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# Spartan Random Fields: Smoothness Properties of Gaussian Densities and Definition of Certain Non-Gaussian Models

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## 1 Introduction

Spartan spatial random fields (SSRFs) were introduced in [10]. Certain mathematical properties of SSRFs were presented, inference of the model parameters from synthetic samples was investigated [10], and methods for the unconditional simulation of SSRFs were developed [11]. This research has focused on the fluctuation component of the spatial variability, which is assumed to be statistically homogeneous (stationary) and normally distributed. The probability density function (pdf) of Spartan fields is determined from an energy functional  $H[X_\lambda(\mathbf{s})]$ , according to the familiar in statistical physics expression for the Gibbs distribution

$$f_x[X_\lambda(\mathbf{s})] = Z^{-1} \exp \{-H[X_\lambda(\mathbf{s})]\}. \quad (1)$$

The constant  $Z$  (called partition function) is the pdf normalization factor obtained by integrating  $\exp(-H)$  over all degrees of freedom (i.e. states of the SSRF). The subscript  $\lambda$  denotes the fluctuation resolution scale. The energy functional determines the spatial variability by means of interactions between neighboring locations. One can express the multivariate Gaussian pdf, typically used in classical geostatistics, in terms of the following energy functional

$$H[X_\lambda(\mathbf{s})] = \frac{1}{2} \int d\mathbf{s} \int d\mathbf{s}' X_\lambda(\mathbf{s}) c_X^{-1}(\mathbf{s}, \mathbf{s}') X_\lambda(\mathbf{s}'), \quad (2)$$

where  $c_X(\mathbf{s}, \mathbf{s}')$  is the centered covariance function; the latter needs to be determined from the data for all pairs of points  $\mathbf{s}$  and  $\mathbf{s}'$ , or (assuming statistical homogeneity) for all distance vectors  $\mathbf{s} - \mathbf{s}'$ . In contrast, the energy functional in Spartan models is determined from physically motivated interactions between neighbors. The name ‘Spartan’ emphasizes that the number  $N_p$  of model parameters to be determined from the data is small. For example,

in the fluctuation – gradient – curvature (FGC) model, the pdf involves three main parameters: the scale factor  $\eta_0$ , the covariance shape parameter  $\eta_1$ , and the correlation length  $\xi$ . Another factor that adds flexibility to the model is the coarse-graining kernel that determines the fluctuation resolution  $\lambda$  [10]. As we show below, the resolution is directly related to smoothness properties of the SSRF. In previous work [10, 11], we have used a kernel with a boxcar spectral density that imposes a sharp cutoff in frequency (wavevector) space at  $k_c \propto \lambda^{-1}$ . We have treated the cutoff frequency as a constant, but it is also possible to consider it as an additional model parameter, in which case  $N_p = 4$ .

A practical implication of an interaction-based energy functional is that the parameters of the model follow from simple sample constraints that do not require the full calculation of two-point functions (e.g., correlation function, variogram). This feature permits fast computation of the model parameters. In addition, for general spatial distributions (e.g., irregular distribution of sampling points, anisotropic spatial dependence with unknown a priori principal directions), the parameter inference does not require various empirical assumptions such as choice of lag classes, number of pairs per class, lag and angle tolerance, etc. [7] used in the calculation of two-point functions. In the case of SSRFs that model data distributed on irregular supports, the definition of the interaction between ‘near neighbors’ is not uniquely defined. Determining the neighbor structure for irregular supports increases the computational effort [10], but the model inference process is still quite fast. Methods for the non-constrained simulation of SSRFs with Gaussian probability densities on the square lattice (by filtering Gaussian random variables in Fourier space and reconstructing the state in real space with the inverse FFT) and for irregular supports (based on a random phase superposition of cosine modes with frequency distribution modeled on the covariance spectral density), have been presented in [11].

