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Efficiently estimating some common geostatistical models from “image-type, possibly incomplete” datasets: the R-package CGEMEV and its extension to unknown nugget-effect

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► To cite this version:

Didier A. Girard, Rémy Drouilhet. Efficiently estimating some common geostatistical models from “image-type, possibly incomplete” datasets: the R-package CGEMEV and its extension to unknown nugget-effect. *Spatial Statistics 2019: Towards Spatial Data Science*, Jul 2019, Sitgès, Barcelone, Spain. , 2019. hal-02174478v1

HAL Id: hal-02174478

<https://hal.science/hal-02174478v1>

Submitted on 5 Jul 2019 (v1), last revised 10 Jul 2019 (v2)

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The problem of estimating the 2 parameters (“range” and “variance”) of a stationary isotropic Gaussian process whose autocorrelation function belongs to the Matérn class, appears in many contexts (e.g. [9,11]). We propose two extensions of the CGEM-EV method (cf. [5,6]) for the important case of unknown “nugget-variance” (3rd parameter), and compare them to the classic maximum likelihood (ML) method, for the Matérn subclass $\nu = 1/2$, and “small image”-type observations

Background

We mainly consider the following statistical model which arises e.g. in remote sensing image analysis: let $Z(\mathbf{s})$, $\mathbf{s} \in \mathbb{R}^2$, be a zero mean stationary Gaussian stochastic process whose autocorrelation function is assumed to belong to the popular isotropic Matérn family. One realization of this process is observed at n sites \mathbf{s}_i , $i = 1, \dots, n$, which are a subset of the $n_1 \times n_2$ regularly spaced locations $\tilde{\mathbf{s}}_k$ in $[0, 1] \times [0, 1]$, with an additive Gaussian white noise whose variance is σ_0^2 (this noise can model either suspected homoscedastic measurement errors or a nugget effect added to Z , see e.g. Zhang and Zimmerman (2007) and references therein). Using a standard lexicographic ordering, the observations thus form a vector \mathbf{y} of size n whose law is Gaussian :

$\mathbf{y} \sim \mathcal{N}(\mathbf{0}, \tau_0^2 \mathbf{R}(\theta_0) + \sigma_0^2 \mathbf{I}_{n,n})$ where $\mathbf{R}(\theta) = \mathbf{J}_{n,n_1 \times n_2} \tilde{\mathbf{R}}(\theta) \mathbf{J}_{n,n_1 \times n_2}^T$ with $\mathbf{J}_{n,n_1 \times n_2}$ denoting the rectangular, “with coefficients in $\{0, 1\}$ ”, incidence matrix, \mathbf{I}_n the identity matrix, and $\tilde{\mathbf{R}}(\theta)$ the autocorrelation matrix of the gridded process i.e. the block Toeplitz matrix (with n_1^2 Toeplitz square blocks, each of size $n_2 \times n_2$) whose coefficients are given by

$$[\tilde{\mathbf{R}}(\theta)]_{j,k} := \rho_{\nu,\theta}(\|\tilde{\mathbf{s}}_j - \tilde{\mathbf{s}}_k\|), \quad j, k = 1, \dots, n_1 \times n_2,$$

$\|\cdot\|$ being the Euclidean norm and $\rho_{\nu,\theta}$ the Matérn function

$$\rho_{\nu,\theta}(x) = \frac{(\theta x)^\nu}{\Gamma(\nu)2^{\nu-1}} K_\nu(\theta x), \quad x > 0, \theta > 0,$$

where K_ν is the modified Bessel function of the second kind of order $\nu > 0$.

We here use the parameters b, θ, σ , with $b_0 = \frac{\tau_0^2}{\sigma_0^2}$ called the true signal-to-noise (SNR). The microergodic-parameter is $c = b\sigma^2\theta^{2\nu}$.

