Multivariate Multiscale Categorical Variable Distributions

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Facies have a significant impact on reservoir flow performance. In geostatistics, facies are treated as categorical variables. They are considered to be mutually exclusive at a small scale and become proportions at larger scales. In the case of facies simulation with coarse grids this assumption may not be valid; mixing of facies inevitably occurs at larger scales. Assessing the uncertainty of facies proportions at a specific scale honoring the sum to unity is a challenging problem. This paper introduces the basic need for multiscale multivariate facies distributions. The analytical form of the univariate marginal distributions of the multivariate multiscale facies proportion distribution in truncated Gaussian simulation framework (TGSIM) has also been investigated.

Introduction

A random variable is a variable, Z , that can take a series of outcomes or realizations $(z_i, i = 1, \dots, L)$ with a given set of probabilities of occurrence $(p_i, i = 1, \dots, L)$. The probabilities are all greater than or equal to zero and must sum to one. When the number L of occurrences is finite, the random variable is discrete (or categorical). If L is infinite the random variable is continuous. The probability distribution of a continuous random variable $Z(\boldsymbol{u}_\alpha)$ is characterized by its cumulative distribution function defined as:

$$F(\boldsymbol{u}_\alpha; z) = Prob\{Z(\boldsymbol{u}_\alpha) \leq z\} \in [0,1] \;\; ; \; \alpha = 1, \dots, N$$

$F(\boldsymbol{u}_\alpha; z)$ is called the univariate cumulative distribution function.

A random function is defined as a set of usually dependent random variables $Z(\boldsymbol{u}_\alpha)$ ($\boldsymbol{u}_\alpha, \alpha = 1, \dots, N$, is the vector of location). The random function can be written as $\{Z(\boldsymbol{u}_\alpha), \alpha = 1, \dots, N\}$, where N is the number of locations or random variables under consideration. The N random variables of the random function form an N −variate cumulative distribution function defined as:

$$F_{MV}(\boldsymbol{u}_1, \dots, \boldsymbol{u}_N; z_1, \dots, z_N) = Prob\{Z(\boldsymbol{u}_1) \leq z_1, \dots, Z(\boldsymbol{u}_N) \leq z_N\}$$

MV stands for multivariate. For categorical variables the multivariate probability density function representation is more relevant (Deutsch 2002) and can be written as:

$$p_{MV}(\boldsymbol{u}_1, \dots, \boldsymbol{u}_N; k_1, \dots, k_N) = Prob\{Z(\boldsymbol{u}_1) \in k_1, \dots, Z(\boldsymbol{u}_N) \in k_N\} \;;$$
$$k_\alpha \; = 1, \dots, K \;\&\; \alpha = 1, \dots, N$$

There are K mutually exclusive facies categories ordered as $k = 1, \dots, K$. k_α is the facies code corresponding to location $\boldsymbol{u}_\alpha$. Once the N −variate probability distribution function is formed, all of the multivariate marginal (with the number of variables less than N) probability density functions can be obtained.

Categorical Variables and Compositional Property

Continuous variables have a natural ranking and are amenable to basic arithmetic (add, subtract, multiply, divide, etc) (Chiles, J. P. and Delfiner, P., 1999). For example, porosity is a continuous variable because it can take any numeric values between 0 and 1. Categorical variables are discrete variables representing elements of classification. In general, we cannot do arithmetic on categorical variables because their values act as labels rather than numbers.

Facies are categorical and assigned by a geologist or petrophysicist using the analysis of cores and available data. In the absence of core measurements, well log data are used to assign facies. Two important assumptions are made in assigning the facies data. These assumptions are the basis for all current facies simulation techniques. The assumptions are (1) mutual exclusivity and (2) exhaustivity. Consider K mutually exclusive and exhaustive facies categories $k = 1, \dots, K$.

