Likelihood analysis for a class of spatial geostatistical compositional models

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Abstract

We propose a model-based geostatistical approach to deal with regionalized compositions. We combine the additive-log-ratio transformation with multivariate geostatistical models whose covariance matrix is adapted to take into account the correlation induced by the compositional structure. Such specification allows the usage of standard likelihood methods for parameters estimation. For spatial prediction we combined a back-transformation with the Gauss-Hermite method to approximate the conditional expectation of the compositions. We analyze particle size fractions of the top layer of a soil for agronomic purposes which are typically expressed as proportions of sand, clay and silt. Additionally a simulation study assess the small sample properties of the maximum likelihood estimator.

Keywords: `Compositional data`, `geostatistical models`, `maximum likelihood`, `regionalized composition`.

1. Introduction

Compositional data are vectors of proportions, specifying fractions of a whole whose elements typically sum to one or 100%. Given the nature of this data, the direct application of usual statistical techniques based on the Gaussian multivariate distribution on the composition values is not suitable. As pointed out by Aitchison (1986), the constant sum constraints not only invalidate the assumption that our response variables are drawn from unbounded random processes, but also induce negative correlations between response variables.

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Compositional data are frequent in earth sciences, such as, in mineralogy, agronomy, geochemistry and hydrology. In such applications, not rarely, compositions are recorded along with their spatial locations, and spatial patterns are of interest, characterizing what is called regionalized compositions (Pawlowsky, 1989). Models accounting for spatial patterns should account for both, the correlation induced by the composition structure and the spatial correlation at a suitable scale.

Practical analysis of compositional data is, in general, based on the seminal work of Aitchison (1982) and the comprehensive monograph by Aitchison (1986). Barceló-Vidal et al. (2001) presented the mathematical background of compositional data as equivalence classes. Further mathematical developments include the definitions of Euclidean vector space structure Pawlowsky-Glahn and Egozcue (2001) and isometric logratio transformation Egozcue et al. (2003). The R package `compositions` (van ver Boogaart and Tolosana-Delgado, 2006) provides a complete toolbox for analysis of compositional data including facilities to deal with regionalized compositions (van den Boogaart and Tolosana-Delgado, 2013).

The literature about regionalized compositions is concentrated around the contributions of Pawlowsky (Pawlowsky, 1989; Pawlowsky and Burger, 1992; Pawlowsky et al., 1995) and its applications (Odeh et al., 2003; Lark and Bishop, 2007). The monograph Pawlowsky-Glahn and Olea (2004) presented the state of the art for the analysis of regionalized compositional data in the year 2000. Tjelmeland and Lund (2003) proposed a model-based approach for the analysis of spatial compositional data under the Bayesian framework. Further developments and references can be found in Tolosana-Delgado (2006) and Pawlowsky-Glahn et al. (2015).

The approach adopted in (Pawlowsky-Glahn and Olea, 2004) can be summarized in three steps: (i) given a vector of B regionalized compositions apply the additive-log-ratio transformation (Aitchison, 1986). (ii) for the transformed vector use the orthodox cokriging approach (Wackernagel, 1998). (iii) adopt an unbiased back-transformation to predict the compositions back on the original compositional scale. Examples of this approach with emphasis on step (iii) can be found in Lark and Bishop (2007). Such approach include the usage of traditional geostatistical techniques with parameter estimation based on the variogram and cross-variogram methods. Alternatively, a model-based geostatistical approach (Diggle et al., 1998) can be considered, allowing the adoption of likelihood based or Bayesian statistical methods for estimation and prediction, inheriting related properties of consistency, asymptotic normality and efficiency. The application of maximum likelihood inference in geostatistics offers several advantages: The method may focus on the parameters of interest (sill, range, anisotropy angle, etc.). The uncertainty of the estimates is easily assessed. The log-likelihood function may be used for model selection. The method is more efficient than others including the variogram and moments-based methods in mean square error terms. The method can also be used for optimum sample design. For more references discussing the advantages of maximum likelihood in the context of geostatistical models, see Pardo-Igúzquiza (1998); Stein (1999); Diggle and Ribeiro Jr (2007).

We adopt the model-based approach to deal with regionalized compositions. Following the aforementioned approach, we apply the additive-log-ratio transformation to obtain transformed response variables, for which we specify a common spatial component multivariate geostatistical model (Diggle and Ribeiro Jr, 2007). For estimation of the model parameters we adopt the maximum likelihood method. For spatial prediction,

we adopt the approach proposed by Pawlowsky-Glahn and Olea (2004) combining a back-transformation and the Gauss-Hermite method to approximate the conditional expectation of the compositions. We also obtain simulations of the predictive distributions. Our approach produces predictions satisfying the required constant sum constraints and has interpretable parameters in the scale of the transformed response variables. We apply our model to analyse a data set about the distribution of mineral particles in the soil. We also present a simulation study to verify the small sample properties of the maximum likelihood estimator.