In all the alternatives to ML we consider, the signal-variance τ_0^2 is “estimated”, given a candidate value for the noise-variance σ^2 , by the naive “bias corrected” empirical variance :

$$\hat{\tau}_{EV|\sigma}^2 := n^{-1} \mathbf{y}^T \mathbf{y} - \sigma^2 \quad (\text{and the “SNR estimate” is } \hat{b}_{EV|\sigma} := \frac{\hat{\tau}_{EV|\sigma}^2}{\sigma^2})$$

Proposed estimators

When the true σ^2 is known, CGEM-EV $|\sigma_0$ (which stands for “Conditional Gibbs-Energy Mean and Empirical Variance”) is quite efficient, both statistically and computationally (using a fast randomized-trace), for many common problems (see [5,6]). Recall that CGEM-EV $|\sigma$ consists of solving (a fixed-point algorithm is used in [2,3,4,7]) the equation in θ defined by

$$\text{LE}_1(\theta | \hat{b}_{EV|\sigma}, \sigma) = 0 \quad \text{with} \quad \text{LE}_1(\theta | b, \sigma) := \frac{1}{n} (\mathbf{A}_{b,\theta} \mathbf{y}, \mathbf{R}(\theta)^{-1} \mathbf{A}_{b,\theta} \mathbf{y}) - b \sigma^2 \frac{1}{n} \text{tr}(\mathbf{A}_{b,\theta}) \quad (1),$$

where the “smoothing matrix” $\mathbf{A}_{b,\theta} := b \mathbf{R}(\theta) (b \mathbf{R}(\theta) + \mathbf{I})^{-1}$ (a.k.a. a Kalman smoother); let us denote “the” root of (1) with $\sigma = \sigma_0$ (the smallest one in case of multiple roots) by $\hat{\theta}_{CGEMEV|\sigma_0}$.

- The first extension of CGEM-EV to the case of unknown σ_0 is a simple (and fast!) “plugin” method: one computes a nonparametric estimator of σ^2 , say $\hat{\sigma}_{VEZ}^2$, by extrapolating at 0_+ the (classic or robust) semi-variogram function as a function of the lag (proposed by [9]) and substitutes $\hat{\sigma}_{VEZ}^2$ for σ_0^2 in the CGEM-EV $|\sigma_0$ equation in θ , producing $\hat{\theta}_{CGEMEV|\hat{\sigma}_{VEZ}}$.

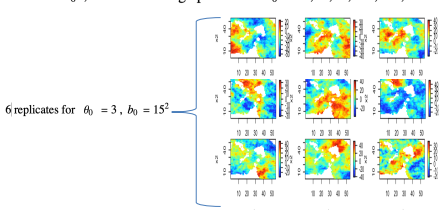
- The second possible extension consists of adding to (1) a well-known equation satisfied by the ML estimate of σ^2 when the signal-to-noise ratio b and θ are fixed; precisely, σ is the root of $\text{LE}_3(\sigma | b, \theta) := \frac{1}{n} (\mathbf{y}, (\mathbf{I} - \mathbf{A}_{b,\theta}) \mathbf{y}) - \sigma^2 \quad (2).$

N.B. : In fact $\text{LE}_3(\sigma | b, \theta)$ (resp. $\text{LE}_1(\sigma | b, \theta)$) is proportional to the partial derivative of the log-likelihood w.r.t. the 3rd (resp. 1st) parameter.

A classic bisection-search of σ , can be used to solve the concentrated CGEM-EV-LE₃ equation $\text{LE}_3(\sigma | \hat{b}_{EV|\sigma}, \hat{\theta}_{CGEMEV|\sigma}) = 0$ in σ , where an inner iteration is used to compute $\hat{\theta}_{CGEMEV|\sigma}$. The final $\hat{\theta}$ -iterate, thus root of (1) and (2), will be denoted by $\hat{\theta}_{CGEMEVLE_3}$.

Experiments setting, VEZ-tuning

- $\nu = 1/2$
- $n_1 = n_2 = 54$. about 20% missing data (fixed locations) : $n=2300$
- signal-to-noise ratios $b_0 = (\frac{\text{var}(Z)}{\text{var}(\epsilon)})$ chosen among: $7^2, 10^2, 15^2, 33^2$
- For each b_0 , inverse-range parameter $\theta_0 = 1, 3, 6, 12, 24, 48$