## 2 FGC Energy Functional

The energy functional involves the SSRF states (configurations)  $X_\lambda(\mathbf{s})$ . For notational simplicity, we will not use different symbols for the random field and its states in the following. As hinted above, the energy functional is properly defined for SSRFs  $X_\lambda(\mathbf{s})$  with an inherent scale parameter ‘ $\lambda$ ’ that denotes the spatial resolution of the fluctuations. At lower scales, the fluctuations are coarse-grained. The fluctuation resolution scale is physically meaningful, since it would be unreasonable to expect a model of fluctuations to be valid for all length scales. In contrast with classical random field representations, which do not have a built-in scale for a fluctuation cutoff, SSRFs provide an explicit ‘handle’ for this meaningful parameter. In practical situations, the fluctuation resolution scale is linked to the measurement support scale and the sampling density. In the case of numerical simulations, the lattice spacing provides

a lower bound for  $\lambda$ . The fluctuation resolution can also exceed the lattice spacing, to allow for smoother variations of the field. The general probability density function of continuum FGC Spartan random fields (FGC-SSRF) in  $\mathbb{R}^d$  is determined from the following functional

$$H_{\text{fgc}}[X_\lambda] = \frac{1}{2\eta_0\xi^d} \int d\mathbf{s} h_{\text{fgc}}[X_\lambda(\mathbf{s}); \eta_1, \xi], \quad (3)$$

where  $\eta_0$  is a scale factor with dimensions  $[X]^2$  that determines the magnitude of the overall variability of the SSRF,  $\eta_1$  is a covariance shape parameter (dimensionless),  $\xi$  is the correlation length, and  $h_{\text{fgc}}$  is the normalized (to  $\eta_0 = 1$ ) local energy at the point  $\mathbf{s}$ . In the case of a Gaussian FGC random field with mean (not necessarily stationary)  $m_{X;\lambda}(\mathbf{s}) = E[X_\lambda(\mathbf{s})]$  and isotropic spatial dependence of the fluctuations, the functional  $h_{\text{fgc}}[X_\lambda(\mathbf{s}); \eta_1, \xi]$  is given by the following

$$h_{\text{fgc}}[X_\lambda(\mathbf{s}); \eta_1, \xi] = [\chi_\lambda(\mathbf{s})]^2 + \eta_1 \xi^2 [\nabla \chi_\lambda(\mathbf{s})]^2 + \xi^4 [\nabla^2 \chi_\lambda(\mathbf{s})]^2, \quad (4)$$

where  $\chi_\lambda(\mathbf{s})$  is the local fluctuation field. The functional (4) is permissible if Bochner's theorem [3] for the covariance function is satisfied. As shown in [10], permissibility requires  $\eta_1 > -2$ . The covariance spectral density follows from the equation

$$\tilde{G}_{x;\lambda}(\mathbf{k}) = \frac{|\tilde{Q}_\lambda(\mathbf{k})|^2 \eta_0 \xi^d}{1 + \eta_1 (k\xi)^2 + (k\xi)^4} \quad (5)$$

where  $\tilde{Q}_\lambda(\mathbf{k})$  is the Fourier transform of the smoothing kernel. If the latter is the boxcar filter with cutoff at  $k_c$ , (5) leads to a band-limited spectral density  $\tilde{G}_{x;\lambda}(\mathbf{k})$ . For negative values of  $\eta_1$  the spectral density develops a sharp peak, and as  $\eta_1$  approaches the permissibility boundary value equal to  $-2$ , the spectral density tends to become singular. For negative values of  $\eta_1$  the structure of the spectral density leads to a negative hole in the covariance function in real space. If  $\tilde{Q}_\lambda(\mathbf{k})$  has no directional dependence, the spectral density depends on the magnitude but not the direction of the frequency vector  $\mathbf{k}$ . Thus, the covariance is an isotropic function of distance in this case.

On regular lattices, the FGC spectral density is obtained by replacing the operators  $\nabla$  and  $\nabla^2$  in the energy functional with the corresponding finite differences. Then, the local energy becomes  $h_{\text{fgc}}[X_\lambda(\mathbf{s}); \eta_1, \xi] = h_{\text{fgc}}[\chi_\lambda\{U(\mathbf{s}); \eta_1, \xi\}]$ , where  $U(\mathbf{s}) = \mathbf{s} \cup \text{nnb}(\mathbf{s})$  is the local neighborhood set that contains the point  $\mathbf{s}$  and its nearest lattice neighbors,  $\chi_\lambda\{U(\mathbf{s})\}$  is the set of the SSRF values at the points in  $U(\mathbf{s})$ , and  $h_{\text{fgc}}[\cdot]$  is a quadratic functional of the SSRF states that defines interactions between the fluctuation values  $\chi_\lambda\{U(\mathbf{s})\}$ . For irregular spatial distributions, there are more than one possibilities for modeling the interactions. One approach, explored in [10], is to define a background lattice that covers the area of interest and to construct interactions between the cells of the background lattice. If  $C_B(\mathbf{s})$  denotes the cell of the background lattice that includes the point  $\mathbf{s}$  and  $\text{nnb}\{C_B(\mathbf{s})\}$  is