Section 2 presents the compositional geostatistical model along with the estimation and spatial prediction procedures. In Section 3 we apply the proposed model to analyse a real data set. Section 4 presents the simulation study. Finally, Section 5 provides some discussions and recommendations for future works. We provide the R code and data set in the supplementary material.

2. The geostatistical compositional model

In this section we describe the geostatistical compositional model as an extension of the bivariate Gaussian common component geostatistical model (Diggle and Ribeiro Jr, 2007). Let $\boldsymbol{X}(\boldsymbol{u})$ be an $n \times B$ matrix of regionalized compositions at spatial locations $\boldsymbol{u} = (u_1, \ldots, u_n)^\top$ i.e., $\boldsymbol{X}_j(\boldsymbol{u}_i) > 0$ and $\sum_{j=1}^{B} \boldsymbol{X}_j(\boldsymbol{u}_i) = 1$ for $i = 1, \ldots, n$. Let $\boldsymbol{Y}(\boldsymbol{u})$ denote an $n \times (B-1)$ matrix of transformed regionalized compositions obtained by the application of the additive-log-ratio transformation on each row of $\boldsymbol{X}(\boldsymbol{u})$. Furthermore, let $\mathcal{Y}(\boldsymbol{u}) = (\boldsymbol{Y}_1(\boldsymbol{u})^\top, \ldots, \boldsymbol{Y}_{B-1}(\boldsymbol{u})^\top)^\top$ be the $n(B-1) \times 1$ stacked vector of transformed regionalized compositions by columns. The geostatistical compositional model assumes that $\mathcal{Y}(\boldsymbol{u})$ is multivariate Gaussian distributed with vector of mean $\boldsymbol{\mu} = (\boldsymbol{D}_1 \boldsymbol{\beta}_1^\top, \ldots, \boldsymbol{D}_{B-1} \boldsymbol{\beta}_{B-1}^\top)^\top$ and covariance matrix $\boldsymbol{\Sigma}$ given by the components,

$$\text{Cov}(\boldsymbol{Y}_r(\boldsymbol{u}_i); \boldsymbol{Y}_r(\boldsymbol{u}_i)) = \sigma_r^2 + \tau_r^2, \qquad \text{Cov}(\boldsymbol{Y}_r(\boldsymbol{u}_i); \boldsymbol{Y}_r(\boldsymbol{u}_{i'})) = \sigma_r^2 \rho(u, \phi), \qquad (1)$$

and

$$\text{Cov}(\boldsymbol{Y}_r(\boldsymbol{u}_i); \boldsymbol{Y}_{r'}(\boldsymbol{u}_{i'})) = \sigma_r \sigma_{r'} \boldsymbol{I_2}(i, i') + \tau_r \tau_{r'} \boldsymbol{I_3}(i, i'), \qquad (2)$$

where the functions $\boldsymbol{I}_2$ and $\boldsymbol{I}_3$ are defined by

$$\boldsymbol{I_2}(i, i') = \left\{ \begin{array}{ll} 1 & , \text{ if } \ i = i', \\ \rho(u, \phi) & , \text{ if } \ i \neq i', \end{array} \right. \qquad \boldsymbol{I_3}(i, i') = \left\{ \begin{array}{ll} \rho_{rr'} & , \text{ if } \ i = i', \\ 0 & , \text{ if } \ i \neq i'. \end{array} \right.$$

respectively. Based on this specification the rth component of the transformed regionalized compositions is given by

$$\boldsymbol{Y}_r(\boldsymbol{u}_i) = \boldsymbol{D}_r \boldsymbol{\beta}_r + \sigma_r \boldsymbol{S}(\boldsymbol{u}_i; \phi) + \tau_r \boldsymbol{Z}, \qquad (3)$$

where $r = 1, \ldots, B - 1$. The model consists of the sum of fixed effects $\boldsymbol{D}_r \boldsymbol{\beta}_r$, spatially correlated $\boldsymbol{S}(\boldsymbol{u}_i; \phi)$ and uncorrelated $\tau_r \boldsymbol{Z}$ random effects. These effects are specified by Equation (1). The parameters τ_r^2 are sometimes called nugget effect. The $n \times p$ design matrix $\boldsymbol{D}_r$ contains values of p covariates and $\boldsymbol{\beta}_r$ is a $p \times 1$ vector of regression parameters.

The spatial random effect $\boldsymbol{S}(\boldsymbol{u}_i; \phi)$ is a unit variance Gaussian random field (GRF) with correlation function $\rho(u; \phi)$ where $\rho \in \Re^d$ is a valid correlation function parametrized

3

by ϕ with d being the dimension of the spatial domain. We assume in particular correlation functions for spatially continuous process depending only on Euclidean distance $u = ||u_i - u_{i'}||$ between pair of points. Popular choices are the exponential, Matérn and spherical. At last, Equation (2) describes the cross-covariance structure composed by a spatial component and a term inducing the cross-correlation, measured by the parameters $\rho_{rr'}$. It is important to highlight that the range parameter is assumed common for all components of the transformed regionalized compositions.

