0
1 0 1 1	9	9.0
1 1 0 0	9	9.9
1 1 0 1	15	15.3
1 1 1 0	1	1.1
1 1 1 1	11	11.0

TABLE 5

Morrison Formation Three-Class Latent Structure

Class	Size	Sandstone	Limestone	Anhydrite	Chert
1	.322	.491	.524	.095	.576
2	.415	.158	.553	.840	1.000
3	.263	.000	.843	.829	.911

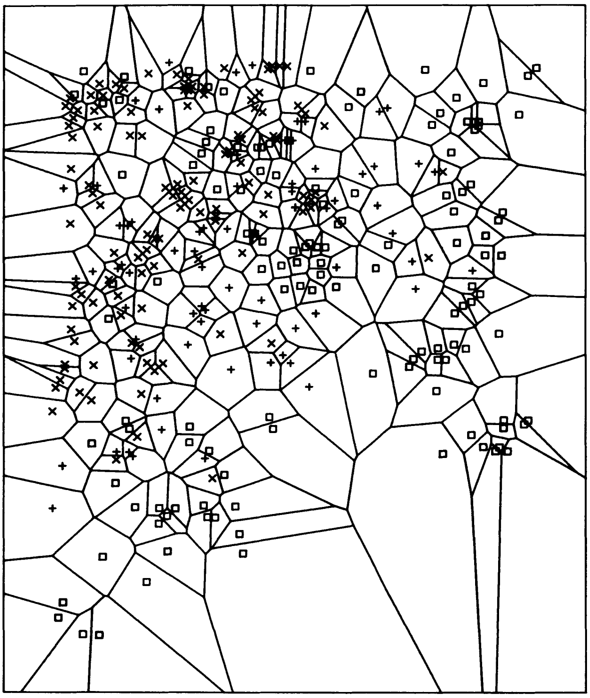

FIG. 5.—Thiessen polygonal tessellation of locations of Morrison Formation drill-cuttings samples.

could be contoured as a single map, because the classification alternatives summed to unity. For the more complex three-class case, each well was classified in terms of one of the three latent facies as dictated by the highest Bayesian probability. The classifications were then used as the basis for a symbolic facies map by assigning the facies of each well to its immediate neighborhood and fusing the results as a composite map. The process can be done automatically by the subdivision of the region into Thiessen polygons (also known as Dirichlet cells or Voronoi polygons). Green and Sibson (1978) describe an algorithm for the construction of a complete tessellation, where each polygon encloses all locations which are closer to the interior data point than to any other point. The result of the Thiessen polygon subdivision of the Morrison Formation well control is shown in figure 5, where the symbols mark well location and latent facies classification.

If the polygons are assigned the facies of their well, and edges are erased between neighboring polygons with common facies, the result is the lithofacies map of figure 6. As would be expected, this map shows essentially the same distribution of clastic facies as the two-class probability map. However, the most striking new feature is the marked segregation of the two chemical latent facies. The northeast-trending clastic belt is paralleled by a zone of chert-anhydrite facies, which is flanked to the northwest by a limestone-chert-anhydrite facies. Since geographic location does not enter the latent class analysis, this character supports the idea that the latent facies subdivision represents geologically meaningful associations rather than mathematical artifacts. The map is easy to interpret when related to the Morrison Formation subdivision proposed by Merriam (1955), who recognized a lower division marked by anhydrite and chert and an upper division with limestone "stringers." The regional features pick up the geographic limits of the lower Morrison chert-anhydrite-shale unit overlapped by the upper unit which grades from nearshore clastics to shallow-water limestones in the northwest. The clastic belt is broken by a major northwest-trending lobe, which may reflect the influence of the Oakley Anticline as a structurally-high feature as suggested by Lee and Merriam

