Vecchia-Laplace approximations of generalized Gaussian processes for big non-Gaussian spatial data

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Abstract

Generalized Gaussian processes (GGPs) are highly flexible models that combine latent GPs with potentially non-Gaussian likelihoods from the exponential family. GGPs can be used in a variety of settings, including GP classification, nonparametric count regression, modeling non-Gaussian spatial data, and analyzing point patterns. However, inference for GGPs can be analytically intractable, and large datasets pose computational challenges due to the inversion of the GP covariance matrix. To achieve computationally feasible parameter inference and GP prediction for big spatial datasets, we propose a Vecchia-Laplace approximation for GGPs, which combines a Laplace approximation to the non-Gaussian likelihood with a computationally efficient Vecchia approximation to the GP. We examine the properties of the resulting algorithm, including its linear complexity in the data size. We also provide numerical studies and comparisons on simulated and real spatial data.

Keywords: Exponential family; Kriging; Geostatistics; Spatial Generalized Linear Mixed Model; Nearest Neighbor

1 Introduction

Dependent non-Gaussian data are ubiquitous in time series, geospatial applications, and more generally in nonparametric regression and classification. A popular model for such data is obtained by combining a latent Gaussian process (GP) with conditionally independent, potentially non-Gaussian likelihoods from the exponential family. This is referred to as a spatial generalized linear mixed model in spatial statistics (Diggle et al., 1998) and a generalized GP (GGP) in machine learning (e.g., Chan and Dong, 2011). GGPs are highly flexible, interpretable, and allow for natural, probabilistic uncertainty quantification. However, inference for GGPs can be analytically intractable, and large datasets pose additional computational challenges due to the inversion of the GP covariance matrix.

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Popular techniques to numerically perform the intractable marginalization necessary for inference are, in order of increasing speed: Markov chain Monte Carlo (MCMC), expectation propagation, variational methods, and Laplace approximations. See Shang and Chan (2013) for a recent review of deterministic techniques, and Filippone and Girolami (2014) for a comparison of MCMC and expectation propagation. Here we consider the Laplace approximation (e.g., Tierney and Kadane, 1986; Williams and Barber, 1998), which approximates the posterior of the vector of latent GP realizations as Gaussian, by carrying out a second-order Taylor expansion of the log-posterior density at its mode. Rue et al. (2009) argue that variational methods and expectation propagation suffer from underestimated or overestimated posterior variances, respectively, and they provide adjustments to increase the accuracy of Laplace approximations.

It has long been recognized that the computational cost for GPs is cubic in the data size. Much work has been done on GP approximations that address this problem in the context of Gaussian noise (as recently reviewed in Heaton et al., 2019). Low-rank approaches (e.g., Higdon, 1998; Wikle and Cressie, 1999; Quinonero-Candela and Rasmussen, 2005; Banerjee et al., 2008; Cressie and Johannesson, 2008; Katzfuss and Cressie, 2011) have limitations in the presence of fine-scale structure (Stein, 2014), but they have proved popular due to their simplicity. Approximations relying on sparsity in covariance matrices (Furrer et al., 2006; Kaufman et al., 2008) by definition can only capture local, short-range dependence. Approaches that take advantage of Toeplitz or Kronecker structure (e.g., Dietrich and Newsam, 1997; Flaxman et al., 2015; Guinness and Fuentes, 2017) are not as generally applicable. Recently, methods relying on sparsity in precision matrices (Rue and Held, 2005; Lindgren et al., 2011; Nychka et al., 2015) have gained popularity due to their accuracy and flexibility.

To apply GGP s to large non-Gaussian datasets, a popular approach is to combine a low-rank GP with an approximation of the non-Gaussian likelihood, as the dimension reduction inherent in the low-rank approximation carries through even to the non-Gaussian case. Sengupta and Cressie (2013) take this approach and estimate parameters using an expectation-maximization algorithm with a Laplace approximation. Sheth et al. (2015) use variational inference to select a set of conditioning points that determine their low-rank approximation. For the case of one-dimensional non-Gaussian time series data, Nickisch et al. (2018) develop state-space models that can perform inference in linear time and memory using a set of knots in time, in what is essentially a low-rank approximation. Alternatively, the intractability issues with GGP s can be avoided completely by using low-rank approximations through alternate priors (e.g., log gamma priors for count data, Bradley et al., 2018).

