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

Didier A. Girard, Rémy Drouilhet

Efficiently estimating some common geostatistical models from «image-type, possibly incomplete» datasets: CGEMEV and its extension to unknown nugget-effect

Rémy Drouilhet[1], Didier Girard[1,2]

[1]Univ. Grenoble Alpes, LJK, France, [2]CNRS, LJK, France

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 $\mathbf{s}_i, i = 1, \cdots, n$, which are a **subset** of the $n_1 \times n_2$ regularly spaced locations $\bar{\mathbf{s}}_k$ 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 $\boldsymbol{y}$ of size n whose law is Gaussian :

$$\boldsymbol{y} \sim \mathcal{N}(\mathbf{0}, \tau_0^2 \boldsymbol{R}(\theta_0) + \sigma_0^2 \boldsymbol{I}_{n,n}) \text{ where } \boldsymbol{R}(\theta) = \boldsymbol{J}_{n,n_1\times n_2} \tilde{\boldsymbol{R}}(\theta) \boldsymbol{J}_{n,n_1\times n_2}{}^T$$

with $\boldsymbol{J}_{n,n_1\times n_2}$ denoting the rectangular, "with coefficients $\in \{0,1\}$", incidence matrix, $\boldsymbol{I}_n$ the identity matrix, and $\tilde{\boldsymbol{R}}(\theta)$ 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

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

$||\cdot||$ 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** :

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

Proposed estimators

When the true σ_0^2 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

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

where the "smoothing matrix" $\boldsymbol{A}_{b,\theta} := b\,\boldsymbol{R}(\theta)\,(b\,\boldsymbol{R}(\theta) + \boldsymbol{I})^{-1}$ (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 $\hat{\theta}_{\text{CGEMEV}|\sigma_0}$.

- 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 $\hat{\sigma}^2_{\text{VEZ}}$, **by extrapolating at 0_+ the (classic or robust) semi-variogram function as a function of the lag** (proposed by [9]) and substitutes $\hat{\sigma}^2_{\text{VEZ}}$ for ${\sigma_0}^2$ in the CGEM-EV$|\sigma_0$ equation in θ, producing $\hat{\theta}_{\text{CGEMEV}|\hat{\sigma}^2_{\text{VEZ}}}$.

- 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

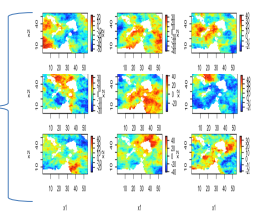
$$\text{LE}_3(\sigma|b,\theta) := \frac{1}{n}\left\langle \mathbf{y}, (\boldsymbol{I} - \boldsymbol{A}_{b,\theta})\,\mathbf{y}\right\rangle - \sigma^2 \quad (2).$$

N.B.: In fact **$\text{LE}_3(\theta|b,\sigma)$** (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-LE$_3$ equation $\text{LE}_3\left(\sigma\middle|\hat{b}_{\text{EV}|\sigma}, \hat{\theta}_{\text{CGEMEV}|\sigma}\right) = 0$ in σ, where an inner iteration is used to compute $\hat{\theta}_{\text{CGEMEV}|\sigma}$. The final $\hat{\theta}$-iterate, thus root of (1) and (2), will be denoted by $\hat{\theta}_{\text{CGEMEVLE}_3}$.

Experiments setting, VEZ-tuning

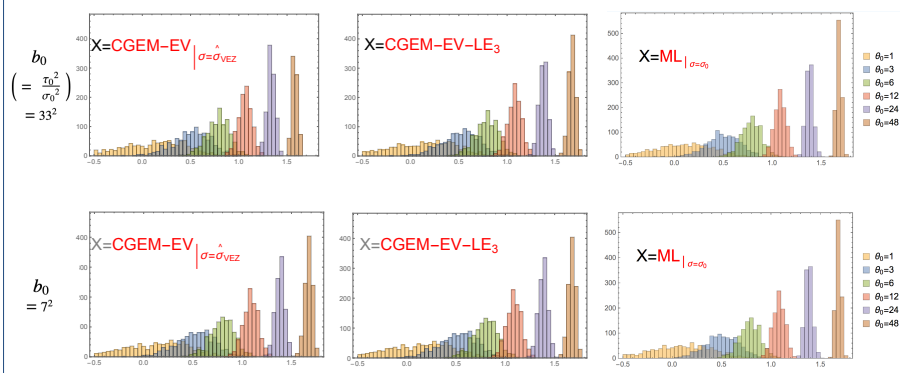
- $\nu = 1/2$
- $n_1 = n_2 = 54$. about 20% missing data (fixed locations) : n=2300
- signal-to-noise ratios b_0 $\left(= \frac{\text{var}(Z)}{\text{var}(\epsilon)}\right)$ chosen among: $7^2, 10^2, 15^2, 33^2$
- For each b_0 , inverse-range parameter $\theta_0 = 1, 3, 6, 12, 24, 48$