The facies are called mutual exclusive and exhaustive because it is assumed that any location $\boldsymbol{u}_\alpha, \alpha = 1, \dots, N$, in the reservoir belongs to one and only one of these K categories. If facies k exists at location $\boldsymbol{u}_\alpha$ then other facies do not exist at $\boldsymbol{u}_\alpha$ on the other hand if facies k does not exist at location $\boldsymbol{u}_\alpha$ then there must exist only one facies, e.g. k', other than k at location $\boldsymbol{u}_\alpha$. The existence and non-existence of facies k at location $\boldsymbol{u}_\alpha$ can be coded as 0 (non-existence) or 1 (existence). Let $i(\boldsymbol{u}_\alpha; k)$ be the indicator variable corresponding to category k at location $\boldsymbol{u}_\alpha$. Therefore,

$$i(\boldsymbol{u}_\alpha; k) = \begin{cases} 1, & if\ location\ \boldsymbol{u}_\alpha\ in\ category\ k \\ 0, & otherwise \end{cases} \quad ; k = 1, \dots, K\ \&\ \alpha = 1, \dots, N$$

In mathematical form the two assumptions of mutual exclusivity and exhaustivity are:

$$i(\boldsymbol{u}_\alpha; k).\, i(\boldsymbol{u}_\alpha; k') = 0 \ ; \quad \forall\, k \neq k'\ \&\ k, k' = 1, \dots, K\ \ \&\ \ \alpha = 1, \dots, N$$

$$\sum_{k=1}^{K} i(\boldsymbol{u}_\alpha; k) = 1\ ; \quad \alpha = 1, \dots, N$$

At each location, the indicator variable is 0 or 1 at a point scale. As the scale increases $i(\boldsymbol{u}_\alpha; k)$ becomes a proportion, $p_k, k = 1, \dots, K$, with values between 0 and 1.

To calculate the proportion of facies k ($p_k, k = 1, \dots, K$), first a neighborhood or scale of location $\boldsymbol{u}_\alpha, \alpha = 1, \dots, N$ should be defined then the volumetric averaging of $i(\boldsymbol{u}_\alpha; k)$ will be performed, therefore:

$$p_k = \frac{1}{V} \int_V i(\boldsymbol{u}_\alpha; k).\, dv \quad ; k = 1, \dots, K\ \&\ \alpha = 1, \dots, N$$

The facies variable changes from categorical to continuous as the scale increases. At point scale ($V = 0$), the value of p_k is 0 or 1. At very large scale (V is the entire reservoir) the value of p_k is the global proportion of facies k. Figure 1 shows a schematic plot of the impact of scale on facies probability distribution function.

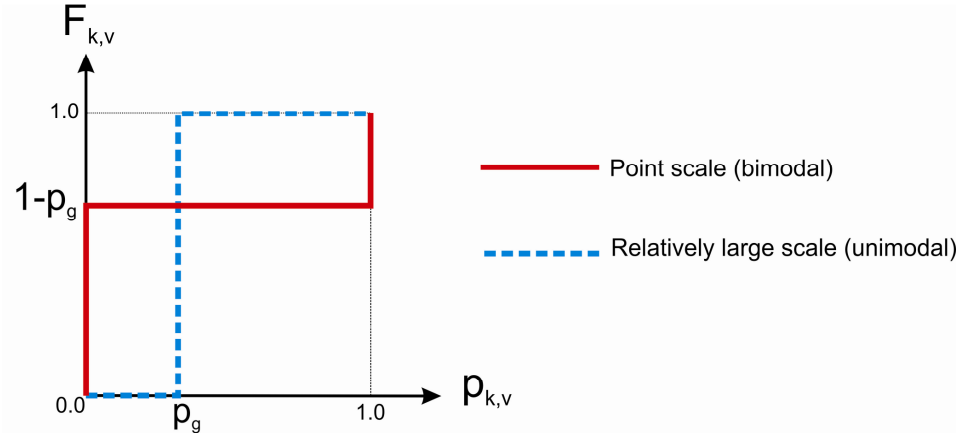

Figure 1 univariate bimodal and unimodal facies distribution at point scale and large scale respectively

The univariate distribution for each indicator variable changes from a bimodal distribution of ones and zeros at point support to the unimodal (global average) at large support. Figure 2 shows the distribution of facies proportions at different scales.

