UNDERSTANDING OF SPATIAL PROBLEM FOR LARGE DATASETS

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1 GAUSSIAN RANDOM FIELD AND ITS CHALLENGE

Gaussian spatial processes has been popular for decades in spatial data contexts like geostatistics where they are known as kriging, and in computer experiments where they are deployed as surrogate models or emulators. More recently, they have become a popular prediction engine in the machine learning literature. The reasons are many, but the most important are probably that: the Gaussian structure affords a large degree of analytic capability not enjoyed by other general-purpose approaches to nonparametric nonlinear modeling; and because they perform well in out-of-sample tests.

Assume there is a response or dependent variable $Y(s)$ at a generic location $s \in \mathbf{D} \subset \mathcal{R}^2$ along with a $p \times 1$ vector of spatially referenced predictors $\mathbf{X}(s)$. A spatial regression model has the form

$$y(s) = \beta \mathbf{X}(s) + w(s) + \epsilon(s) \tag{1}$$

where β is the vector of regression coefficients. The residual from the regression is decomposed into two independent parts: a spatial process, $w(s)$, modelling spatial association, and an independent process, $\epsilon(s)$, also known as the nugget effect, modelling measurement error.

The nugget effect $\epsilon(s)$ is often assumed to follow a normal distribution with variance τ^2 for every location s. The spatial process $w(s)$ in (1) is often referred to as spatial random effects, capturing the effect of unmeasured or unobserved covariates with spatial pattern.

The most common specification for $w(s)$ is $w(s) \sim GP(0, \mathbf{C}(\cdot,\cdot))$, a zero-mean Gaussian process with a valid covariance function $\mathbf{C}(s, s')$. It is often reasonable to assume a constant process variance and thus we specify $\mathbf{C}(s, s') = \sigma^2 \rho(s, s'; \theta)$, where $\rho(s, s'; \theta)$ is a correlation function and θ is a vector of correlation parameters which needs to be estimated from a finite number of observations, $\mathbf{Y} = (y(s_1). \cdots, y(s_n))'$.

Therefore, $y(s)$ follows a spatial Gaussian process, and thus we have the log-likelihood function for $(\beta, \tau^2, \sigma^2, \theta)$:

$$l(\beta, \tau^2, \sigma^2, \theta) \propto -\frac{1}{2} \log |\mathbf{\Sigma}| - \frac{1}{2} (\mathbf{Y} - \beta \mathbf{X})' \mathbf{\Sigma}^{-1} (\mathbf{Y} - \beta \mathbf{X}) \tag{2}$$

where $\mathbf{\Sigma} = \mathbf{C} + \tau^2 \mathbf{I}$. Then best linear unbiased prediction (BLUP) at an unobserved location s_0 can be obtained by the kriging equation:

$$\hat{y}(s_0) = \beta \mathbf{X}(s_0) + \mathbf{S}'_{s_0} \mathbf{\Sigma}^{-1} (\mathbf{Y} - \beta \mathbf{X}) \tag{3}$$

where $\mathbf{S}_{s_0} = (\mathbf{\Sigma}(s_0, s_1), \ldots, \mathbf{\Sigma}(s_0, s_n))'$.

However, with large or massive data, direct implementation of these statistical process, including parameter etimation by (2) and interpolation by (3), becomes computationally prohibitive, since evaluating the log-likelihood in (2) and solving the kriging equation (3) involve the Cholesky factorization of an $n \times n$ covariance matrix for data of size n, which requires $O(n^3)$ operations and $O(n^2)$ memory in general(see Porcu et al. [2012], Sang and Huang [2012], Heaton et al. [2019], Ma and Kang [2020]).

2 SEVERAL APPROACHES TO OVERCOME THE COMPUTATIONAL PROBLEM

From an **approximation** point of view, the approximation of the likelihood in either the spatial or spectral domain is fundamental solution to overcome computational obstacles. These solutions focus on model development, the design of efficient and parallel algorithms, and the improvement and efficient use of modern computing platforms (e.g. Using TensorFlow and GPU).