the set of nearest neighbors of the cell  $C_B(\mathbf{s})$ , the local neighborhood set involves the sampled points that belong to the cell  $C_B(\mathbf{s})$  and its neighbors, i.e.  $U(\mathbf{s}) = \mathbf{s}' \in C_B(\mathbf{s}) \cup nnb\{C_B(\mathbf{s})\}$ .

### 3 Model Inference

The problem of model inference from available data is a typical inverse problem. In order to determine the model parameters experimental constraints need to be defined that capture the main features of the spatial variability in the data. These constraints should then be related to the interactions in the SSRF energy functional. The experimental constraints used in [10] for the square lattice are motivated by the local ‘fluctuation energy measures’  $S_0(\mathbf{s}) = \chi_\lambda^2(\mathbf{s})$ ,  $S_1(\mathbf{s}) = \sum_{i=1}^d [\nabla_i \chi_\lambda(\mathbf{s})]^2$ , and  $S_2(\mathbf{s}) = \sum_{i,j=1}^d \Delta_2^{(i)} [\chi_\lambda(\mathbf{s})] \Delta_2^{(j)} [\chi_\lambda(\mathbf{s})]$ , where  $\Delta_2^{(i)}$  denotes the centered second-order difference operator. The respective experimental constraints are then given by  $\overline{S_0(\mathbf{s})}$  (sample variance),  $\overline{S_1(\mathbf{s})}$  (average square gradient) and  $\overline{S_2(\mathbf{s})}$ , where the bar denotes the sample average. The respective stochastic constraints are  $E[S_m(\mathbf{s})]$ ,  $m = 0, 1, 2$  and they can be expressed in terms of the covariance function. For the isotropic FGC model, calculation of the stochastic constraints involves a one-dimensional numerical integration over the magnitude of the frequency. Matching of the stochastic and experimental constraints is formulated as an optimization problem in terms of a functional that measures the distance between the two sets [10] of constraints. Minimization of the distance functional leads to a set of optimal values  $\eta_0^*, \eta_1^*, \xi^*$  for the model parameters. Use of  $k_c$  as a fourth parameter needs further investigation. It should be noted that constraint matching is based on the ergodic assumption, and thus a working approximation of ergodicity should be established for the fluctuation field.

### 4 Smoothness of FGC Spartan Random Fields

The probability density of the FGC-SSRF involves the first- and second-order derivatives of the field’s states. This requires defining the energy functional in a manner consistent with the existence of the derivatives. In general, for Gaussian random fields [1, 15], the  $n$ th-order derivative  $\partial^n X_\lambda(\mathbf{s}) / \partial s_1^{n_1} \dots \partial s_d^{n_d}$  exists in the mean square sense if (i) the mean function  $m_{X;\lambda}(\mathbf{s})$  is differentiable, and (ii) the following derivative of the covariance function exists [1, 15]

$$\left. \frac{\partial^{2n} G_{X;\lambda}(\mathbf{s}, \mathbf{p})}{\partial s_1^{n_1} \dots \partial s_d^{n_d} \partial p_1^{n_1} \dots \partial p_d^{n_d}} \right|_{\mathbf{s}=\mathbf{p}}, n = n_1 + \dots + n_d. \quad (6)$$

Since the FGC covariance function is statistically homogeneous and isotropic, the above condition simply requires the existence of the isotropic derivative

of order  $2n$  at zero pair separation distance, i.e. the existence of the following quantity

$$G_{\mathbf{x};\lambda}^{(2n)}(0) = (-1)^n \left[ \frac{d^{2n} G_{\mathbf{x};\lambda}(\mathbf{r})}{dr^{2n}} \right] \Big|_{\mathbf{r}=\mathbf{0}} \quad (7)$$