Haas et al (2002), Biver et al (2002) and Deutsch et al (2008) proposed analytical techniques to model the probability density function of categorical independent variables at different scales. They started with multinomial distribution of facies. It can be proved mathematically that if the variables are independent binary (0 and 1) categorical variables and are upscaled to a larger support, the probability density function becomes binomial. As a generalization for multiple categories the probability density function becomes multinomial but it should be noted that this law is correct for independent variables and not for dependent variables.

Haas et al (2002) and Deutsch et al (2008) tried to fit some analytical family of distributions such as, multinomial distribution, beta distribution, ordinary beta distribution, Dirichlet distribution to multivariate multiscale facies distribution. The counting algorithm is used in this paper to find the univariate marginals of multivariate multiscale facies distributions.

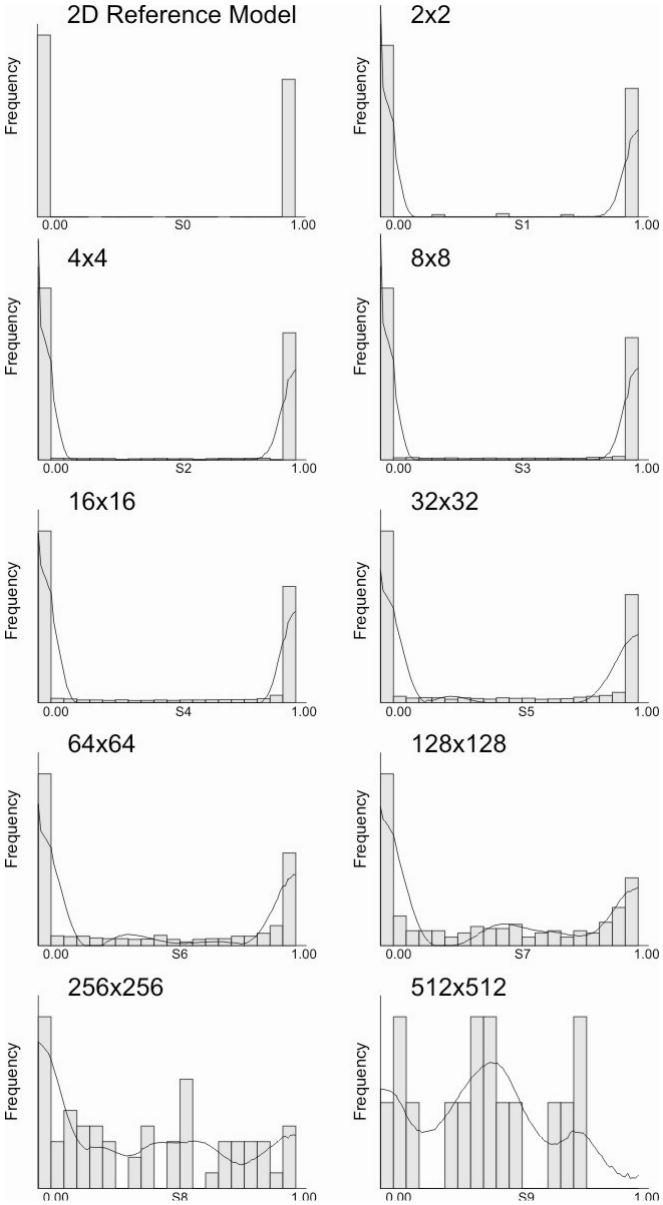

Figure 2 Distribution of facies proportions at different scales

At a specific scale of V, p_k takes a value from a set of $\left\{0, \frac{1}{V}, , \ldots, \frac{v}{V}, \ldots, \frac{V-1}{V}, 1\right\}$ with a specific probability of $p_{k,v}; k = 1, \ldots, K \;\&\; v = 0,1,2, \ldots, V$. For example if the upscaled value is calculated using eight point scale locations (e.g. upscaled grid dimensions $V = 2 \times 2 \times 2$) p_k can take any numbers from the set of $\left\{0, \frac{1}{8}, \frac{2}{8}, \frac{3}{8}, \frac{4}{8}, \frac{5}{8}, \frac{6}{8}, \frac{7}{8}, 1\right\}$ with probability of $p_{k,v}$. $p_{k,v}$ is the univariate marginal distribution of facies k at scale v. The purpose of this paper is to calculate $p_{k,v}$ analytically.