Model:

1) Conditional distributions: Michael L. Stein (The restricted likelihood, 2004);
2) Sparse covariance by tapering method: Reinhard Furrer(2006); Douglas Nychka(bias correction, 2008); Michael L. Stein(Statistical Properties, 2013);
3) Low-Rank methods: Noel Cressie (FRK, 2008), Sudipto Banerjee (Predictive process, 2008); Matthias Katfuss(multiresolution approximation, 2017) by basis-function;
4) Sparse precision: Douglas Nychka(lattice kriging, 2015) by basis-function; Finn Lindgren (GRMF Approximations, 2011) by SPDE; Abhi Datta (NNGP, 2016a, 2016b, 2016c, 2019) by conditional distributions;
5) Spectral method: Montserrat Fuentes and Joe Guinness(Circulant embedding, 2017 and Periodic Embeddings, 2007, 2019).
6) Discrete process convolutions. Dave Higdon(2002); Bruno Sansó(2009); Francky Fouedjio(2016).
7) Vecchia's approximation: Zilber and Katzfuss [2020], Katzfuss et al. [2020] and Jurek and Katzfuss [2020].

Algorithms and platforms:

1) INLA: Haavard Rue.
2) Parallel algorithm: Matthias Katfuss.
3) TensorFlow: Andrew Zammit-Mangion.

Table 1: Scope of application

Model	**non-stationary**	**space-time**	**multivariate data**
FRK	√	√	√
Predictive process	√		√
MRA	√	√	
Tapering			√
Spatial partitioning			
LatticeKrig	√	×	×
SPDE	√	√	√
NNGP	√	√	√
Whittle's approximation	×	×	×

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3 LIKELIHOOD APPROXIMATIONS IN THE SPECTRAL DOMAIN

3.1 Whittle's likelihood

The spectral methods are computationally efficient by avoiding the calculation of determinants and can be easily adapted to model nonstationary processes as a mixture of independent stationary processes.

Fuentes [2007], [Guinness, 2019] and [Guinness and Fuentes, 2017] propose the use of small domain expansions and imputing data in a periodic fashion on the expanded lattice and presented a version of Whittle's approximation to the Gaussian negative log-likelihood by introducing a lattice process which can be used to deal with irregularly spaced data. Additional computational savings were obtained by truncating the spectral representation of the lattice process. The calculation requires $O(m \log_2 m + n)$ operations where m is lattice size. However, the flexibility of the spectral methods mentioned above are disputable in prediction with out of sample data, since the expanded lattice is pre-difined.

4 LIKELIHOOD APPROXIMATIONS IN THE SPATIAL DOMAIN

4.1 Low rank methods

Comment: The reduced rank based methods usually fail to accurately capture the local, small scale dependence structure [Sang and Huang, 2012].

4.1.1 *Fixed rank Kriging*

FRK ([Cressie and Johannesson, 2006], [Cressie and Johannesson, 2008]) aims to approximate the spatial process $w(s)$ in (1) by a linear combination of K ($\ll n$) **multi-resolution bisquare** basis functions:

$$w(s) = \sum_{r=1}^{R} \sum_{k=1}^{K_r} h_{rk}(s) w^{\star}_{rk} \tag{4}$$

where $K = \sum_{r=1}^{R} K_r$ and the coefficients $w^{\star}$ is an K-dimensional Gaussian vector with mean zero and exponential covariance defined by some small basic areal units. which ensures that all estimation and prediction equations only contain inverses of matrices of size $K \times K$.

4.1.2 *Gaussian predictive processes (GPP)*

With regard to the challenge of computational cost on covariance matrices, Banerjee et al. [2008] proposed a class of models based on the idea of a spatial predictive pro-

cess which is motivated by Kriging equation in (3). The predictive process projects the original process, $w(s)$ in (1), onto a subspace generated by realizations of the original process at a specified set of locations (or knots), e.g. $s_1^\star, \cdots, s_K^\star, K \ll n$. The approach is in the same spirit as process modeling approaches using basis functions and kernel convolutions, that is, specifications which attempt to facilitate computations through lower dimensional process representations, i.e.

$$w(s) = \mathbf{c}'_{s_0} \boldsymbol{\Sigma}^{-1}_{w^\star} w^\star_{rk} \tag{5}$$

where $\mathbf{c}_{s_0} = \left(\mathbf{C}(s_0, s_1^\star), \ldots, \mathbf{C}(s_0, s_K^\star)\right)'$, and then $\mathbf{c}'_{s_0} \boldsymbol{\Sigma}^{-1}_{w^\star}$ plays the same role as h in (4), and thus can be regarded as some basis functions.