Equation (7) is equivalent to the existence of the corresponding integral of the covariance spectral density

$$\left[ \frac{d^{2n} G_{\mathbf{x};\lambda}(\mathbf{r})}{dr^{2n}} \right] \Big|_{\mathbf{r}=\mathbf{0}} = \eta_0 \xi^d S_d \int_0^\infty dk \frac{\left| \tilde{Q}_\lambda(k) \right|^2 k^{d+2n-1}}{1 + \eta_1 (k\xi)^2 + (k\xi)^4} \quad (8)$$

where  $S_d = \int d\hat{\mathbf{k}} = 2\pi^{d/2}/\Gamma(d/2)$  denotes the surface of the unit sphere in  $d$  dimensions. Note that if  $\left| \tilde{Q}_\lambda(k) \right|^2 = 1$ , i.e. in the absence of smoothing, the above integral does not exist unless  $d+2n < 4$ , which can be attained only for  $d = 1$  and  $n = 1$ . If the smoothing kernel has a sharp cutoff  $k_c$  (band-limited spectrum), the  $2n$ -th order derivative is expressed in terms of the following integral

$$\frac{d^{2n} G_{\mathbf{x};\lambda}(\mathbf{r})}{dr^{2n}} \Big|_{\mathbf{r}=\mathbf{0}} = \eta_0 \xi^{-2n} S_d \int_0^{k_c \xi} d\kappa \frac{\kappa^{d+2n-1}}{1 + \eta_1 \kappa^2 + \kappa^4}. \quad (9)$$

The integral in 9 exists for all  $d$  and  $n$ . However, if the correlation length  $\xi$  exceeds significantly the resolution scale, i.e.  $\xi \gg \lambda$  and  $k_c \xi \gg 1$ , for  $\kappa \gg 1$  the integrand behaves as  $\kappa^{d+2n-5}$ . Then, it follows  $G_{\mathbf{x};\lambda}^{(2n)}(0) = \text{regular} + \alpha_d \xi^{-2n} (k_c \xi)^{d+2n-4}$ , where ‘regular’ represents the bounded contribution of the integral, while for fixed  $\xi$  the remaining term increases fast with  $k_c \xi$ . The constant  $\alpha_d$  depends on the dimensionality of space. Hence, for  $d \geq 2$  the singular term in  $G_{\mathbf{x};\lambda}^{(2n)}(0)$  leads to large values of the covariance derivatives for  $n \geq 1$ . In [10] we focused on the case  $k_c \xi \gg 1$ , which leads to ‘rough’ Spartan fields. Based on the above, the Gaussian FGC-SSRF can, at least in principle, interpolate between very smooth Gaussian random fields (e.g., Gaussian covariance function) and non-differentiable ones (e.g., exponential, spherical covariance functions). The ‘degree’ of smoothness depends on the value of the combined parameter  $k_c \xi$ . Hence, the FGC-SSRF in effect has four parameters,  $\eta_0, \eta_1, k_c, \xi$ , and the value of  $k_c \xi$ , which controls the smoothness of the model. This property of smoothness control is also shared by random fields with Matérn class covariance functions [14].

## 5 Non-Gaussian Probability Densities

An issue of significant practical importance is the ability of geostatistical models to capture fluctuations with non-Gaussian distributions. Such distributions can be developed in the Spartan-Gibbs framework by adding suitable

(higher than second order) interaction terms in the energy functional. An example is the energy functional of the Landau model e.g. [10], which includes non-Gaussian terms and exhibits a transition between exponential and power-law spatial dependence of the covariance function. Geostatistical probability density models provide sufficient flexibility for fitting various types of non-Gaussian data. The approaches typically used in geostatistics for modeling asymmetric distributions with higher-than-normal weight in their tails employ the logarithmic and the Box-Cox transforms. In the former approach, the initial distribution is assumed to be approximately lognormal. The logarithmic mean  $m_Y(\mathbf{s}) = E[\log X_\lambda(\mathbf{s})]$  is first estimated. Then, the fluctuations  $y_\lambda(\mathbf{s}) = \log[X_\lambda(\mathbf{s})] - m_Y(\mathbf{s})$  follow the Gaussian distribution, and they can be modeled by means of the FGC-SSRF normalized energy density  $h_{\text{fgc}}[y_\lambda(\mathbf{s}); \eta_1, \xi]$ . If the logarithm of the random field deviates from the Gaussian distribution, it is possible to modify the energy functional by adding a non-Gaussian term as follows

