ODDS AND ENDS OF VARIOGRAM MODELLING

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Introduction

Although modelling and estimation of the variogram is the most crucial step of kriging, the standard methodology lacks solutions for all day problems of variogram estimation. These problems include the unbiased estimation of the variogram in the presence of external drift, the handling of clearly nonstationary random fields, simple unbiased estimation of the sill, precision of the estimated variogram and the kriging error for non Gaussian processes, spatial hypothesis testing, and optimal prediction with estimated variogram.

Prior knowledge

A good geostatistical analysis is not only based on the observed data, but also on our scientific knowledge of the landscape under consideration. In most cases we have a conceptual physical model of genesis of our random field, although our physical understanding is not deep enough to express the landscape as the unique solution of physically motivated differential equations. However the conceptual model gives us some qualtitative prior information, such as assumed stationarity or isotropy, as crucial ingredients of the variogram modeling process. Both come from the supposition that the randomness should have the same symmetry properties as the underlying physics.

Kriging with nonstationary trend models

Physical laws are invariant under translation (stationarity) and rotation (isotropy). Anyway in many real cases the random field under consideration physically depends on some well known external influence such as the local topography (and derived quantities such as direction of water flow or sun exposition), geology or mineralogy. In this cases we could still assume stationarity, when the underling influence is stationary as well, however the process conditional to the surrounding geology is by no means stationary and we ignore our geological knowledge when disregarding this secondary information. A first and simple way to take secondary information into account is universal kriging with external drift or cokriging. While universal kriging leads to difficult problems in variogram estimation, cokriging imposes the additional assumption for the influence process to be stationary. A method for variogram estimation with nonstationary trend models was proposed in (Boogaart and Brenning 2001).

Many ideas to estimate the variogram in case of trend models can be found in literature as shown in (Boogaart, Brenning 2001) most of them yield based estimates excluding the IRFk-theory, which is confined to special trend models (polynomial, harmonic) not appropriate for external drifts, and the maximum likelihood approach, which is confined to known distributions models, especially gaussian random fields. A more generally applicable method estimating the variogram without distributional assumptions from its second order moment properties only has been developed (Boogaart, Brenning 2001). The idea is to compare covariance of the residuals after removing the trend to the covariance the residuals would have after trend removel, when the field had the model variogram as true variogram. The estimate is given by the set of parameters yielding the minimum difference between the expected and observed covariance of the residuals:

$$\hat{\theta} = \arg\min \left\| P\Gamma_\theta P + P_{ZZ}^t P \right\|^2$$

with some residual projector PF=0 and the usual notations for the universal kriging equation system (cf. Cressie 1993)

$$\hat{Z}(x) = \begin{pmatrix} z^t & 0 \end{pmatrix} \begin{pmatrix} \lambda \\ l \end{pmatrix} = \begin{pmatrix} z^t & 0 \end{pmatrix} \begin{pmatrix} \Gamma & F \\ F & 0 \end{pmatrix}^{-1} \begin{pmatrix} \vec{\gamma} \\ f \end{pmatrix}$$

The estimator is shown to be unbiased for variance component models, such as the empirical variogram (which itself is biased due to misspecification). The argmin is unique up to equivalence classes of variograms $\gamma(x,y)$ defined by trend model dependent subspace $J := \langle \mathrm{f(x)g(y)} + \mathrm{f(y)g(x)} : \mathrm{f, g} \in \mathrm{I} \rangle$

where $I := \bigcap_{h \in R^d} \left\{ f(x) = \sum_{i=1}^{d} \beta_d f_d(x+h) : \beta_1, ..., \beta_d \in R \right\}$ is the translation invariant subspace of the trend model

$$f(x) = \sum_{i=1}^{d} \beta_d f_d(x)$$

For polynomial trend models J is equivalent to the factor spaces of generalized covariances and variograms defined by IRFk. Variograms or covariance functions, which differ only by a function in this subspace all yield the same kriging predictor and the same kriging variance. The same identifiability property shows up with maximum likelihood estimators and all other estimators. Thus unbiased variogram estimation for the purpose of kriging is possible by this method for all trend models and universal kriging yields the correct predictor. However we therefore use a more rich class of generalized covariograms and variograms here und thus this theory is a joint generalization of universal kriging and IRFk-kriging combining the advantage of identifiable variograms in the IRFk-theory and the full range of possible trend models of universal kriging as well as the advantage of being free of possibly violated gaussian assumptions. Anyway in case of Gaussian random fields we should use maximum likelihood estimators instead of the method of moments estimator given here, since parametric methods are superior, whenever their assumptions are met.