We use the "best performing" VEZ pour this setting, precisely:
- classic variogram,
- maximum-lag := 3/54

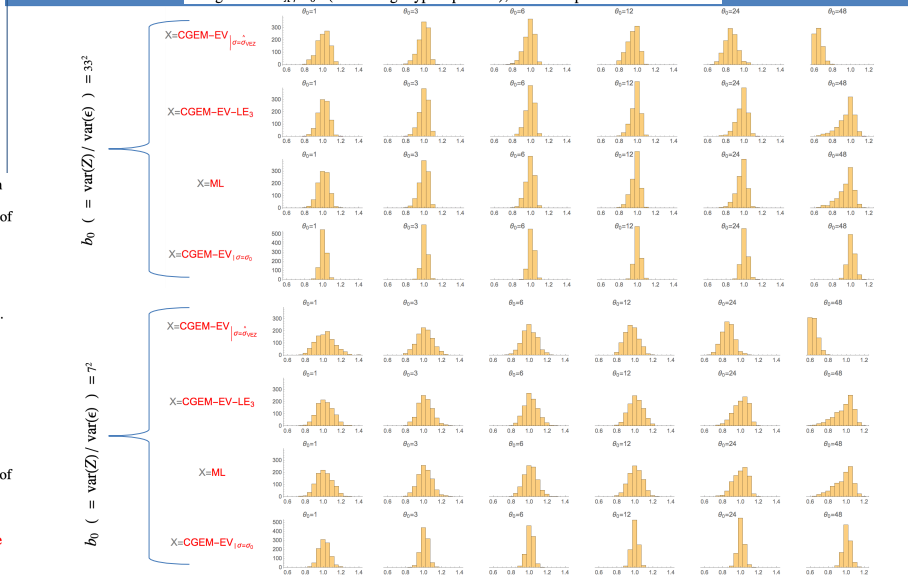
Estimation of the inverse-range parameter θ_0 .

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-LE$_3$ only causes a very small additional inaccuracy, even when compared with "ML given the true σ_0". The simplest CGEMEV $|\hat{\sigma}_{\text{VEZ}}$ is almost as good, except for the largest θ_0's.

- Concerning the estimation of the micro-ergodic-parameter c_0, CGEMEV $|\hat{\sigma}_{\text{VEZ}}$ 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-LE$_3$ 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 $|\hat{\sigma}_{\text{VEZ}}$ 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-LE$_3$

References

[1] Drouilhet R., Girard D.A. (2019) "Simple and efficient procedures for fitting isotropic Matérn covariance models to large (noisy) data sets " To appear

[2] Girard D.A. (2014) "Estimating a Centered Ornstein-Uhlenbeck Process under Measurement Errors," *Wolfram Demonstrations Project*, Published: July 1, 2014.

[3] Girard D.A. (2015) "Three Alternatives to the Likelihood Maximization for Estimating a Centered Matérn (3/2) Process, " *Wolfram Demonstrations Project*,

[4] Girard D.A. (2015) " Estimating a Centered Matérn (1) Process: Three Alternatives to the Likelihood Maximization via conjugate gradient linear solvers" *Wolfram Demonstrations Project*,

[5] Girard D.A. (2016 & 2019). "Asymptotic Near-Efficiency of the 'Gibbs-Energy and Empirical-Variance' Estimating Functions for Fitting Matérn Models, I: Densely sampled processes, & II: Accounting for measurement errors via conditional GE mean," *Stat. Prob. Letters* & arxiv.org/pdf/0909.1046v3.pdf.

[6] Girard D.A. (2017) . "Efficiently estimating some common geostatistical models by 'energy-variance matching' or its randomized 'conditional-mean' versions," *Spatial Statistics*, 21(Part A), 1-26

[7] Girard D.A. (2018) "Estimators of a Noisy Centered Ornstein-Uhlenbeck Process and Its Noise Variance, " *Wolfram Demonstrations Project*,

[8] Kaufman C.G., Shaby, B.A. (2013). "The Role of the Range Parameter for Estimation and Prediction in Geostatistics," *Biometrika* 100 (2), pp. 473-484.

[9] Katzfuss and N. Cressie, "Bayesian Hierarchical Spatio-temporal Smoothing for Very Large Datasets," *Environmetrics* , 23(1), 2012 pp. 94-107.

[10] Zhang H. (2012). "Asymptotics and Computation for Spatial Statistics," in *Advances and Challenges in Space-time Modelling of Natural Events (Lecture Notes in Statistics, Vol. 207)* (E. Porcu, J. M. Montero, and M. Schlather, eds.), New York: Springer, pp. 239-252.

[11] Zhang, H., Zimmerman, D.L., 2007. "Hybrid estimation of semivariogram parameters," *Mathematical Geology* 39 (2), 247-260.

Work developed in the framework of Grenoble Alpes Data Institute, supported by the French National Research Agency under the " Investissements d'avenir" program (ANR-15-IDEX-02).