$$H_{\text{ng}}[y_\lambda(\mathbf{s}); \eta_0, \eta_1, \xi, \mathbf{q}] = H_{\text{fgc}}[y_\lambda(\mathbf{s}); \eta_0, \eta_1, \xi] + \delta H[y_\lambda(\mathbf{s}); \mathbf{q}], \quad (10)$$

where  $\delta H$  is the non-Gaussian term that involves a parameter vector  $\mathbf{q}$ . For simplicity, below we are going to express (10) as  $H = H_G + \delta H$ , where  $H$  is the entire energy functional, and  $H_G = H_{\text{fgc}}$  is the Gaussian FGC contribution. Now one has to determine the entire set of model parameters  $\eta_0, \eta_1, \xi, \mathbf{q}$  (and possibly  $k_c$ ) simultaneously from the sample. The deviation of the distribution from the Gaussian dependence is captured by means of additional constraints, e.g. based on the local terms  $S_3(\mathbf{s}) = y_\lambda^3(\mathbf{s})$  and  $S_4(\mathbf{s}) = y_\lambda^4(\mathbf{s})$ . The corresponding distance functional then becomes

$$\begin{aligned} \Phi_s[X_\lambda(\mathbf{s})] = & \left| 1 - \sqrt{\frac{\bar{S}_1}{\bar{S}_0}} \frac{E[S_0]}{E[S_1]} \right|^2 + \left| 1 - \sqrt{\frac{\bar{S}_2}{\bar{S}_0}} \frac{E[S_0]}{E[S_2]} \right|^2 + \\ & \left| 1 - \sqrt{\frac{\bar{S}_3}{\bar{S}_0^{3/2}}} \frac{E[S_0]^{3/2}}{E[S_3]} \right|^2 + \left| 1 - \sqrt{\frac{\bar{S}_4}{\bar{S}_0^2}} \frac{E[S_0]^2}{E[S_4]} \right|^2 \end{aligned} \quad (11)$$

The ratio  $\bar{S}_3/\bar{S}_0^{3/2}$  represents the sample skewness coefficient, while  $\bar{S}_4/\bar{S}_0^2$  the sample kurtosis coefficient. In the case of the Gaussian FGC-SSRF model, the stochastic moments  $E[S_m]$ ,  $m = 0, 1, 2$  (which are used in determining the model parameters) are expressed exactly in terms of the two-point covariance function. The covariance spectral density also follows directly from the energy functional. Such explicit expressions are not available for non-Gaussian energy functionals. The moments must be calculated either by numerical integration (e.g., Monte Carlo methods) for each set of parameters visited by the optimization method or by approximate, explicit methods that have been developed in the framework of many-body theories, e.g. [5, 8, 9, 13].

In statistical physics, e.g. [4, 5, 6] there is a long literature on approximate but explicit methods (variational approximations, Feynman diagrams, renormalization group, replicas) that address calculations with non-Gaussian

probability densities. Preliminary efforts to apply these methods in geostatistical research [9, 12], and references therein] should be followed by further research on closed-form expressions for non-Gaussian Spartan densities and the accuracy of such approximations in various areas of the parameter space. In the variational approach [2, 5, 8], the non-Gaussian probability density is expanded around an ‘optimal’ Gaussian. The variational Gaussian can then be used as the zero-point approximation for low-order or diagrammatic perturbation expansions of the moments [9, 13]. Below, we outline the application of the variational method [2, 4, pp. 198–200, 5, pp. 71–77].

### 5.1 The Variational Method

We present the formalism of the variational method assuming that the SSRF is defined in a discretized space (e.g. on a lattice). The fluctuation random field and its states are denoted by the vector  $\mathbf{y}$ . The characteristic function  $Z[\mathbf{J}]$  corresponding to the energy functional  $H$  is defined as

$$Z[\mathbf{J}] = \text{Tr} [\exp(-H + \mathbf{J} \cdot \mathbf{y})]. \quad (12)$$

The symbol ‘Tr’ denotes the trace over all the field variables in  $H$ . For a lattice field the trace is obtained by integrating over the fluctuations at every point of the lattice. The cumulant generating functional (CGF) is defined by

$$F[\mathbf{J}] = -\log Z[\mathbf{J}]. \quad (13)$$

The cumulants of the distribution are obtained from the derivatives of the CGF with respect to  $\mathbf{J}$ . For example, the mean is given by

$$E[y(\mathbf{s}_i)] = -\left. \frac{\partial F[\mathbf{J}]}{\partial J_i} \right|_{\mathbf{J}=0}, \quad (14)$$

and the covariance function by

$$G_{y;\lambda}(\mathbf{s}_1, \mathbf{s}_2) = \left. \frac{\partial^2 F[\mathbf{J}]}{\partial J_1 \partial J_2} \right|_{\mathbf{J}=0}. \quad (15)$$