Similar to what we shall propose, some authors have combined a sparse-precision approach with a non-Gaussian approximation. A prominent example is Lindgren et al. (2011), in which an integrated nested Laplace approximation (INLA) is combined with a sparse-precision approximation of the GP. Datta et al. (2016) proposed to apply the GP approximation of Vecchia (1988) to a latent GP, but did not explicitly study the case of non-Gaussian data. While both Lindgren et al. (2011) and Datta et al. (2016) limit the number of nonzero entries per row or column in the precision matrix to a small constant, the computational complexity for decomposing this sparse \( n \times n \) matrix is not linear in \( n \), but rather \( \mathcal{O}(n^{3/2}) \) in two dimensions (Lipton et al., 1979, Thm. 6), and at least \( \mathcal{O}(n^2) \) in higher dimensions. In the Gaussian setting, this scaling problem can be overcome by applying a Vecchia approximation to the observed data (Vecchia, 1988) or to the joint distribution of the observed data.
and the latent GP (Katzfuss and Guinness, 2017).

To handle both scaling and intractability, we propose a Vecchia-Laplace (VL) approximation for GGP$s. The posterior mode necessary for the Laplace approximation is typically found using the Newton-Raphson algorithm, which can be viewed as iterative GP inference based on Gaussian pseudo-data. At each iteration of our VL algorithm, the joint Gaussian distribution of the pseudo-data and the latent GP realizations is approximated using the general Vecchia framework (Katzfuss and Guinness, 2017; Katzfuss et al., 2018). By modeling the joint distribution of pseudo-data and GP realizations at each iteration, we are able to overcome the scaling issues of the sparse-matrix approaches mentioned above. Specifically, our VL approach ensures sparsity and guarantees linear scaling in $n$ for any dimension. We discuss the implied integrated likelihood for parameter inference, and provide an approach for obtaining predictions at unobserved locations. In addition, we show how VL can be used for the analysis of point patterns by approximating a log-Gaussian Cox process. As shown in Katzfuss and Guinness (2017), the general Vecchia approximation includes many other GP approximations (e.g., Finley et al., 2009; Snelson and Ghahramani, 2007; Sang et al., 2011; Katzfuss, 2017; Katzfuss and Gong, 2019) as special cases, and so our VL algorithm also offers a way to combine these approaches with a Laplace approximation.

The remainder of this document is organized as follows. In Section 2, we review the Laplace approximation and general Vecchia. In Section 3, we introduce our VL methods and describe their properties. In Sections 4 and 5, we study and compare the performance of VL on simulated and real data, respectively. Detailed calculations are left to the appendix. A separate Supplementary Material document contains Sections S1–S6 with additional derivations, simulations, and discussion. The methods and algorithms proposed here are implemented in the R package GPvecchia available at https://github.com/katzfuss-group/GPvecchia, and all results and figures can be reproduced using the code and data at https://github.com/katzfuss-group/GPvecchia-Laplace.

2 Review of techniques

2.1 Generalized Gaussian processes

Let $y(\cdot) \sim GP(\mu, K)$ be a latent Gaussian process with mean function $\mu$ and kernel or covariance function $K$ on a domain $D \subset \mathbb{R}^d$, $d \in \mathbb{N}^+$. Observations $z = (z_1, \ldots, z_n)'$ at locations $s_i \in D$ are assumed to be conditionally independent, $z_i | y \overset{\text{ind.}}{\sim} g_i(z_i | y_i)$, where $y = (y_1, \ldots, y_n)'$ and $y_i = y(s_i)$. We assume that the observation densities or likelihoods $g_i$ are from the exponential family. Parameters $\theta$ in $\mu$, $K$, or the $g_i$ will be assumed fixed and known for now.

Our goal is to obtain an approximation of the posterior of $y$, which takes the form

$$p(y | z) = \frac{N_n(y | \mu, K) \prod_{i=1}^n g_i(z_i | y_i)}{p(z)},$$

where $\mu = (\mu(s_1), \ldots, \mu(s_n))'$, and $K$ is an $n \times n$ covariance matrix with $(i, j)$ entry $(K)_{ij} = K(s_i, s_j)$. Once an approximation of the posterior (1) has been obtained, it is conceptually straightforward to extend this result to other quantities of interest, such as the integrated
likelihood for inference on parameters $\theta$ (see Section 3.3), and prediction of $y(\cdot)$ at unobserved locations (see Section 3.4).