The constraint of sum to unity is preserved at all scales, that is, at each location and at all scales the sum of the facies proportions is 1. If we plot all of the facies proportions in a K dimensional space, all of the points fall on a hyperplane or more specifically a standard or unit $(K-1)-$ simplex. For example consider a three dimensional facies model that contains two facies. Each grid cell has two values for the proportion of facies 1 and 2 (regardless of scale). A plot of the proportions of facies 1 versus the proportions of facies 2 will fall on a line. The set of plotted proportion points is a unit 1-simplex with the equation of $p_1 + p_2 = 1$ (with vertices of (1, 0) and (0, 1)) or if we have three facies, the set of plotted

proportion points is an equilateral triangle plane or a unit 2-simplex with the equation of $p_1 + p_2 + p_3 = 1$ (with vertices of (1, 0,0), (0, 1,0) and (0, 0,1)).

Figure 3 shows a typical 2-simplex (an equilateral triangle in three dimensional space). Each point on the unit $(K-1)-$simplex corresponds to a location in reservoir model. For example in the case of three facies of sand, shaley-sand and shale; a grid block that contains 20 % sand, 50 % shaley-sand and 30 % shale sand can be shown as (0.2,0.5,0.2). This point will fall on the unit 2-simplex.

The standard or unit $(K-1)-$simplex can be written as below (Aitchison, 1986):

$$\Delta^{K-1} = \left\{ (p_1, \dots, p_K) \in \mathbb{R}^K \middle| \sum_{k=1}^{K} p_k = 1 \ \ and \ \ p_k \geq 0 \ for \ all \ k \right\}$$

Note that the above definition for unit $(K-1)-$simplex satisfies the condition of $p_k \leq 1$. The matrix of vertices of unit $(K-1)-$simplex is a unit matrix:

$$\boldsymbol{I}_{K\times K} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix}_{K\times K}$$

Each row in above unit matrix is one of the vertices of the unit $(K-1)-$simplex. Therefore the K vertices can be written as below:

$$\begin{gathered} e_1 = (1,0,0,\dots,0,\dots,0) \\ e_2 = (0,1,0,\dots,0,\dots,0) \\ e_3 = (0,0,1,\dots,0,\dots,0) \\ \vdots \\ e_k = (0,0,0,\dots,1,\dots,0) \\ \vdots \\ e_K = (0,0,0,\dots,0,\dots,1) \end{gathered}$$

The facies proportion points at point scale fall exactly on the vertices of unit $(K-1)-$simplex and at infinite scale they become a point (global proportion point) on the unit $(K-1)-$simplex.

The facies proportions $p_k, k = 1, \dots, K$ form a $K-$variate probability distribution function. The total number of feasible facies proportion points, $S(K,V)$, from the set of $\left\{0, \frac{1}{V}, , \dots, \frac{v}{V}, \dots, \frac{V-1}{V}, 1\right\}$ that fall on the Δ^{K-1} is calculated as (Chasalow and Brand 1995):

$$S(K,V) = C(V+K-1,V) = \frac{(V+K-1)!}{V! \cdot (K-1)!}$$

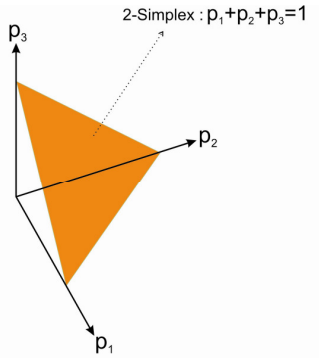

Figure 3 a 2-simplex with three vertices of (1,0,0), (0,1,0) and (0,0,1)

Scaling Law

Before getting into the scaling law it is needed to recall the definition of the variogram and two important assumptions of first and second order stationarity. The variogram is a two-point statistic that spatially relates two random variables $Z(\mathbf{u})$ and $Z(\mathbf{u}+\mathbf{h})$:

$$2\gamma(\mathbf{h}) = E\{[Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})]^2\}$$