2.1. Estimation and Inference

In this section we describe the likelihood approach used to estimate the model parameters. We divide the set of parameters into two subsets, $\boldsymbol{\theta} = (\boldsymbol{\beta}^\top, \boldsymbol{\lambda}^\top)^\top$. In this notation $\boldsymbol{\beta} = (\boldsymbol{\beta}_1^\top, \ldots, \boldsymbol{\beta}_{B-1}^\top)^\top$ denotes a $P \times 1$ vector containing all regression parameters. Similarly, we let
$\boldsymbol{\lambda} = (\sigma_1^2, \ldots \sigma_{B-1}^2, \tau_1^2, \ldots, \tau_{B-1}^2, \phi, \rho_1, \ldots, \rho_{(B-1)(B-2)/2})^\top$ be a $Q \times 1$ vector of all covariance parameters. We use the convention to stack the correlation parameters $\rho_{rr'}$ by columns. For a vector of observed transformed regionalized compositions $\mathcal{Y}(\boldsymbol{u})$, the log-likelihood function is given by,

$$l(\boldsymbol{\theta}; \mathcal{Y}(\boldsymbol{u})) = -\frac{(n(B-1))}{2} \ln(2\pi) - \frac{1}{2} \ln|\boldsymbol{\Sigma}| - \frac{1}{2}(\mathcal{Y}(\boldsymbol{u}) - \boldsymbol{D}\boldsymbol{\beta})^\top \boldsymbol{\Sigma}^{-1}(\mathcal{Y}(\boldsymbol{u}) - \boldsymbol{D}\boldsymbol{\beta}). \quad (4)$$

The maximum likelihood estimator is obtained by the maximization of the log-likelihood function (4) with respect to the parameter vector $\boldsymbol{\theta}$ whose components are orthogonal (Hürlimann, 1992; D. R. Cox, 1987). For the regression parameters we can obtain a closed-form,

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{D}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{D})^{-1}(\boldsymbol{D}^\top \boldsymbol{\Sigma}^{-1} \mathcal{Y}(\boldsymbol{u})). \quad (5)$$

For the covariance parameters we adopt the `L-BFGS-B` algorithm as implemented in the `R` (R Core Team, 2015) function `optim()` for numerical maximization of the profile log-likelihood function obtained by substituting (5) in the expression (4). Note that, in order to have an authorized model, i.e. positive definite covariance matrix, we need to restrict the covariance parameters to the positive real values and the correlation parameter in the $(-1, 1)$ interval. For this reason, we used the `L-BFGS-B` algorithm, since this algorithm allows us to introduce these restrictions on the parameter space. The algorithm requires the calculation of the score function, first derivative of (4) with respect to the covariance parameters either numerically or analytically. We opt to compute the score function analytically obtaining

$$\frac{\partial l(\boldsymbol{\theta}; \mathcal{Y}(\boldsymbol{u}))}{\partial \boldsymbol{\lambda}_q} = -\frac{1}{2}\text{tr}\left(\boldsymbol{\Sigma}^{-1}\frac{\partial \boldsymbol{\Sigma}}{\partial \boldsymbol{\lambda}_q}\right) - \frac{1}{2}(\mathcal{Y}(\boldsymbol{u}) - \boldsymbol{D}\hat{\boldsymbol{\beta}})^\top \left(-\boldsymbol{\Sigma}^{-1}\frac{\partial \boldsymbol{\Sigma}}{\partial \boldsymbol{\lambda}_q}\boldsymbol{\Sigma}^{-1}\right)(\mathcal{Y}(\boldsymbol{u}) - \boldsymbol{D}\hat{\boldsymbol{\beta}}) \quad (6)$$

where $\frac{\partial \boldsymbol{\Sigma}}{\partial \boldsymbol{\lambda}_q}$ denotes the partial derivative of $\boldsymbol{\Sigma}$ with respect to the element $\boldsymbol{\lambda}_q$ for $q = 1, \ldots, Q$. Such derivatives are easily computed using matrix calculus (Wand, 2002).

Let $\hat{\boldsymbol{\theta}}$ be the maximum likelihood estimator of $\boldsymbol{\theta}$. Then the asymptotic distribution of $\hat{\boldsymbol{\theta}}$ is

4

$$\begin{pmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\lambda}} \end{pmatrix} \sim N\left(\begin{pmatrix} \boldsymbol{\beta} \\ \boldsymbol{\lambda} \end{pmatrix} ; \begin{pmatrix} \mathrm{I}_{\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}) & \mathbf{0} \\ \mathbf{0} & \mathrm{I}_{\boldsymbol{\lambda}}(\hat{\boldsymbol{\lambda}}) \end{pmatrix}^{-1}\right) \tag{7}$$

where $\mathrm{I}_{\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}) = \boldsymbol{D}^{\top}\hat{\boldsymbol{\Sigma}}\boldsymbol{D}$ and $\mathrm{I}_{\boldsymbol{\lambda}}(\hat{\boldsymbol{\lambda}})$ are the Fisher information matrices for $\boldsymbol{\beta}$ and $\boldsymbol{\lambda}$, respectively. The adopted asymptotic regime is compatible with the increasing domain framework, for further references see Chang et al. (2013); Pardo-Igúzquiza (1998); Diggle and Ribeiro Jr (2007). It is not possible to obtain a closed-form for $\mathrm{I}_{\boldsymbol{\lambda}}(\hat{\boldsymbol{\lambda}})$. Thus, we replace it by the observed information matrix obtained numerically using the Richardson method as implemented in the R package numDeriv (Gilbert and Varadhan, 2012).