### 2.2 Review of the Laplace approximation

The first difficulty with the posterior distribution in (1) is that the normalizing constant $p(z)$ is not available in closed form for non-Gaussian likelihoods. A popular approach to avoid this issue is the Laplace approximation (e.g., Tierney and Kadane, 1986; Williams and Barber, 1998; Rasmussen and Williams, 2006, Section 3.4), which is obtained by a second-order Taylor expansion of the log-posterior log $p(y|z)$ at its mode, and is equivalent to assuming that the posterior is Gaussian with mean and precision matrix equal to the mode and negative Hessian at the mode, respectively, of log $p(y|z)$. To make this approximation more precise, consider the first and second derivative of log $g_i$ and define

$$u_i(y_i) = \frac{\partial}{\partial y_i} \log g_i(z_i|y_i) \quad \text{and} \quad d_i(y_i) = -\left(\frac{\partial^2}{\partial y_i^2} \log g_i(z_i|y_i)\right)^{-1}, \quad i = 1, \ldots, n.$$  

Stacking these quantities as $u_y = (u_1(y_1), \ldots, u_n(y_n))'$ and $D_y = \text{diag}(d_1(y_1), \ldots, d_n(y_n))$, it is easy to show that $\frac{\partial}{\partial y} \log p(y|z) = K^{-1}(y - \mu) + u_y$ and $-\frac{\partial^2}{\partial y^2} \log p(y|z) = K^{-1} + D_y^{-1}$. Hence, the Laplace approximation is given by

$$\hat{p}_L(y|z) = \mathcal{N}_n(y|\alpha, W^{-1}_\alpha),$$

where $\alpha = \arg\max_{y \in \mathbb{R}^n} \log p(y|z)$ and $W_y = K^{-1} + D_y^{-1}$.

The mode $\alpha$ can be obtained using a Newton-Raphson algorithm. Starting with an initial value $y^{(0)}$, one updates the current guess for $l = 0, 1, 2, \ldots$ until convergence as $y^{(l+1)} = h(y^{(l)})$, where

$$h(y) = y - \left(\frac{\partial^2}{\partial y \partial y} \log p(y|z)\right)^{-1} \left(\frac{\partial}{\partial y} \log p(y|z)\right).$$  

(2)

The crucial observation for our later developments is that this Newton-Raphson update is equivalent to computing the posterior mean of $y$ given Gaussian pseudo-data $t_y = y + D_yu_y$ with noise covariance matrix $D_y$ (e.g., Rasmussen and Williams, 2006, Section 3.4.1). Specifically, we can write the Newton-Raphson update in (2) as:

$$h(y) = \mu + W_y^{-1}D_y^{-1}(t_y - \mu) = \mathbb{E}(y|t_y),$$  

(3)

which is the conditional mean of $y$ given Gaussian pseudo-data $t_y|y \sim \mathcal{N}_n(y, D_y)$. The derivation of (3) is straightforward and included in Appendix A for completeness. This means we can obtain the mode $\alpha$ by iteratively computing pseudo-data $t_y^{(l)}$ with $i$th entry $y_i^{(l)} + d_i(y_i^{(l)})u_i(y_i^{(l)})$ and obtaining the posterior mean $y^{(l+1)}$ of $y$ given $t_y^{(l)}$ assuming independent Gaussian noise with variances $d_1(y_1^{(l)}), \ldots, d_n(y_n^{(l)})$.

Some examples of popular likelihoods and the corresponding pseudo-data and pseudo-variances are summarized in Table 1. The Bernoulli and Poisson cases are also illustrated in Figure 1.
distribution | likelihood $g(z | y)$ | pseudo-data $t_y$ | pseudo-variance $d(y)$
--- | --- | --- | ---
Gaussian | $\mathcal{N}(y, \tau^2)$ | | $\tau^2$
Bernoulli | $\mathcal{B}(\text{logit}(y))$ | $y + \frac{(1+e^y)^2}{e^y}(z - e^y)\frac{z}{1+e^y}$ | $(1 + e^{-y})(1 + e^y)$
Poisson | $\mathcal{P}(e^y)$ | $y + e^{-y}(z - e^y)$ | $e^{-y}$
Gamma | $\mathcal{G}(a, ae^{-y})$ | $y + (1 - z^{-1}e^y)$ | $aze^{-y}$

Table 1: Examples of popular likelihoods, together with the Gaussian pseudo-data and pseudo-variances implied by the Laplace approximation. The non-canonical logarithmic link function is used for the Gamma likelihood to ensure that the second parameter, $ae^{-y}$, is positive.