Where $\mathbf{u}$ and $\mathbf{h}$ are location and lag vectors, respectively, in domain of study. The assumption of stationarity requires that the proposed geostatistical model based on our sampled data, can adequately describe the behaviour of the population. The goal is to infer the population based on the sample data. So, we should make an informed decision regarding what information we can use to describe the region of interest, this is called the decision of stationarity (Kelkar and Perez, 2002). In geostatistical study two kinds of stationarities can be defined, they are first order and second order stationarities. The first order stationarity is as below:

$$E\{Z(\mathbf{u})\} = E\{Z(\mathbf{u}+\mathbf{h})\} = m$$

Where m is the mean of data. It means that the expected value of a random variable at $\mathbf{u}$ is the same as the expected value of a random variable $\mathbf{h}$ lag distance away. Therefore first order stationarity means that the expected value across the region is the same. If we divide the region into small subregions and calculate the mean within each subregion then the means should be approximately the same in the case of first order stationarity (Kelkar and Perez, 2002). If the mean varies significantly from a subregion to another subregion, then there is a trend in the data. One of the most important parts of geostatistical modelling is to find the correct trend model if the data show a systematic trend. The trend function can be developed by a regression technique, inverse distance weighting and moving window averaging. This trend should be removed before variogram modelling and geostatistical simulation. Second order stationarity uses the variance at each location, and it assumes that the variance is constant across the region. Therefore,

$$Var\{Z(\mathbf{u})\} = Var\{Z(\mathbf{u}+\mathbf{h})\} = \sigma^2$$

By using the first and second order stationarities the relationship between the covariance and variogram can be obtained:

$$\gamma(\mathbf{h}) = \sigma^2 - C(\mathbf{h})$$

Where $\sigma^2$is the variance of data, $\gamma(\mathbf{h})$ is the variogram and $C(\mathbf{h})$ is the covariance function.

The scaling law requires the assumption of stationarities. Journel and Huijbregts (1978) developed a series of theoretical concepts and theorems for volume scaling. Given two different volumetric supports v and V, there are three important concepts: dispersion variance $D^2(v,V)$, average variogram $\bar{\gamma}(v,V)$ and mean covariance $\bar{C}(v,V)$ which are defined as (Journel and Huijbregts, 1978):

$$D^2(v,V) = E\{[m_v - m_V]^2\}$$

$$\bar{\gamma}(v,V) = \frac{1}{v.V}\int_v \int_V \gamma(\mathbf{y}-\mathbf{y}').d\mathbf{y}.d\mathbf{y}'$$

$$\bar{C}(v,V) = \frac{1}{v.V}\int_v \int_V C(\mathbf{y}-\mathbf{y}').d\mathbf{y}.d\mathbf{y}'$$

Where m_v and m_V are average values at the scale v and V respectively. The average values of variogram, $\bar{\gamma}(v,V)$, and covariance, $\bar{C}(v,V)$, are the average values of the point variogram, $\gamma(\mathbf{h})$, and covariance, $C(\mathbf{h})$, where one extremity of the distance vector $\mathbf{h}$ falls in the volume of v and the other extremity independently falls in the volume of V. The following results are well known (Journel and Huijbregts, 1978):

$$D^2(v,V) = D^2(v,\Omega) - D^2(V,\Omega)$$

$$\sigma^2(v,V) = \bar{C}(v,v) - \bar{C}(V,V) = \bar{\gamma}(V,V) - \bar{\gamma}(v,v)$$

In above relations two assumptions are made, they are: (1) $\sigma^2(\cdot,\cdot) = 0$ and (2) $\bar{\gamma}(\Omega,\Omega) = D^2(\cdot,\Omega)$. "$\cdot$" denotes the point scale. There are other previous works on scaling law. Isaaks and Srivastava (1989) presented the scaling laws with a practical study. Deutsch and Frykman (1999) discuss variogram modeling at different scales.

Analytical Form of Univariate Marginals

Truncated Gaussian simulation (TGSIM) was first introduced by Matheron et al (1987) and then developed by Beucher et al (1993) and Xu and Journel (1993). The goal in TGSIM is to generate realizations of a continuous Gaussian variable and then truncate them at a series of thresholds to create categorical realizations. Suppose that a very fine scale facies model with K categories (facies) is created using TGSIM

and upscaled to a V scale using arithmetic averaging. The upscaled block contains V point scale data. K facies are assigned to these V points. These V points are correlated to each other using the covariance matrix, $\Sigma_{V\times V}$. The proportions of facies k for this upscaled block take values from the set $\left\{0,\frac{1}{V},,\dots,\frac{v}{V},\dots,\frac{V-1}{V},1\right\}$ with the probability mass function of $p_{k,v}$.