We shall show in Section 4 through of simulation studies that often this type of asymptotic result does not work well for covariance parameters. In the context of geostatistical analysis of compositional data we are particularly interested in the covariance parameters. Thus, we recommend to use the profile likelihood approach to compute confidence intervals for covariance parameters, mainly when analysing small or medium sized data sets. Details about how to implement profile likelihood computations in R can be found in Bolker (2012).

2.2. Spatial prediction

In this section we describe the spatial prediction in the context of geostatistical compositional models. The procedure we shall present in this section is often called additive logistic normal kriging or ALN-kriging for short (Tolosana-Delgado, 2006; Pawlowsky-Glahn and Olea, 2004). The objective is to predict the values of $\mathcal{Y}_0(\boldsymbol{u}_0)$ additional random variables at any arbitrary spatial locations $\boldsymbol{u}_0$ within the study region. The best linear unbiased predictor of $\mathcal{Y}_0(\boldsymbol{u}_0)$ is the conditional expectation of $\mathcal{Y}_0(\boldsymbol{u}_0)|\mathcal{Y}(\boldsymbol{u})$ whose expression is presented in Equation (8) along with the expression for the conditional covariance. We suppress the spatial indexes for convenience.

$$\mathrm{E}(\mathcal{Y}_0|\mathcal{Y}) = \mathrm{E}(\mathcal{Y}_0) + \boldsymbol{\Sigma}_{\mathcal{Y}_0\mathcal{Y}}\boldsymbol{\Sigma}_{\mathcal{Y}\mathcal{Y}}^{-1}(\mathcal{Y} - \mathrm{E}(\mathcal{Y})), \qquad \mathrm{Cov}(\mathcal{Y}_0|\mathcal{Y}) = \boldsymbol{\Sigma}_{\mathcal{Y}_0\mathcal{Y}_0} - \boldsymbol{\Sigma}_{\mathcal{Y}_0\mathcal{Y}}\boldsymbol{\Sigma}_{\mathcal{Y}\mathcal{Y}}^{-1}\boldsymbol{\Sigma}_{\mathcal{Y}\mathcal{Y}_0}. \tag{8}$$

In practice, the unknown parameters in the expectation and covariance structures are replaced by the maximum likelihood estimates. Note that from this procedure we obtain predictions for the stacked regionalized transformed compositions at non-observed spatial locations $\boldsymbol{u}_0$. The next objective is to back-transform these predictions to the original composition scale i.e., the unit simplex. For a single spatial location, let $\boldsymbol{\mu}_{\boldsymbol{Y}}$ and $\boldsymbol{\Sigma}_{\boldsymbol{Y}}$ be the expectation and covariance matrix of the additive-log-ratio transformed variable $\boldsymbol{Y}$ obtained by Equation (8). The probability density function of $\boldsymbol{X}$ is given by

$$f(\boldsymbol{X}) = (2\pi)^{-\frac{B-1}{2}}|\boldsymbol{\Sigma}_{\boldsymbol{Y}}|^{-\frac{1}{2}}\exp\left\{-\frac{1}{2}(\mathrm{alr}(\boldsymbol{X}) - \boldsymbol{\mu}_{\boldsymbol{Y}})^{\top}\boldsymbol{\Sigma}_{\boldsymbol{Y}}^{-1}(\mathrm{alr}(\boldsymbol{X}) - \boldsymbol{\mu}_{\boldsymbol{Y}})\right\}\left(\prod_{i=1}^{B} X_i\right)^{-1}, \tag{9}$$

where $\mathrm{alr}(\boldsymbol{X})$ denotes the additive-log-ratio transformation applied on the vector of compositions $\boldsymbol{X}$. The Equation (9) is recognizable as the multivariate Gaussian distribution with an additional term, which is the Jacobian of the back-transformation (Pawlowsky-Glahn and Olea, 2004). By assuming that the B-part simplex is a constraint subset of