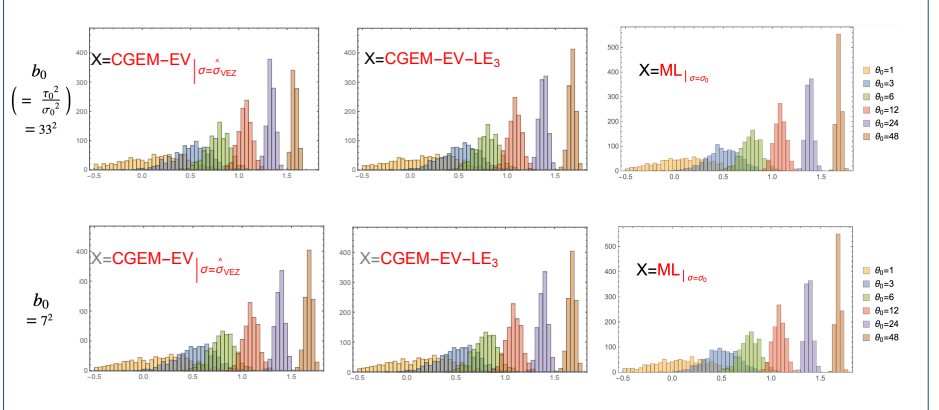


We use the “best performing” VEZ pour this setting, precisely:

- classic variogram, □ maximum-lag := 3/4

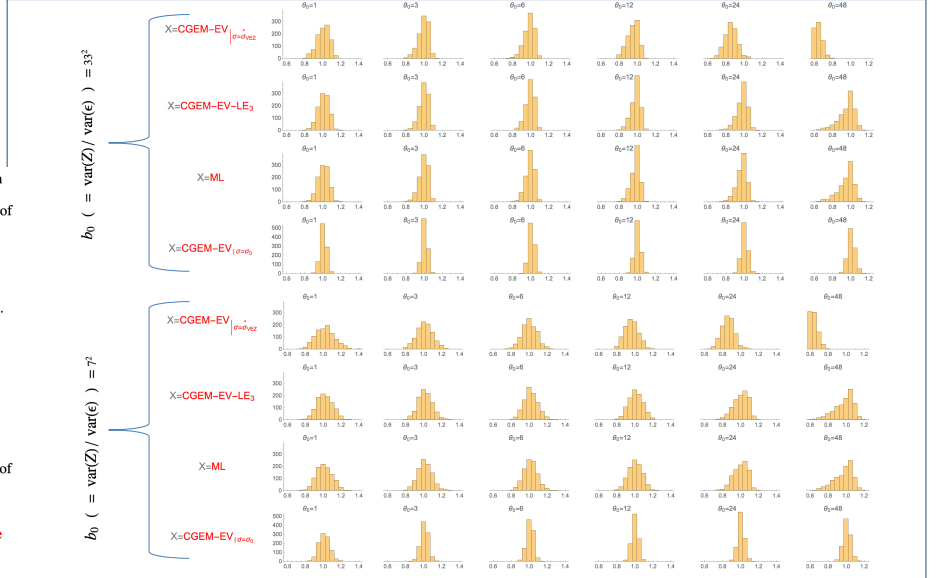
Estimation of the inverse-range parameter θ_0

histograms of $\log_{10}(\hat{\theta}_X)$ (1000 image-type replicates), observed pixels number $n=2300$



Estimation of the micro-ergodic parameter c_0

histograms of \hat{c}_X / c_0 (1000 image-type replicates), observed pixels number $n=2300$



Conclusions

- Concerning the estimation of the range-parameter θ_0 , estimating the nugget-variance via CGEM-EV-LE₃ only causes a very small additional inaccuracy, even when compared with “ML given the true σ_0 ”. The simplest CGEMEV $|\hat{\sigma}_{VEZ}$ is almost as good, except for the largest θ_0 's.

- Concerning the estimation of the micro-ergodic-parameter c_0 , CGEMEV $|\hat{\sigma}_{VEZ}$ is clearly not efficient for the two largest θ_0 's (and also for $\theta_0 \geq 6$, in case of strong SNR). But CGEM-EV-LE₃ is always nearly as efficient as ML (also note that the ideal “ML given the true σ_0 ” would much better estimate c_0). The simplest method CGEMEV $|\hat{\sigma}_{VEZ}$ is almost as good, except for the largest θ_0 's.

R-package CGEMEV : ongoing work is an assessment of various versions of the “bisection with inner iterations” [1] mentioned above for implementing CGEM-EV-LE₃



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