The univariate marginals, $p_{k,v}$, can be calculated using the combinatorial and counting techniques because of the discrete behavior of facies codes. The univariate marginal distribution of facies k for the upscaled block which contains V points is written and summarized as below:

$$p_{k,v}=\sum_{j=1}^{K^V}\delta[v_k(j),v].p(j)\ ;\ k=1,\dots,K\ \&\ v=0,1,\dots,V$$

In Microsoft Excel 2007 the function for $p_{k,v}$ can be written as below:

$$\begin{cases}p_{k,v}=SUMIF(range,criteria,[sum\_range])\\range=v_1(j),\dots,v_K(j)\\criteria=n\\[sum\_range]=p(1),\dots,p(K^V)\end{cases}$$

Where $p(j)$ is the integral below the $V-$ variate Gaussian distribution of point scale locations for the probability class index j and can be calculated as below:

$$p(j)=\int_{a_{k,k_V(j)-1}}^{x_{c,k_V(j)}}\dots\int_{x_{c,k_v(j)-1}}^{x_{c,k_v(j)}}\dots\int_{x_{c,k_1(j)-1}}^{x_{c,k_1(j)}}g_X(x_1,\dots,x_v,\dots,x_V).dx_1\dots dx_v\dots dx_V$$

$\delta[v_k(j),v]$ is the Dirac delta function with the value of 0 or 1 based on the below definition:

$$\delta[v_k(j),v]=\begin{cases}1 & ;\ if\ v_k(j)=v\\0 & ;\ if\ v_k(j)\neq v\end{cases}\ ;\ v=0,1,\dots,V$$

$v_k(j)$ is the total number of facies k which make the probability class index j :

$$v_k(j)=\sum_{v=1}^{V}\delta[k_v(j),k]$$

Again $\delta[k_v(j),k]$ is the Dirac delta function with value of 0 or 1 based on the following definition:

$$\delta[k_v(j),k]=\begin{cases}1 & ;\ if\ k_v(j)=k\\0 & ;\ if\ k_v(j)\neq k\end{cases}\ ;\ k=1,\dots,K$$

In Microsoft Excel 2007 the function for $v_k(j)$ can be written as below:

$$\begin{cases}v_k(j)\ =COUNTIF(range,criteria)\\range=k_1(j),\dots,k_V(j)\\criteria=k\end{cases}$$

$k_v(j)$ is the vth index of the probability class index j and can be written as:

$$j=1+\sum_{v=1}^{V}[k_v(j)-1].K^{v-1}\quad\rightleftarrows\quad k_v(j)=1+int\left(\frac{j-1}{K^{v-1}}\right)-K.int\left(\frac{j-1}{K^v}\right)$$

The $V-$ variate Gaussian distribution of point scale locations is defined as:

$$g_X(x_1,\dots,x_V)=\frac{1}{\sqrt{(2\pi)^V.|\Sigma|}}.exp\left[-\frac{1}{2}(\boldsymbol{x})^T.\Sigma^{-1}.(\boldsymbol{x})\right]$$

$$\boldsymbol{x}=\begin{bmatrix}x_1\\x_2\\\vdots\\x_{V-1}\\x_V\end{bmatrix}_{N\times N}\ \text{and}\ \Sigma=\begin{bmatrix}1 & \rho_{1,2} & \dots & \rho_{1,V-1} & \rho_{1,V}\\\rho_{2,1} & 1 & \dots & \rho_{2,V-1} & \rho_{2,V}\\\vdots & \vdots & \ddots & \vdots & \vdots\\\rho_{V-1,1} & \rho_{V-1,2} & \dots & 1 & \rho_{N-1,V}\\\rho_{V,1} & \rho_{V,2} & \dots & \rho_{V,V-1} & 1\end{bmatrix}_{V\times V}\ \text{and}\ \Sigma\ \text{is symmetric.}$$

Example

Suppose that we have three facies categories and the number of point scale values is two (scale), therefore $K=3,V=2$. The 3^2different probability classes are shown in Figure 4.