Figure 1: Pseudo-data $t_\alpha$ plus or minus half the standard deviation of the pseudo-noise for simulated data $z$ in one spatial dimension, along with the latent posterior mode $\alpha$ plus or minus half the posterior standard deviation. Note that the data are on a different scale than the pseudo-data due to the link function.

Once the algorithm has converged (i.e., $y^{(l)} = \alpha$), the Laplace approximation can be viewed as an approximation of the likelihood based on pseudo-data,

$$\hat{p}_L(z | y) = p(t_\alpha | y) = \mathcal{N}_n(t_\alpha | y, D_\alpha),$$

or equivalently as an approximation of the posterior conditional on pseudo-data,

$$\hat{p}_L(y | z) = p(y | t_\alpha) = \mathcal{N}_n(y | \alpha, W^{-1}_\alpha).$$

2.3 Review of the general Vecchia approximation

The Laplace approximation described in Section 2.2 allows us to deal with non-Gaussian likelihoods, but it still requires decomposing the $n \times n$ matrix $K$ and thus scales as $O(n^3)$. To achieve computational feasibility even for data sizes $n$ in the tens of thousands or more, we also apply a general Vecchia approximation (Katzfuss and Guinness, 2017; Katzfuss et al., 2018), which we will briefly review here.
Assume that $y \sim \mathcal{N}(\mu, K)$ is a vector of GP realizations and $t|y \sim \mathcal{N}(y, D)$ a vector of noisy data, where $D$ is diagonal. Then, consider a vector $x = y \cup t$ consisting of the $2n$ elements of $y$ and $t$ in some ordering (more details below). It is well known that the density function, $p(x)$, can be factored into a product of univariate conditional densities,

$$p(x) = \prod_{i=1}^{2n} p(x_i|x_{1:i-1}),$$

where $c(i) \subset \{1, \ldots, i - 1\}$ is a conditioning index set of size $m$ (or of size $i - 1$ for $i \leq m$). If $m$ is small, the approximation can lead to enormous computational savings.

As $y_i = y(s_i)$ and $t_i$ is the corresponding noisy observation, the ordering within $y$ and within $t$ is determined by an ordering of the observed locations, $s_1, \ldots, s_n$. We will use a coordinate-based (left-to-right) ordering in one spatial dimension. In higher-dimensional spaces, we recommend a maxmin ordering (Guinness, 2018; Schäfer et al., 2017), which sequentially chooses each location in the ordering to maximize the minimum distance to previous locations in the ordering.

By straightforward extension of the proof of Prop. 1 in Katzfuss and Guinness (2017) to the case $\mu \neq 0$, it can be shown that the approximation in (6) implies a multivariate normal joint distribution, $\hat{p}(x) = \mathcal{N}(\mu_x, Q^{-1})$, where $\mu_{x,i} = \mu(s_j)$ if $x_i = y_j$ or $x_i = t_j$, $Q = UU'$, and $U$ is the sparse upper triangular Cholesky factor based on a reverse row-column ordering of $Q$. We write this as $U = rchol(Q) := rev(chol(rev(Q)))$, where $rev(\cdot)$ reverse-orders the rows and columns of its matrix argument. The nonzero entries of $U$ are computed directly based on the covariance function $K$ as described in Appendix B.

Let $U_y$ and $U_t$ be the submatrices of $U$ consisting of the rows of $U$ corresponding to $y$ and $t$, respectively. Then, $W = U_y U_y$ is the general Vecchia approximation to the posterior precision matrix of $y$ given $t$. Defining $V := rchol(W)$, we can obtain the posterior mean of $y$ as $E(y|t) = \mu - (V')^{-1} V^{-1} U_y U_t^t (t - \mu)$.

### 3 Vecchia-Laplace methods

We now introduce our Vecchia-Laplace (VL) approximation, which allows fast inference for large datasets modeled using GGPs, by combining the general Vecchia and Laplace approximations.