5

the B-dimensional real space, along with the induced Euclidean geometry and Lebesgue measure, an unbiased predictor of $\boldsymbol{X}$ can be obtained by computing the expectation of $\boldsymbol{X}$ i.e.,

$$\mathrm{E}(\boldsymbol{X}) = \int \boldsymbol{X} f(\boldsymbol{X}) d\boldsymbol{X}, \tag{10}$$

we adopt the Gauss Hermite method to solve the intractable integral. Basically, the Gauss Hermite method changes the intractable integral by a weighted finite sum,

$$\int_{\Re^{B-1}} f(\boldsymbol{G}) \exp\left\{-\boldsymbol{G}\boldsymbol{G}^\top\right\} d\boldsymbol{G} \approx \sum_{i_1=1}^{K} \cdots \sum_{i_{(B-1)}=1}^{K} w_{i_1}, \ldots, w_{i_{(B-1)}} f(G_{i_1}, \ldots, G_{i_{(B-1)}}), \tag{11}$$

where K is the number of points used for the approximation, $\boldsymbol{G}$ are roots of the Hermite polynomial $H_k(\boldsymbol{G})(i = 1 < 2, ..., K)$ and w_i are weights given by,

$$w_i = \frac{2^{K-1} K! \sqrt{\pi}}{K^2 [H_K(G_i)]^2}.$$

The Gauss Hermite method is easily implemented in R, as the function `gauss.quad()` from package `statmod` (Smyth et al., 2013) provides the weights and the Gauss Hermite points. Pawlowsky-Glahn and Olea (2004) show that the auxiliary function $f(\boldsymbol{G})$ required in Equation (11) is given by,

$$f(\boldsymbol{G}) = \pi^{-\frac{B-1}{2}} \mathrm{agl}(\sqrt{2}\boldsymbol{R}^\top \boldsymbol{G} + \boldsymbol{\mu_Y}), \tag{12}$$

where agl denotes the additive generalized logistic (back-transformation) and $\boldsymbol{R}$ denotes the Cholesky decomposition of $\boldsymbol{\Sigma_Y}$. Note that, the agl back-transformation guarantees that the predicted values satisfy the required constant sum constraints (Odeh et al., 2003). A related matter corresponds to the calculation of confidence intervals for the predicted compositions. There is no straightforward way to build consistent and optimal confidence intervals for the predicted compositions. In general, it is due to the assumed space structure of the data support, i.e. bounded values, modelled by assuming the additive logistic normal distribution, which in turn assumes to be embedded in the whole real space, with the usual real space structure and Lebesgue measure. For a detailed discussion about the limitations of ALN-kriging as well as assumed conditions, we refer the interested reader to (Tolosana-Delgado, 2006). In this paper, we do not pursue in this problem, however, we present an alternative approach based on Monte Carlo simulation of the predictive distribution.

Our approach follows the lines of (Tjelmeland and Lund, 2003), thus for estimated $\boldsymbol{\mu_Y}$ and $\boldsymbol{\Sigma_Y}$ simulating values from this multivariate Gaussian distribution is straightforward. We denote simulated values by $\boldsymbol{Y}_s$. We apply the back-transformation on the simulated values to obtain values $\boldsymbol{X}_s$. An unbiased predictor of $\boldsymbol{X}$ is the sample mean of $\boldsymbol{X}_s$. An appealing feature is that prediction of other quantities of interest, linear and non-linear can be also obtained applying the functional of interest to the simulated values. Furthermore, confidence intervals for the predicted compositions can be replaced by intervals based on quantiles, which in turn are easily obtained based on the simulated values.

3. Data analysis

In this section we report analysis of particle size fractions of sand, silt and clay measured at an experimental plot within the Areão experimental farm belonging to the Escola Superior de Agricultura Luiz de Queiroz, Piracicaba, São Paulo State, Brazil. The soil was sampled in the soil layer of 0 to 20 centimetres at 82 points and on a regular grid with 20 metres spacing, Figure 1 shows the data as a ternary diagram, histograms for each component of the composition along with normal quantile plot and a scatterplot for the transformed response variables.
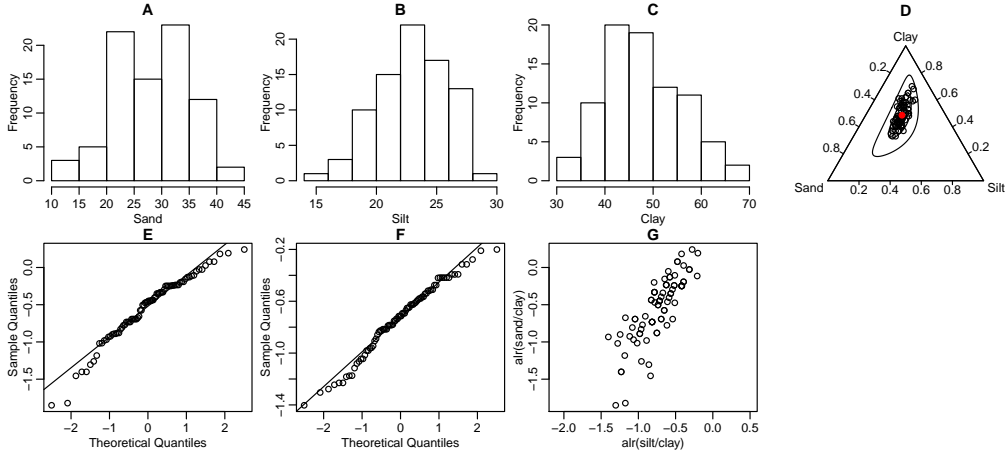

Figure 1: Histograms (A to C) for the proportions of sand, silt and clay. Ternary diagram and geometric mean (red dot) of particle size fractions (D). Normal quantile plot for the additive-log-ratio (alr) transform of sand (E) and silt (F) contents, with clay as the denominator of the ratio. Scatterplot relating the alr transform of sand over clay with alr transform of silt over clay (G).