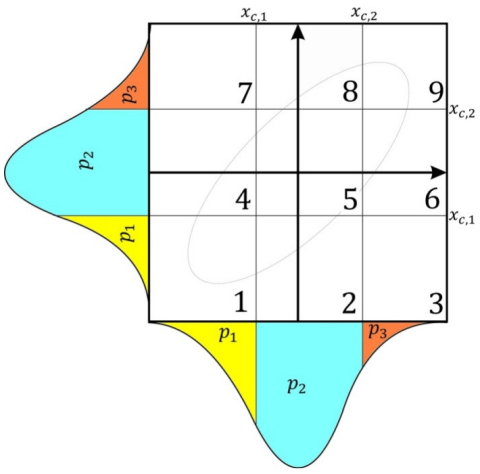

Figure 4 Nine different probability classes in the case of three facies and two point scale facies model

Below table shows the formulas for the univariate marginals of multivariate multiscale facies proportions, $p_{k,v}$:

k	v	$p_{k,v}$
1	0	$p_{1,0} = p(5)+p(6)+p(8)+p(9)$
1	1	$p_{1,1} = p(2)+p(3)+p(4)+p(7)$
1	2	$p_{1,2} = p(1)$
2	0	$p_{2,0} = p(1)+p(3)+p(7)+p(9)$
2	1	$p_{2,1} = p(2)+p(4)+p(6)+p(8)$
2	2	$p_{2,2} = p(5)$
3	0	$p_{3,0} = p(1)+p(2)+p(4)+p(5)$
3	1	$p_{3,1} = p(3)+p(6)+p(7)+p(8)$
3	2	$p_{3,2} = p(9)$

Another example is also presented using two facies and three point scale locations $K = 2, V = 3$, therefore we have 2^3different probability classes. Table below shows formulas for the univariate marginals of multivariate multiscale facies proportions, $p_{k,v}$:

k	v	$p_{k,v}$
1	0	$p_{1,0} = p(8)$
1	1	$p_{1,1} = p(4)+p(6)+p(7)$
1	2	$p_{1,2} = p(2)+p(3)+p(5)$
1	3	$p_{1,3} = p(1)$
2	0	$p_{2,0} = p(1)$
2	1	$p_{2,1} = p(2)+p(3)+p(5)$
2	2	$p_{2,2} = p(4)+p(6)+p(7)$
2	3	$p_{2,3} = p(8)$

Future work

Jointing these univariate marginal distributions in such a way that all of marginal distributions (k variate) are honored and correct in the presence of sum to unity and spatial correlation of data constraints with and without assumption of data conditioning might be the future work. The same algorithm can be performed to get the bivariate, trivariate, etc marginal distributions. This work can improve the facies simulation techniques at scales where mixing of facies is important and facies are not mutual exclusive any more.

List of Notations

$p_{k,v}$: The univariate marginal probability mass function for facies k at the scale of v

$p(j)$: The probability of class index j

v : Discrete random variable (location index) for all of the formula presented the range of v is $0,1,\dots,V$ except for $k_v(j)$ which has the range of $1,\dots,V$.

j : Probability class index with the range of $0,1,\dots,K^V$

K : Total number of facies ($K \geq 2$)

V : Total number of nodes in the upscaled block of interest (scale index)

$k_v(j)$: The vth component for the probability class index;

$$j \equiv \left(k_1(j),\dots,k_v(j),\dots,k_V(j)\right)$$

The $k_v(j)$ values are between 1 to K

$v_k(j)$: The total number of facies k in probability class j

The $v_k(j)$ values are between 0 to V

$x_{c,k_v(j)}$: The $k_v(j)-th$ threshold for truncating the simulated Gaussian values; for the notation purposes it is assumed that $x_{c,0}=-\infty$, $x_{c,K}=+\infty$

$\boldsymbol{x}$: The $V \times 1$ vector of stationary standard (zero mean and unit variance) multivariate normal RF

Σ : $V \times V$ covariance matrix between locations to be upscaled

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