#### 3.1 The VL algorithm

To apply a Laplace approximation, it is first necessary to find the mode of the posterior density of $y$. As discussed in Section 2.2, this is usually done using a Newton-Raphson algorithm, which can be viewed as iteratively computing a new value $y^{(l+1)}$ as the posterior mean of the latent GP realization $y$ based on Gaussian pseudo-data $t = t_y^{(l)}$. Our VL algorithm applies a general Vecchia approximation $\hat{p}(x)$ to the joint distribution of $x = y \cup t$ at each iteration $l$, and computes the posterior mean of $y$ given $t$ under this approximate
The resulting VL algorithm is presented as Algorithm 1. After convergence, we obtain the approximation

\[ \hat{p}_{VL}(y|z) = N_n(y|\alpha_V, W_V^{-1}). \]  

**Algorithm 1 Vecchia-Laplace (VL)**

1: procedure \textsc{Vecchia-Specify}(\(S, m\)) \Comment{Define Vecchia Structure}
2: \hspace{1em} Order locations \(S\) using coordinate (in 1D) or maxmin ordering (in 2D or higher)
3: \hspace{1em} For VL-IW, determine variable ordering and conditioning as in Sect. 3.2.1
4: \hspace{1em} For VL-RF, determine variable ordering and conditioning as in Sect. 3.2.2
5: \hspace{1em} return ordering and conditioning info in Vecchia Approximation Object \(\text{VAO}\)
6: end procedure

7: procedure \textsc{VL-Inference}(\(z, \text{VAO}, g_i, \mu, K\)) \Comment{Maximize GP Posterior}
8: \hspace{1em} Derive \(u_i(\cdot) = \frac{\partial}{\partial y} \log g_i|_{(\cdot)}\) and \(d_i(\cdot) = \frac{\partial^2}{\partial y^2} \log g_i|_{(\cdot)}\)
9: \hspace{1em} Initialize \(y^{(0)} = \mu\)
10: \hspace{1em} for \(l=0,1,\ldots\) do
11: \hspace{2em} Compute \(u = (u_1(y_1^{(l)}), \ldots, u_n(y_n^{(l)}))^T\) and \(D = \text{diag}(d_1(y_1^{(l)}), \ldots, d_n(y_n^{(l)}))\)
12: \hspace{2em} Update pseudo-data \(t = y^{(l)} + Du\)
13: \hspace{2em} Compute \(U\) (see Appendix B) based on \(D, K,\) and \(\text{VAO}\)
14: \hspace{2em} Extract submatrices \(U_y\) and \(U_t\)
15: \hspace{2em} Compute \(W = U_y U'_y\) and \(V = \text{rchol}(W)\)
16: \hspace{2em} Compute the new posterior mean: \(y^{(l+1)} = \mu - (V')^{-1}V^{-1}U_y U'_t(t - \mu)\)
17: \hspace{2em} if \(\|y^{(l+1)} - y^{(l)}\| < \epsilon\) then
18: \hspace{3em} return \(\alpha_V = y^{(l+1)}\) and \(W_V = W\) \Comment{Posterior Mode Estimate}
19: \hspace{2em} end if
20: \hspace{1em} end for
21: end procedure

Once the algorithm has converged and the posterior mean \(\alpha_V\) and precision \(W_V\) have been obtained, the posterior distribution in (7) can be used for estimation of the integrated likelihood (Section 3.3) and for prediction at unobserved locations (Section 3.4). As we will see in our simulation studies later, even for moderate \(m\), the VL procedure in Algorithm 1 essentially finds the exact mode of the posterior.

### 3.2 Specific Vecchia approximations

We now consider two specific approximations within the general Vecchia framework, which are based on how the elements of \(y\) and \(t\) are ordered in the vector \(x\) in (6): Interweaved (IW) ordering and response-first (RF) ordering. IW ordering is recommended for the integrated likelihood (Section 3.3) and for Algorithm 1 in one spatial dimension. RF ordering is recommended for Algorithm 1 when working in more than one dimension.
3.2.1 Interweaved (IW) ordering

Vecchia-Interweaved (IW) is the sparse general Vecchia approach proposed for likelihood inference in Katzfuss and Guinness (2017), reviewed briefly here. It is a special case of general Vecchia in (6), in which \(x = (y_1, t_1, y_2, t_2, \ldots, y_n, t_n)'\) is specified using an interweaved ordering of the latent \(y\) and (pseudo-)data \(t\). We consider the following specific expression for (6):

\[
\hat{p}_{IW}(x) = \prod_{i=1}^{n} p(t_i|y_i) p(y_i|y_{q_y(i)}, t_{q_t(i)}).
\]  