Higher-order cumulants are given by higher order derivatives of the CGF. The CGF of the Gaussian part  $H_0 - \mathbf{J} \cdot \mathbf{y}$  is denoted as  $F_0[\mathbf{J}]$ . Let us now consider a variational Gaussian energy functional  $H_0$ , which is in general different than the Gaussian component  $H_G$  of  $H$ . The average of an operator  $A$  with respect to the pdf with energy  $H_0$ , is obtained by means of

$$\langle A \rangle_0 = \frac{\text{Tr} A e^{-H_0}}{\text{Tr} e^{-H_0}}. \quad (16)$$

The following inequality [5] is valid for all  $H_0$

$$F[\mathbf{J}] \leq F_0[\mathbf{J}] + \langle H - H_0 \rangle_0. \quad (17)$$

The optimal  $\hat{H}_0$  that gives the best approximation of  $F[\mathbf{J}]$ , is obtained by minimizing the variational bound  $F_0 + \langle H - H_0 \rangle_0$  with respect to the parameters of  $H_0$ . The optimal Gaussian pdf has energy  $\hat{H}_0$  and provides approximate estimates of the non-Gaussian covariance function.

It is possible to improve on the variational approximation by expressing the energy functional  $H$  as follows

$$H = \hat{H}_0 + (H - \hat{H}_0) = \hat{H}_0 + (H_G - \hat{H}_0 + \delta H), \quad (18)$$

and treating the component  $H_{\text{pert}} = H_G - \hat{H}_0 + \delta H$  of the energy functional as a perturbation around the optimal Gaussian  $\hat{H}_0$ . Corrections of the stochastic moments can then be obtained either by means of simple (low-order) perturbation expansions, or by means of diagrammatic perturbation methods. However, there is no a priori guarantee that such corrections will lead to more accurate estimates, and such approximation must be investigated for each energy functional.

## 5.2 Example of Variational Calculation

Here we present a simple example for a univariate non-Gaussian pdf, which illustrates the application of the variational method. Consider the non-Gaussian energy functional

$$H(y) = a^2 y^2 + \beta^4 y^4, \quad (19)$$

where  $y$  is a fluctuation with variance  $E[y^2]$ , and the average is over the pdf  $p(y) = Z^{-1} \exp(-H)$ . The following Gaussian variational expression is used as an approximation of the non-Gaussian pdf

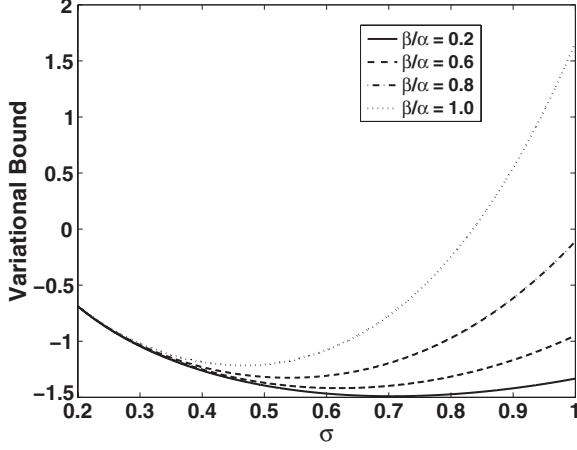
$$p_0(y) = \left( \sqrt{2\pi}\sigma \right)^{-1} \exp(-y^2/2\sigma^2). \quad (20)$$

Hence, the variational energy functional is  $H_0 = y^2/2\sigma^2$  and  $\sigma$  is the variational parameter. It follows that  $F_0 = -\log(\sqrt{2\pi}\sigma)$  and  $\langle H - H_0 \rangle_0 = a^2 \sigma^2 + 3\beta^4 \sigma^4 - 1/2$ . The variational bound given by (17) is a convex upward function of  $\sigma$ , as shown in Fig. 1. The bound is minimized for the following value of  $\sigma$

$$\hat{\sigma} = \frac{\alpha}{6\beta^2} \left\{ 3 \left[ \sqrt{1 + 12\rho^4} - 1 \right] \right\}^{1/2} = \frac{\alpha^{-1}}{6\rho^2} \left\{ 3 \left[ \sqrt{1 + 12\rho^4} - 1 \right] \right\}^{1/2}. \quad (21)$$