The silt fractions have smaller values and variability whereas clay is the predominant component with the largest variability. In general the Normal quantile plots (E and F) support our assumption of marginal Gaussian distribution for the transformed response variables. The scatterplot shows a clear positive correlation between the transformed response variables. This example illustrates a fairly common situation in agriculture where the application of geostatistical compositional model is required. The distribution of mineral particles between size fractions, typically sand, silt and clay, affects many properties of the soil, such as water relations, chemistry, organic carbon dynamics and mechanical properties. In general the main goal of this type of spatial analysis is to predict the particle size fractions of the soil at a grid covering the area to define areas for possible different management practices. Interest can be in mean values, maxima and minima as well as exceedance of critical values.

We computed the additive-log-ratio transform of sand and silt contents, with clay, the most abundant content, as the denominator of the ratio. For the transformed regionalized compositions we fitted the geostatistical compositional model with exponential correlation function. Parameter estimates, standard errors (SE) and asymptotic 95% confidence intervals are shown in Table 1.

Table 1: Parameter estimates, standard errors (SE) and asymptotic 95% confidence intervals.

Parameter	Estimate	SE	2.5%	97.5%
β_1	-0.7864	0.2561	-1.2883	-0.2845
β_2	-0.7943	0.0694	-0.9304	-0.6583
σ_1	0.4705	0.1827	0.1125	0.8285
σ_2	0.1168	0.0690	-0.0185	0.2520
τ_1	0.2838	0.0491	0.1875	0.3800
τ_2	0.2619	0.0220	0.2187	0.3050
ϕ	81.4365	80.4313	-76.2059	239.0789
ρ	0.9589	0.0559	0.8492	1.0685

Following the notation introduced in the Section 2, β_1 and β_2 denote the means for the transformed response variables `alr(Sand/Clay)` and `alr(Silt/Clay)`, respectively. Results on Table 1 show that the variability of the first transformed component is larger than of the second. The cross-correlation is large and the proportion of variability attributed to the spatial effect is larger for the first component. The value of the common range parameter $\hat{\phi} = 81.43$ indicates the presence of spatial structure, although the asymptotic confidence interval include artefactual negative values. Artefactual negative values are also included in the confidence interval for σ_2. It is a well-known result that, in general, the asymptotic result (7) does not work well for covariance parameters, specially with small data sets, such are the data considered here. We recommend to use the profile likelihoods to quantify the uncertainty associated with these estimates. Figure 2 shows profile likelihoods expressed in terms of the square root of the profile deviances for the covariance parameters in the geostatistical compositional model considered here.
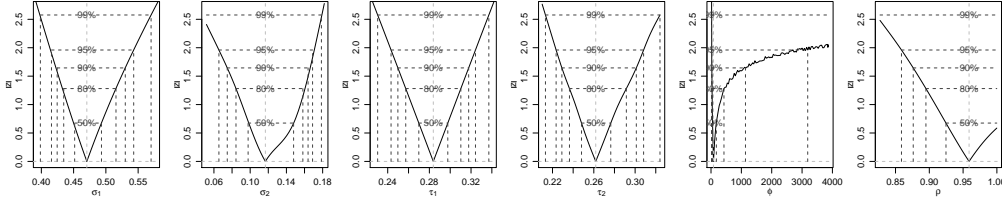

Figure 2: Profile likelihoods for covariance parameters.

The plots in Figure 2 are compatible with a quadratic profile likelihood except for the range parameter ϕ that show a heavy right tail. The results confirm the worth of the spatial effect. Based on the fitted model and using the two methods described in Section 2.2 we perform the spatial prediction of the compositions. Maps of predicted values are shown in Figure 3.

In general the results returned by the two approaches agree. Predictions based on simulations are a noisy version of the ones obtained with the Gauss-Hermite method.