(8)

If \(x_j = t_i\), we only condition on \(y_i\), because \(D\) is diagonal and therefore \(t_i\) is conditionally independent of all other variables in \(y\) and \(t\) given \(y_i\). If \(x_j = y_i\), we condition on \(y_{q_y(i)}\) and \(t_{q_t(i)}\), where \(q(i) = q_y(i) \cup q_t(i)\) is the conditioning index vector consisting of the indices of the nearest \(m\) locations previous to \(i\) in the ordering. For splitting \(q(i)\) into \(q_y(i)\) and \(q_t(i)\), we attempt to maximize \(q_y(i)\) subject to sparse-general-Vecchia rules (Katzfuss and Guinness, 2017). Specifically, for \(i = 1, \ldots, n\), we set \(q_y(i) = (k_i) \cup (q_y(k_i) \cap q(i))\), where \(k_i \in q(i)\) is the index whose latent-conditioning set has the most overlap with \(q(i)\): \(k_i = \arg \max_{j \in q(i)} |q_y(j) \cap q(i)|\), choosing the closest \(k_i\) in space to \(s_i\) in case of a tie. In one-dimensional space with coordinate ordering, this results in \(q_y(i) = q(i) = \{\text{max}(1, i-m), \ldots, i-1\}\) and \(q_z(i) = \emptyset\). In higher-dimensional space, we may not be able to condition entirely on \(y\), so the remaining conditioning indices are assigned to \(q_t(i) = q(i) \setminus q_y(i)\). This conditioning under sparse-general-Vecchia rules guarantees that \(U\) and \(V\) are both highly sparse with at most \(m\) nonzero off-diagonal elements per column. Katzfuss and Guinness (2017) showed that these matrices, and the resulting posterior mean and precision matrix, can be obtained in \(O(nm^3)\) time.

3.2.2 Response-first (RF) ordering

For approximating predictions at observed locations in Algorithm 1 in more than one dimension, we recommend the new RF-full method described in Katzfuss et al. (2018), reviewed briefly here. RF-full orders first all pseudo-response variables, then all latent variables: \(x = (t', y')' = (t_1, \ldots, t_n, y_1, \ldots, y_n)'\). We consider the following specific expression for (6):

\[
\hat{p}_{RF}(x) = \prod_{i=1}^{n} p(t_i) p(y_i|y_{q_y(i)}, t_{q_t(i)}).
\]

The data \(t_i\) do not condition on anything and are considered independent; this implies a poor approximation to \(p(t)\), but it does not affect the posterior distribution \(p(y|t)\), which is the relevant quantity in the VL algorithm. We now assume \(q(i) = q_y(i) \cup q_t(i)\) to be set of indices corresponding to the \(m\) locations closest to \(s_i\) (including \(s_i\)), not considering the ordering. For any \(j \in q(i)\), we then let \(y_i\) condition on \(y_j\) if it is ordered previously in \(x\); otherwise, we condition on \(t_j\). More precisely, we set \(q_y(i) = \{j \in q(i) : j < i\}\) and \(q_t(i) = \{j \in q(i) : j \geq i\}\). Similar to IW, RF-full inference can be carried out in \(O(nm^3)\) time (Katzfuss et al., 2018).
3.3 Integrated likelihood for parameter inference

In the case of unknown parameters \( \theta \) in \( \mu, K \), or in the \( g_i \), we would like to carry out parameter inference based on the integrated likelihood,

\[
\mathcal{L}(\theta) = p(z|\theta) = \int p(z|y, \theta)p(y|\theta)dy.
\]

However, this quantity is exactly the unknown normalizing constant in the denominator of (1), and the integral can generally not be carried out analytically. Instead, we will base parameter inference on the integrated likelihood implied by our VL approximation. In the following, we will again suppress dependence on \( \theta \) for ease of notation.