Comment:

1) One advertised advantage of using the GPP approach as opposed to FRK or LatticeKrig is that the GPP basis functions are completely determined by the choice of covariance function $C(\cdot,\cdot)$, and note that the subsequent Multiresolution approximations is in step with GPP in this regard.

2) At the same time, however, when $C(\cdot,\cdot)$ is governed by unknown parameters (which is nearly always the case) the GPP basis functions need to be calculated iteratively rather than once as in FRK or LatticeKrig which will subsequently increase computation time.

4.1.3 *Multi-resolution approximations*

In contrast to FRK or LatticeKrig, the multi-resolution approximation (MRA) basis functions and the prior distribution of the corresponding weights $w_r^\star$ are chosen using the predictive-process approach to automatically adapt to any given covariance function $\mathbf{C}_r$, and so the MRA can adjust flexibly to a desired spatial smoothness and dependence structure. The MRA allows the number of basis functions to be approximately the same as the data by the two ways to do. The one is by increasing sparsity of the covariance matrices of the corresponding weights (achieved by tapering method, see [Katzfuss and Hammerling, 2017]), the other is by recursively partitioning the spatial domain (see [Katzfuss, 2017]).

4.2 Sparse covariance methods

4.2.1 *Tapering*

Including tapering for estimation (e.g. approximation log-likelihood function by a tapered covariance. See Kaufman et al. [2008]) and tapering for Kriging (or for interpolation or for prediction, e.g. approximation kriging equation by replacing the original covariance by a tapered version. See Furrer et al. [2006] and some R packages: spam, 2010; KriSp, 2006; fields, 2017.

Comment: The covariance tapering has shown great computational gains, but it also has its own drawbacks.

1) The covariance tapering may not be effective in accounting for **spatial dependence with long range**.

2) The accuracy of the tapering approximation for **nonstationary problems** remains an open question, and the application of tapering techniques to **multivariate random fields** (e.g. [Bevilacqua et al., 2016]) remains to be explored due to the lack of flexible compactly supported cross-covariance functions, see Porcu et al. [2012].

4.2.2 *Spatial partitioning*

By dividing region $\mathbf{D}$ into m disjoint subregions ($d = 1, 2, \cdots, m$), and then the modeling approach based on spatial partitioning is to again assume the model in (6) but take on the assumption of independence between observations across subregions.

$$y_d = \beta X_d + H_d w + \xi_d + \epsilon_d \tag{6}$$

where H_d is a matrix of spatial basis function for subregions d.
Comment:

1) Notice that, in (6) each subregion shares common β and w parameters which allows smoothing across subregions in spite of the independence assumption. Further, the assumption of independence across subregions effectively creates a block-diagonal structure for Σ and allows the likelihood to be computed in parallel (with one node per subregion), thereby facilitating computation.

2) The key to implementing the spatial partitioning approach is the choice of partition and the literature is replete with various options. A priori methods to define the spatial partitioning include partitioning the region into equal areas ([Sang et al., 2011]), partitioning based on centroid clustering ([Kim et al., 2005]), hierarchical clustering based on spatial gradients ([Heaton et al., 2017]). Alternatively, model-based approaches to spatial partitioning include treed regression([Konomi et al., 2014]) and mixture modeling (Neelon et al. [2014]), but these approaches typically require more computation.

4.3 Sparse precision methods

The sparse precision methods focus on basis function and conditional likelihood.

4.3.1 *LatticeKrig*

LatticeKrig (LK, [Nychka et al., 2015]) uses nearly the same setup as is employed by FRK. Here is just a list of the differences:

1) FRK uses families of **bisquare** basis functions that are organized on are organized on irregular basic areal units (BAUs), and LK uses families of **radial** basis functions that are organized on regular grids of increasing resolution.

2) Covariance matrix, Σ_r, of the coefficients $w_r^\star$ in (4) is constrained by a exponential function, the exponential function is defined on the centroids of the BAUs, and precision matrix, Q_r, of the coefficients $w_r^\star$ in LK is constrained to a spatial autoregressive (SAR) model, SAR model is defined on the regular lattice.