Modelling instationary variograms

On the other hand the physical surrounding does not only influence the mean, but also the covariance structure. In smooth areas the range can be larger; boundaries and faults diminish the correlation across the boundary; directions of water flow or structural elongation direct the physical anisotropy; In different geological regions the variability and thus the sill might be different; and according to the physical process (pores or clefts) the local roughness might be different. All of these implies nonstationarity and location dependent anisotropy of the variogram. Two main problems had to be solved to allow the estimation of nonstationary variogram models. First of all the whole variogram estimation theory of kriging is crucially based on stationarity. A way out was the definition of generic stationarity given in (Brenning, Boogaart 2001) based on the conceptual physical model, that the random structure should functionally depend on the local geology. The functional dependence itself should be stationary. Roughly speaking, when we find the same geology in an other place, both locations should have the same probability law. Indeed external drift models are a special case of generic stationarity, where local mean functionally depends on the values of the external drift variable. The functional dependence itself is unknown due to the unknown drift parameters and it is translation invariant, what means here: when the external drift variable is shifted the trend surface would also be shifted.

Variogram estimation gets possible, when the functional dependence of the variogram is simple and can be described by a small set of parameters. Thus we need a model of the functional dependence of the variogram. And there from evolves the second major problem: How to construct meaningful instationary variogram models. (Perrin 1977) just constructs them using stationary ones on a deformed space. This way he solves a major problem: It is difficult to construct negativ semidefinit functions - thats why we normally use one of our standard variogram models. However not all conceptual models of instationarity an be expressed in terms of space deformation. Therefore we proposed a computationally more demanding approach based on local weight functions w(x,y;θ,geology), which may depend in any way on the local geology. The nonstationary covariance function is then modeled by:

$$\operatorname{cov}(Z(x_1), Z(x_2)) = c_\theta(x_1, x_2) := \int w(x_1, y; \theta, \text{geology}) w(x_2, y; \theta, \text{geology}) dy$$

These models are guaranteed to be be positive definite and with slight generalization exhaustive. On the other hand many conceptual models can be expressed and easily modeled in terms of weight functions. These conceptual models include space deformation, non-euclidean geometry neighborhoods (which is not possible in space deformation, but common on the hilly earth), boundaries (even ending boundaries such as limited faults, and shifts on faults with filled gaps), nonlinear transport models, areal, rotating and treelike anisotropy, physical laws in terms of differential equations. The approach therefore allows to use the fullness of information present in the GIS and in scientists mind.

Kriging of tensors and geometric data

Let us return from nonstationary models back to more all day problems. The random fields under consideration are not always scalars. Multivariate Kriging (e.g. Wackernagel 1998) allows the kriging of vectors. However multivariate entities are not always tuples of scalars, but sometimes they are tensors – i.e. they have a geometric relation to the space - or representatives of special data types such as compositions or geometrical quantities (e.g. directions, axes or orientations). Examples of tensors are vectorial tensors such as displacement, flowspeed, gravity, matrix tensors such as stress, strain, permeability, curvature, seismic velocity, and higher order tensors such the Hook tensor. Axes and orientation are not by it self members of an euclidean vector space. They need to be mapped into an euclidean vector space before kriging can be applied to them (Boogaart, Schaeben, Apel 2001), just as this can be done for compositional data. (Pawlowsky)

Types of isotropy of nonscalar random fields

For tensors and geometrical quantities the concept of isotropy gets a new totally new meaning: Physical laws are invariant under rotations of the coordinate system. But a rotation of the coordinate system rotates the locations as well as the observations. On the other hand some processes could be invariant under rotation of the observations only, when the direction in the observable quantity is unrelated to the external direction between two locations. This results in four different types of isotropy a tensorial or geometrical random variable can have (Boogaart, Schaeben 2002).