First, rearranging terms in (1), we have \( p(z) = p(z|y)p(y)/p(y|z) \). The Laplace approximation approximates the posterior in the denominator as \( \hat{\mathcal{L}}(y|z) = p(y|t_\alpha) \) (see (5)). Noting that rearranging the definition of a conditional density gives \( p(y) = p(y, t)/p(t|y) \), we obtain the Laplace approximation of the integrated likelihood:

\[
\mathcal{L}_L(\theta) = \hat{\mathcal{L}}(z) = \frac{p(y, t)}{p(y|t)} \cdot \frac{p(z|y)}{p(t|y)} = p(t) \cdot \frac{p(z|y)}{p(t|y)},
\]

where the terms are evaluated at \( y = \alpha \) and \( t = t_\alpha \). In this form, the approximation of the integrated likelihood of the data \( z \) can be interpreted as a product of the integrated likelihood of the Gaussian pseudo-data \( p(t) \), times a correction term given by the ratio of the true likelihood to the Gaussian likelihood of the pseudo-data:

\[
p(z|y)/p(t|y) = \prod_{i=1}^n g_i(z_i|y_i)/\mathcal{N}(t_i|y_i, d_i).
\]

To achieve scalability, we approximate the density \( p(t) = p(x)/p(y|t) \) as implied by the IW approximation \( \hat{\mathcal{L}}_W(x) \) in (8). The resulting expression for \( \hat{\mathcal{L}}_W(t) \) is derived in Katsfuss and Guinness (2017) for the case of \( \mu = 0 \). We show in Section S1 that the approximate density essentially has the same form if the prior mean is not zero:

\[
-2 \log \hat{\mathcal{L}}_W(t) = -2 \sum_i \log U_{ii} + 2 \sum_i \log V_{ii} + \tilde{t}'\tilde{t} - \tilde{t}'\tilde{t} + n \log 2\pi,
\]

where \( \tilde{t} = U'_t(t - \mu) \) and \( \tilde{t} = V^{-1}U_y\tilde{t} \).

Thus, for a specific parameter value \( \theta \), we run Algorithm 1 based on \( \theta \) to obtain \( \alpha_V \), set \( y = \alpha_V \), \( t = t_\alpha \), and \( d_i = (D_{\alpha_V})_{ii} \), and then evaluate the VL integrated likelihood as

\[
\mathcal{L}_{VL}(\theta) = \hat{\mathcal{L}}_{VL}(z|\theta) = \hat{\mathcal{L}}_{IW}(t) \prod_{i=1}^n \frac{g_i(z_i|y_i)}{\mathcal{N}(t_i|y_i, d_i)}.
\]

We can plug \( \mathcal{L}_{VL}(\theta) \) into any numerical likelihood-based inference procedure, such as numerical optimization for finding the maximum likelihood estimator of \( \theta \), or sampling-based algorithms for finding the posterior of \( \theta \). In an iterative inference procedure, we recommend initializing \( y^{(0)} \) in Algorithm 1 at the mode \( \alpha_V \) obtained for the previous parameter value. Our integrated likelihood can also be used directly to evaluate the posterior of \( \theta \) over a grid of high-probability points (Rue et al., 2009, Sect. 3.1). An extension to the integrated nested Laplace approximation (INLA) that improves the accuracy of the marginal posteriors of the \( y_i \) (Rue et al., 2009, Sect. 3.2) is straightforward.
3.4 Predictions at unobserved locations

We now consider making predictions at \( n^\star \) unobserved locations, \( \mathcal{S}^\star = \{s_1^\star, \ldots, s_n^\star\} \), by obtaining the posterior distribution of \( y^\star = (y_1^\star, \ldots, y_n^\star)' \) with \( y_i^\star = y(s_i^\star) \). Using the Laplace approximation as expressed in (4), GGP predictions are approximated as GP predictions given Gaussian pseudo-data \( t_\alpha \) with noise covariance matrix \( D_\alpha \).

Hence, to obtain scalable predictions at unobserved locations, we use the recommended prediction methods in Katzfuss et al. (2018) that apply Vecchia approximations to the multivariate normal vector \( \tilde{x} = t \cup y \cup y^\star \). For one-dimensional space, we use an extension of IW called LF-auto in Katzfuss et al. (2018), and for higher-dimensional space we use the RF-full method of Katzfuss et al. (2018). In both cases, the pseudo-data \( t = t_\alpha_v \) and the noise variances \( D = D_\alpha_v \) are evaluated at the approximate mode \( \alpha_v \) obtained using Algorithm 1. Based on this approximation, we can compute the implied posterior distribution of \( \tilde{y} = y \cup y^\star \) as described in Section 2.3: \( \tilde{p}(\tilde{y}|t) \sim \mathcal{N}(\tilde{\mu}, (\tilde{V}\tilde{V}')^{-1}) \). Katzfuss et al. (2018) describe how to efficiently extract quantities of interest from this distribution, including the posterior mean and variances at unobserved locations. Finally, summaries or samples from the posterior of \( \tilde{y} \) can be transformed to the data scale using the likelihood function \( g(z|y) \), if desired. Sometimes it is difficult to compute certain predictive summaries at the data scale analytically, but it is always possible to approximate them via sampling.