3) Furthermore, because $\mathbf{Q}_r$ is sparse, LK can set K to be very large (e.g. $K > n$) without much additional computational cost. However, the FRK does not achieve this effect.

4.3.2 *Gaussian Markov random field approximations by SPDE*

Rue and Held [2005] rigorously suggest to approximate Gaussian random fields through Markov fields with a huge increase in speed for the simulations, and then Lindgren et al. [2011] show the construction of the corresponding GMRFs can be used to represent the Matérn field on a triangulated lattice (i.e. the finite element construction).

Similar to FRK or LatticeKrig, the spatial process $w(s)$ in model (1) is represented by the basis function, this method use piecewise linear functions on a triangulation of the domain as basis functions $h(\cdot)$ in (4), and then this yields sparse matrices $\mathbf{C}$ and $\mathbf{G}$ such that the appropriate precision matrix for the weights $w^\star$ is given by (see [Blangiardo and Cameletti, 2015])

$$\mathbf{\Omega} = \tau^2(\kappa^4\mathbf{C} + 2\kappa^2\mathbf{G} + \mathbf{G}\mathbf{C}^{-1}\mathbf{G}).$$

One particular advantage of this approach is that assigning the Gaussian distribution $w^\star \sim N(0, \mathbf{\Omega}^{-1})$ can generate continuously defined functions $\mathcal{X}(s) = \sum_{k=1}^{m} h_k(s) w_k^\star$ that are approximative solutions to the following SPDE (in a stochastically weak sense):

$$(\gamma^2 - \Delta)^{\alpha/2}(\tau(\mathcal{X}(s))) = \mathcal{W}, \quad s \in \mathbf{D},$$

where Δ is the Laplacian, γ is the spatial scale parameter, α controls the smoothness of the realisations, τ controls the variance. The right-hand side of the equation, $\mathcal{W}(s)$, is a Gaussian spatial white noise process. Note that the stationary solutions on $\mathcal{R}^d$ have Matern covariances.

The drawback of Lindgren et al. [2011] is that we can only find the explicit form of GMRFs for those Gaussian random fields that have a Matérn covariance structure at certain integer smoothnesses. Subsequently, Bolin and Kirchner [2020] extend this method to fractional order by the rational approximation.

Comment:

1) The numerical factorization of the precision matrix using sparse matrix algorithms can be done at a typical cost of $O(n^{3/2})$ for two-dimensional GMRFs.

2) SPDE can be extended to model Matérn covariances on the sphere, non-stationary locally isotropic Gaussian random fields (e.g. by using spatially varying parameters), Gaussian random fields with oscillating correlation functions, and non-isotropic fields.

3) The SPDE approach also facilitates extensions to Multivariate random fields, see Hu et al. [2013], Hu and Steinsland [2016], Bolin and Wallin [2020].

4.3.3 *The nearest neighbor Gaussian process*

Similar to the pre-defined knots for Gaussian predictive processes, the starting point of nearest neighbor Gaussian process (NNGP) approach is to choose a fixed collection (e.g. S) of distinct locations in $\mathbf{D}$, where S need not coincide with or be

apart of the observed locations, so its size k need not equal the size of the dataset n (or even larger than the size n). The set S is called as reference set by Datta et al. [2016a].

A directed acyclic graph is defined on the reference set S, and then the joint distribution of spatial process $w(s)$ from the reference set is represented by the product of conditional densities which is motivated by Vecchia's approximation [Vecchia, 1988] ideas, where a careful choice of suitable conditional sets is required, and this conditional set is constrained to be the m nearest neighbors by the NNGP approach and thereby facilitating computation in estimation and prediction problem (for more details on those problems, see [Finley et al., 2017] and Finley et al. [2019]). Based on these results, the NNGP can be well-defined.

1) Total operations is $O((n+k)m^3)$ where $m(\approx 20)$ is the size of conditioning set or neighbor set.

2) NNGP can also be extended to large spatio-temporal data (Datta et al. [2016b]) and non-stationary process(Konomi et al. [2019]), [Risser and Turek, 2020].

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