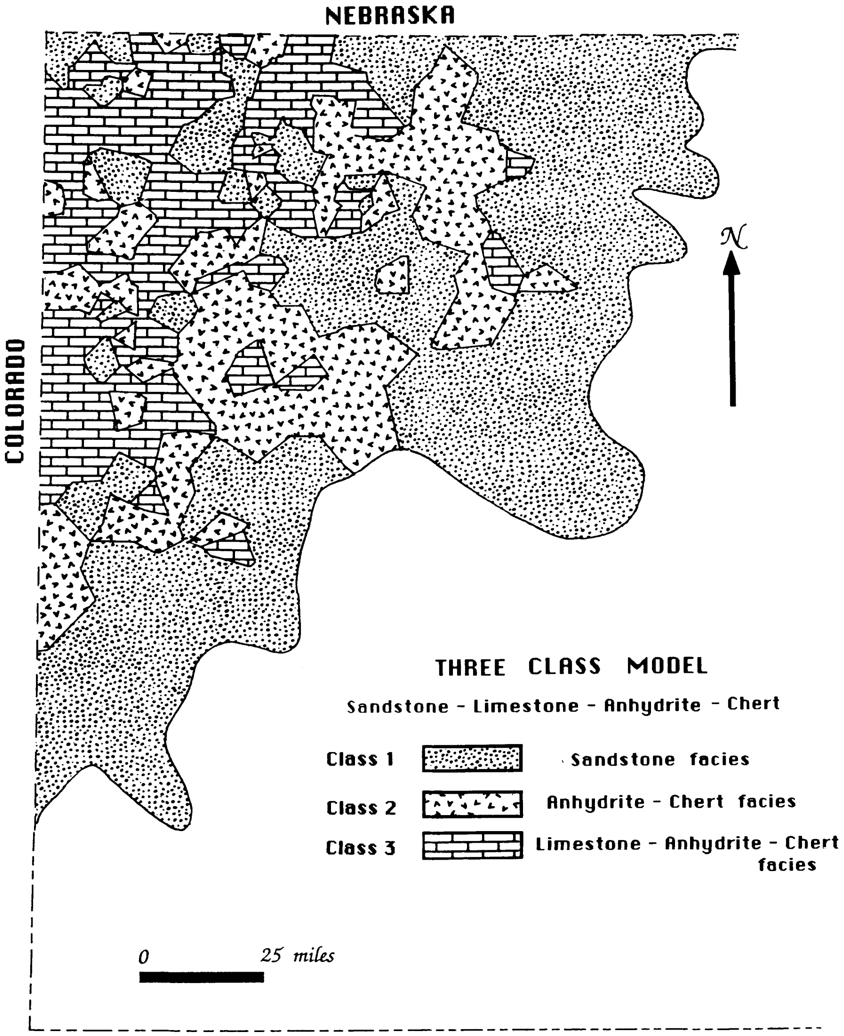

FIG. 6.—Three-class latent lithofacies map of the Morrison Formation in Kansas.

(1954). In a similar way, the Cambridge Arch may also have been active (Merriam 1963) and may be linked with the west-trending clastic feature in the extreme north.

DISCUSSION

The philosophy of latent class analysis as a mathematical model is similar to factor analysis, because a few hidden classes are postulated to account for the observed variety of response patterns. This is not an alien concept to geologists who commonly attempt to define facies as an ensemble of observable features. However, classical sedimentary facies are rooted in models of genesis (usually based on modern analogs), which are then linked with properties observed in the field. The "latent facies" of this paper extract distinctive variable associations empirically, and these are considered to be diagnostic of causal processes. The potential "meaning" of the latent facies must be drawn from the geological context. Their parameters and mapped variation may reflect lateral facies changes and/or the regional distribution of stratigraphic subdivisions.

The latent model has the simple intuitive appeal of its elementary probability concepts and its nominal data requirements make no high demands on precision. These qualities make it a useful method for many geological data sets where observations are either descriptive or weakly numerical. The use of probability also accommodates observation errors within the analysis. Unlike factor analysis, latent class models have no rotation problem. This is because the assumption of normal distribution limits factor analysis to pairwise correlations, whereas latent class analysis uses joint frequencies of three or more items to fix the appropriate rotation. As Everitt (1984, p. 77) notes the cumbersome methods described by early workers in latent class analysis (such as Lazarsfeld and Henry 1968) "are now only of historical interest since with modern computers and optimization algorithms it is fairly straightforward to use maximum likelihood methods." In common with factor analysis, latent structure analysis is not a technique of statistical inference, but a recasting of the data based on variable associations. Since the geographic coordinates of the observations are not used within the latent facies analysis, the appearance of coherent patterns and distinctive trends on the final maps are the best criteria as to the likely success of an application.

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