1. Isotropy under rotation of the locations (classical isotropy for multivariate fields)
2. Isotropy under rotation of the observations (unbelievable)
3. Isotropy under change of the coordinate system for locations and observations (physical isotropy for tensors and geometric quantities)
4. Isotropy under rotation of locations and under rotation of observations (unbelievable, but leeds to enormous simplifications)

In all four cases the rotation can be constrained to rotations around the vertical, which we have called geographic isotropy. Depending on the special problem we need to choose the right type of isotropy, because they all lead to different constraints and simplifications of the variogram listed in (Boogaart, Schaeben 2002).

Differential equations and kriging

A more sophisticate conceptual model can include physically motivated partial differential equations the realization of the random field solves for physical reasons. Examples are simple linear partial differential equations as the Laplace differential equation for source free potentials (cf. Chiles, Delfiner 1999) and by the incompressibile displacement field with small deformations (Boogaart, Drobniewski 2002) or the condition for force fields or strain tensors to be solve by gradients $\frac{\partial f_i}{\partial x_j} = \frac{\partial f_j}{\partial x_i}$ of the potential field or displacement field respectively or nonlinear partial differential equations such as true incompressibility $\nabla\zeta = 1$, laws of continuum mechanics relating a random field of material properties to a displacment field and many more. Linear partial differential equations LZ=k impose constraints to the variogram model $\gamma(L_\gamma(x,y)=0)$ the trend model $\mu(x) = f_0(x) + \sum_i f_i(x)$ ($Lf_i=0$, $Lf_0=k$), which imply -- when met - that the kriging predictor and the conditional simulations solve the differential equation (cf. Boogaart 2001). Thus linear differential equations can fully be used within the environment of kriging. This approach can be generalized towards nonlinear differential equations into a general framework of nonlinear kriging (cf. Boogaart 2003a). Unfortunately the predictor does no longer solve the differential equation due to the nonlinear character of the solution space. However the information can still be very useful for the identification of the stochastic structure.

Finite Elements, stochastic differential equations and kriging with differential equations

The introduction of differential equations as stronghold of deterministic modelling brings geostatistics in direct competition to finite element models and to stochastic differential equations and we need to clarify each domain of application. Finite element methods solve a differential equation based on boundary conditions which fully specify a unique solution. Stochastic differential equations fully specify distributions based on the differential relation of a known random process (such as white noise) to the random function of interest. While kriging with differential equations neither uses enough data to specify unique solutions nor uses differential relations sufficient to specify the distribution or even the moments of the random process. It only uses conditions for the process to be solved and estimates all other parameters from the realization during the variogram modelling step. It is therefore the method with the least necessary a-priory knowledge and therefore well suited for earth science applications, where we seldom know all boundary conditions or all relevant physical processes.

Smoothness and interpretation of derivatives

A more simplicistic view on the differential theory of kriging is based on the observation that the derivatives $\frac{\partial^{2d}}{\partial x^d \partial y^d} c(x, y)$ of the covariance function c(x, y) are nothing more than the covariance function of the derivatives $\frac{\partial^d}{\partial x^d} Z(x)$ of the process Z(x). When they not exist (at least in generalized sense) the process is not such often differentiable. When they are large for x = y, the process has a large variability in the d-th order derivatives, and when they have a short pseudo range, the d-th order derivative of the process is volatile. Negative values in the derived covariance function correspond to anticorrelation of the d-th order derivative making it difficult to interpret the derived process in its own right. Often we have an intuitive or physically motivated presumption on the smoothness of the processes and its derivatives. This can be used in variogram modelling especially, because the weight function models combined by variance component models provide the tools to construct valid variogram models with requested smoothness properties in the interesting derivatives.