The results obtained by Monte Carlo methods are reassuring in the sense they validate the integral approximations. Furthermore, they allow for computing not only predicted means and variances but also general predictands which otherwise would be prohibited by analytical methods. A typical example is the prediction of non-linear functions of
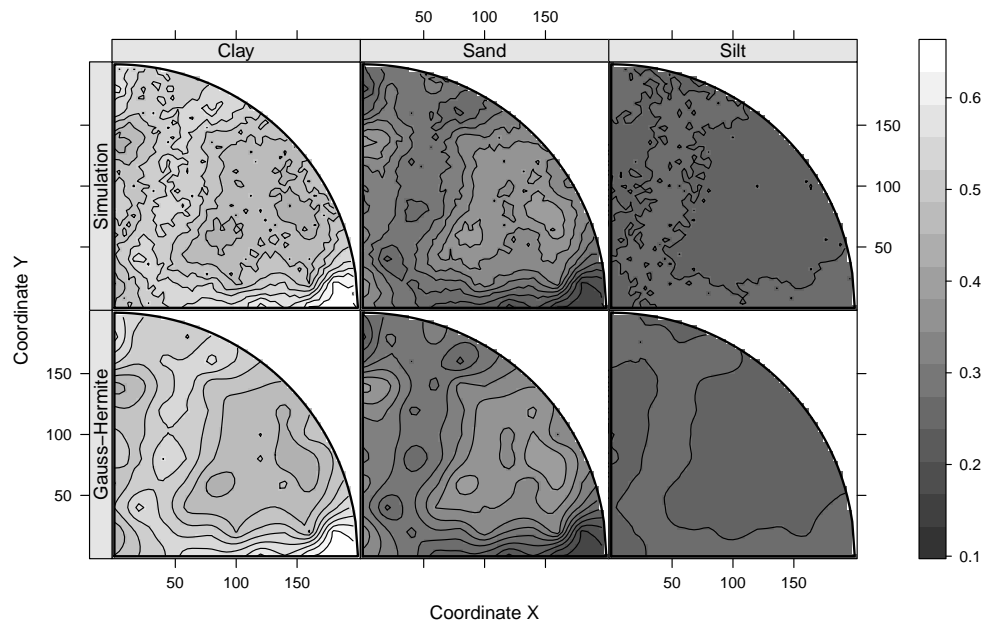
Figure 3: Prediction maps of particle size fraction of clay, silt and sand by Gauss Hermite and simulation methods.

the underlying fields. In order to illustrate this fact, we show in Figure 4 the prediction maps of the 5% and 95% quantile values for the soil fractions. Such quantities can be even more important than the means for defining soil classifications and management.
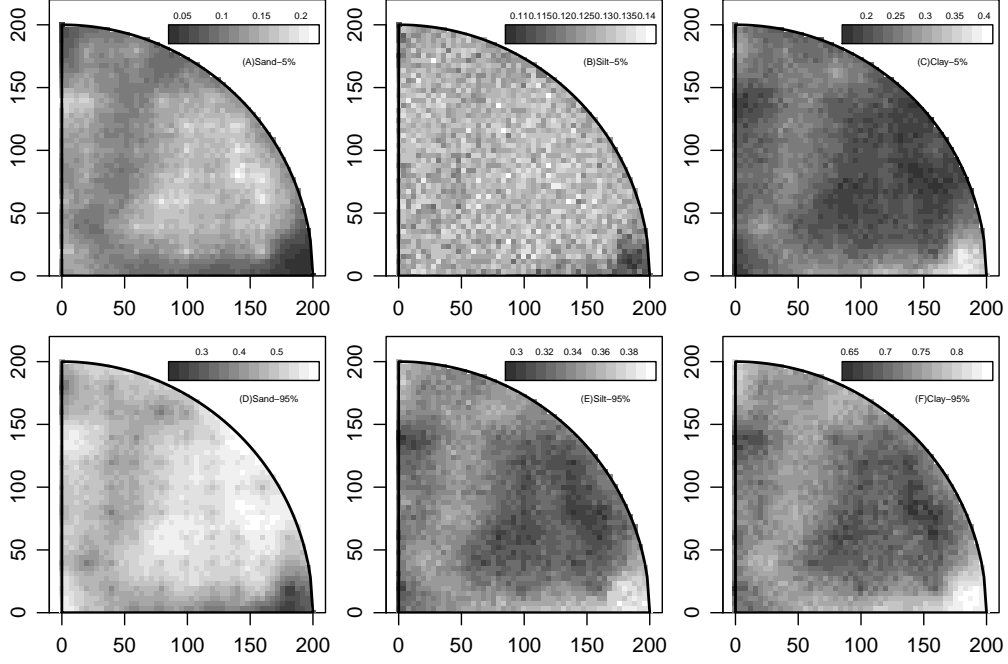

Figure 4: Prediction maps of the 5% and 95% quantile values of particle size fraction of sand, silt and clay.

4. Simulation study

We now turn to a simulation study to evaluate the bias and coverage rate of the maximum likelihood estimators in the context of geostatistical compositional models. We simulated 1000 data sets considering compositions with $B = 3$ components along with two sample sizes $n = 100$ and $n = 250$. We show results for data simulated on a regular grid within the unit squared and adopt the exponential correlation function. We also consider three parameter configurations, in order to obtain different patterns of the compositional data. Table 2 presents the parameter values and Figure 5 shows ternary diagrams for one sample of each of the configurations.

Table 2: Parameters values used in the simulation study.