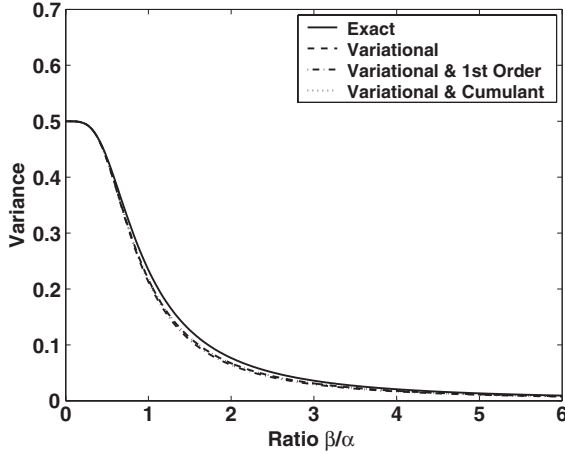
In the above,  $\rho = \frac{\beta}{\alpha}$  is the dimensionless ratio of the quartic over the quadratic pdf parameters that measures the deviation of the energy functional from the Gaussian form. The value of  $\hat{\sigma}^2$  is the variational estimate of the variance. The exact variance, calculated by numerical integration, and the variational approximation for various values of the dimensionless coefficient ratio  $\rho = \beta/\alpha$





**Fig. 1.** Plots of the variational bound as a function of  $\sigma$  for four different values of the ratio  $\beta/\alpha$

are plotted in Fig. 2, which shows that the variational estimate is an excellent approximation of the exact result even for large values of the ratio  $\rho$ . Estimates based on first-order and cumulant perturbation expansions around the optimal Gaussian (these will be presented in detail elsewhere) are also shown in Fig. 2. The additional corrections do not significantly alter the outcome of the variational approximation for the variance, since all three plots almost coincide. However, such corrections will be necessary for calculating higher moments of non-Gaussian distributions. For example, the kurtosis of the



**Fig. 2.** Plots of the exact variance (numerical) and approximate estimates based on the variational approach as well as combinations of variational and perturbation methods (first order and cumulant expansion)

variational Gaussian is equal to 3, and thus it is not an accurate approximation of the kurtosis of the non-Gaussian distribution except for very small values of  $\beta$ .

## 6 Discussion

Spartan random fields provide an alternative to classical geostatistics for modeling the local variability of spatial processes. Spartan models are computationally efficient for large samples. In addition, they allow quantifying the variability of spatially sparse data sets, since the model parameters can be determined from a small number of measurements, in contrast with models based on variograms. The SSRFs also include a resolution scale that controls the smoothness of the field.

For SSRFs the structure of the energy functional, which may involve only short-range interactions, also determines the spatial dependence at large distances. In principle, the impact of this property on geostatistical modeling is mixed: On one hand, it does not allow estimating long-range dependence directly from the data. On the other hand, the estimation of the variogram at large distance often suffers from significant uncertainty due to insufficient number of pairs. Hence, the ability of SSRFs to model the long-range behavior of spatial processes needs to be investigated. It should also be mentioned that it is possible to modify the energy functional of the SSRFs by adding explicit long-range interactions.

Non-Gaussian distributions can be handled by means of the standard logarithmic transform. It is also possible to define interactions in the energy functional that lead to specific non-Gaussian probability densities. The complexity of the inference problem in this case increases compared to the Gaussian case. Certain methods that may be helpful for calculations with non-Gaussian densities were suggested in this paper, and the variational method was presented in more detail with the help of a specific univariate example.

Certain other methodological and numerical issues of SSRFs require further investigation. The methodological issues include estimation at unsampled points, Monte Carlo simulation, application to real data sets, formulation of estimation uncertainty, stability of model parameters to uncorrelated noise, modelling of spatial processes with multiple scales of variability and anisotropic structures. Estimation has been briefly discussed in [10], and unconditional simulation in [11]. Numerical issues involve efficient algorithms for optimization (model inference process), simulation, and the processing of spatial information in problems with irregular supports.

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