The Variance of the field and of the variogram

After all these involved hints on how to construct the best of all variograms and how estimate them with generically stationary trend and variogram models, we are left with a set of questions: 1) Was is the right model? 2) How precise are the parameters estimated? 3) What, if they are not precise enough? 4) How large is the kriging error really, considering the estimation of the variogram? One possible basis to the answers of these questions is the estimation theory for variances of spatially correlated observations given in (Boogaart 2002c). This gives as a first corrolary an unbiased estimator of the variance of the field, which is the sill of the semivariogram, when an upper limit r_{max} of the range is known:

$$\hat{s}^2 := \frac{1}{n}\sum_{i=1}^{n} Z(x_i)^2 - \frac{1}{N^C}\sum_{(i,j)\in N^c} Z(x_i)Z(x_j) \text{, with } N^C = \left\{(i,j) : \left\|x_i - x_j\right\| > r_{\max}\right\}$$

As discussed in (Boogaart 2003a) the approach of (Boogaart 2000c) can be used for the estimation of the estimation error of the empirical variogram, which might - as discussed below - allow to check whether the model is consistent with the empirical variogram, and the variogram parameters, which gives an estimated precision of the variogram. More efficient approaches applicable to gaussian random fields are given in (Pardo-Iguzquiza 1998; Pardo-Iguzquiza, Dowd 2001). With an error in mind the question is whether the estimated variogram is precise enough for kriging and for a reliable calculation of the kriging error? Precise enough for kriging means: Is kriging with the estimated variogram better than kriging with a fixed variogram (i.e. deterministc interpolation)? With any weights λ based on any variogram the true kriging error is given by (using the notations from above):

$$\operatorname{var}\left(\hat{Z}(x) - Z(x)\right) = 2\lambda(\hat{\gamma})^t \vec{\gamma}(\gamma) - \lambda(\hat{\gamma})^t \Gamma(\gamma)\lambda(\hat{\gamma})$$

where γ denotes the true unknown variogram and $\hat{\gamma}$ the actually estimated variogram. $\Gamma(\gamma)$ and $\vec{\gamma}(\gamma)$ and $\lambda(\gamma)$ denote the matrix and vector entries of the kriging equation system, written as functions of the variogram γ. The estimated kriging error is given by:

$$\hat{e}^2(x) = 2\lambda(\hat{\gamma})^t \vec{\gamma}(\hat{\gamma}) - \lambda(\hat{\gamma})^t \Gamma(\hat{\gamma})\lambda(\hat{\gamma})$$

Up to higher order terms (higher than 2) in $\Delta\vec{\gamma} := \vec{\gamma}(\hat{\gamma}) - \vec{\gamma}(\gamma), \Delta\Gamma = \hat{\Gamma} - \Gamma$, and $\Delta\gamma = \hat{\gamma} - \gamma$ the expectations of the difference (und thus the bias of the estimator) is up to calculation errors and most lazy notation given by:

$$E\left[\hat{e}^2(x) - \mathrm{var}(\hat{Z}(x) - Z(x))\right] \approx 3\lambda(\hat{\gamma})\,\mathrm{cov}(\Delta\Gamma, \Delta\gamma)\frac{\partial}{\partial\hat{\gamma}}\lambda(\hat{\gamma})$$

$$- 4trace\left(\mathrm{cov}(\Delta\vec{\gamma}, \Delta\gamma)\frac{\partial}{\partial\hat{\gamma}\lambda(\hat{\gamma})}\right) + o(\Delta\gamma^3)$$

Thus we could use the estimated covariance of the estimation errors of $\hat{\gamma}$ to correct for this bias term in the kriging error. Due to the influence of the covariances this bias is distribution dependent and can therefore not be calculated by gaussian simulation for nongaussian fields. The precision of the kriging error can be estimated by using the first order approximation based on

$$\hat{e}^2(x) - \mathrm{var}(\hat{Z}(x) - Z(x)) = 2\lambda(\hat{\gamma})^t\Delta\vec{\gamma}(\gamma) - \lambda(\hat{\gamma})^t\Delta\Gamma(\gamma)\lambda(\hat{\gamma})$$

by error propagation.

Outlook: towards spatial hypothesis testing

The works on hypothesis testing in (Boogaart 2002b) show a way to construct asymptotic α-level test for spatially correlated data based on variance estimators of spatially correlated data. Unfortunately these tests are still not very efficient and need a large amount of data to converge, especially in situations of far range dependency. However such tests could be used to check variogram models based on their estimated errors. Much to do is left here.

Conclusions

There is an increasing lot of possibilities to introduce scientic knowledge into the geostatistical analysis. And we will need new methods guiding us, which method and model to choose and to take as much efforts as necessary but not as possible.

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