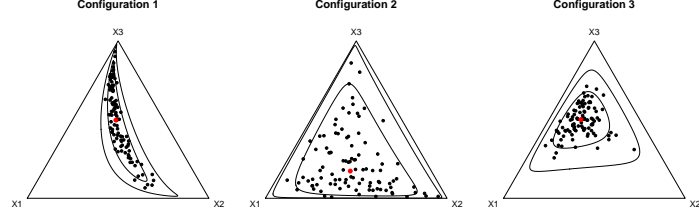| Configuration	β_1	β_2	σ_1	σ_2	τ_1	τ_2	ϕ	ρ
1	-0.2	-0.5	1	1.5	0.3	0.3	0.25	0.9
2	1	1	1.2	1.5	0.9	0.5	0.25	0.5
3	-0.5	-1	0.45	0.13	0.3	0.5	0.1	0

10

Figure 5: Ternary diagrams and geometric mean (red dot) of data simulated from each parameter set considered in the simulation study.

The configurations 1, 2 and 3 generate samples which displays the ternary diagram: concentrated in the middle, spread all over and concentrated on the left side, respectively.

For each parameter configuration we simulated 1000 data sets and fit the geostatistical compositional model proposed in Section 2. The confidence intervals were obtained using the asymptotic result (7). Table 3 presents the bias and coverage rate by sample size and parameter set.

Table 3: Bias (BS) and coverage rate (CR) by sample size and parameter set.

| Parameter | Configuration 1 | | | | Configuration 2 | | | | Configuration 3 | | | |
| | n = 100 | | n = 225 | | n = 100 | | n = 225 | | n = 100 | | n = 225 | |
	BS	CR	BS	CR	BS	CR	BS	LC	BS	CR	BS	CR
σ_1	-.067	.909	-.050	.853	-.035	.966	-.059	0.912	-.048	.814	.009	.894
σ_2	-.101	.901	-.077	.834	-.046	.974	-.072	0.916	-.005	.962	.005	.957
τ_1	.004	.881	-.026	.878	-.120	.964	-.051	0.966	-.039	.788	-.062	.945
τ_2	-.004	.891	-.042	.897	-.179	.960	-.073	0.980	-.021	.956	-.007	.958
ϕ	-.001	.868	-.019	.776	-.029	.732	-.037	0.718	.039	.902	-.004	.807
ρ	-.021	.868	.004	.931	-.400	.926	-.108	0.978	-.109	.924	-.134	.973

The results show that the maximum likelihood estimators underestimate the covariance parameters at all cases. The largest bias appears in the configuration 2 and for the cross-correlation parameter. In general, as expected, the bias decreases when the sample size increases. For most cases the coverage rate is slightly smaller than the expected nominal level (95%) with worse results for the range parameter.

5. Discussion

We presented a model-based geostatistical approach to deal with regionalized compositional data. The model combines the additive-log-ratio transformation and multivariate geostatistical models whose covariance structure was adapted to take into account for the correlation induced by the compositional structure. This allows for the use of standard likelihood methods for estimation of the model parameters. A critical point in the analysis of regionalized compositional data is the spatial prediction. We adopted the approach

11

proposed by Pawlowsky-Glahn and Olea (2004) combining a back-transformation and the Gauss-Hermite method to approximate the conditional expectations.

We also obtain simulations of the predictive distribution which can be used for assessing quality of the results given the analytical approximation of the back-transformation and, possibly more important, to obtain predictions of general functionals of interest. The simulation approach also provides a straightforward way to estimate the conditional probability of discrete textural classes Lark et al. (2012). Results of the predictions returned by our model satisfies the required constant sum constraints.

We applied the geostatistical compositional model to analyse a data set about particle size fractions of sand, silt and clay. In general, in this type of analysis the main goal is to obtain predictions for the fractions in a form of a map covering the study area. We showed through the data set that the two presented prediction methods provide similar and reasonable results. Through a simulation study we showed that in general the maximum likelihood estimators have a small negative bias for the covariance parameters. The coverage rate is slightly smaller than the expected nominal level. Thus, we recommend to use the profile likelihood approach to quantify the uncertainty associated with these estimates, mainly when analysing small and medium data sets.

The proposed model is based on the additive-log-ratio transformation. Thus, the last component in the composition is treated differently from the other elements. In our data set example, we opted to take the clay as the denominator of the ratio. Such a choice was based on the fact that the clay is the most abundant component of our compositions, which in turn makes the computation of the additive-log-ratio more stable computationally. We also fitted the models using sand and silt as the denominator of the ratio. In general, the predictions were virtually the same. However, further studies are required to conclude if it was a particular result for our data set or a general feature of the model based on the additive-log-ratio transformation.

Possible topics for further investigation and extensions include to improve the R code, and to increase the flexibility of the spatial modelling by allowing alternatives correlation functions, as the Matérn and spherical. Also, there is scope for the development of model-based inferential approach for models based on the Aitchison geometry such as presented in Pawlowsky-Glahn et al. (2015). The computational overhead are due to computations with the dense variance-covariance matrix. This overhead may be alleviated by adopting methods such as covariance tapering (Furrer et al., 2006; Kaufman et al., 2008), predictive processes (Eidsvik et al., 2012), low rank kriging (Cressie and Johannesson, 2008) and SPDE models (Lindgren et al., 2011).

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Supplementary material

http://leg.ufpr.br/doku.php/publications:papercompanions:compositional