Algorithm 2 in Section S2 provides pseudo-code for maximum-likelihood estimation of parameters and for prediction.

3.5 Properties

3.5.1 Simplifications for Gaussian likelihoods

In the special case of Gaussian observation distributions, the VL algorithm will converge in a single iteration, as the pseudo-data and -variances do not depend on \( y \) and are equal to the actual data and noise variances, respectively (see Table 1). In addition, the data likelihoods in the integrated likelihood in (9) will cancel. Hence, the VL methods introduced here are a generalization of the general Vecchia likelihood (Katzfuss and Guinness, 2017) and general Vecchia prediction (Katzfuss et al., 2018), with identical results in the case of Gaussian noise.

3.5.2 Complexity

Inference for GPs with independent Gaussian noise using the Vecchia approximations considered here requires \( O(nm^3) \) time (Katzfuss and Guinness, 2017; Katzfuss et al., 2018), where \( m \) is the maximum size of the conditioning sets \( q(i) \). This computation time is dominated by the cost of computing \( U \), which can be done in parallel for the \( n \) columns of \( U \). Our VL Algorithm 1 iteratively computes the Vecchia approximations multiple times until convergence, as mentioned in Sections 3.2.1 and 3.2.2. The only added cost relative to the Gaussian Vecchia approximation at each iteration is the computation of the pseudo-data \( t_y^{(i)} \), which can be achieved in \( O(n) \) time. Hence, assuming that \( k \) iterations are required until convergence, the overall cost of the VL algorithm is \( O(knm^3) \), where \( k \) is often very small (typically smaller than 10).
Once $\alpha_V$ has been determined using Algorithm 1, evaluating the integrated likelihood (10) for parameter inference requires $O(nm^3)$ time (Katzfuss and Guinness, 2017), and prediction at $n^*$ unobserved locations requires $O((n + n^*)m^3)$ time (Katzfuss et al., 2018).

Thus, all computational costs are linear in $n$ for fixed $m$.

### 3.5.3 Approximation errors

Our VL approximation $\hat{p}_{VL}(y|z) = N_n(y|\alpha_V, W_V^{-1})$ in (7) has two sources of error relative to the true posterior $p(y|z)$: the Vecchia approximation and the Laplace approximation.

General Vecchia approximations are exact for any $m \geq n - 1$ (e.g., Katzfuss and Guinness, 2017, Sect. 2.3), in which case our VL approximation reverts to a Laplace approximation. Often, computational feasibility will require considerably smaller $m$, but as our numerical examples in Section 4 will show, our VL approximation can be virtually identical to the Laplace approximation for $m \approx 5$ in one-dimensional space, and $m \approx 40$ in two-dimensional space. In addition, the distribution $\hat{p}_{RF}(y|t)$ obtained at every iteration of Algorithm 1 converges to the exact distribution $p(y|t)$ in terms of Kullback-Leibler divergence as $m$ increases (Katzfuss et al., 2018, Prop. 2.4).

The error due to the Laplace approximation is more difficult to examine. In the case of a Gaussian likelihood, the Laplace approximation is exact and the VL approximation reverts to the general Vecchia approximation (see Section 3.5.1). Rue et al. (2009, Section 4.1) discuss the error of the Laplace approximation for models with latent Gaussian variables. Briefly, they cite the results of Tierney and Kadane (1986) that a Laplace approximation of a posterior distribution has relative error $O(n^{-1})$ under conditions such as unimodality, while normalizing the posterior improves the error rate to $O(n^{-3/2})$. They then point out that the latent Gaussian models routinely fail said conditions, and the error rate cannot be generally determined. Aside from an MCMC simulation of infinite length, there is no direct way to calculate the error between the exact posterior and the Laplace approximation when the likelihoods are not Gaussian. Rue et al. (2009) conclude that the error is related to the effective or “actual” dimension of the latent Gaussian variables. We illustrate numerically in Section 4.1 that our VL approach can be more accurate than a popular MCMC method whose computation time is several orders of magnitude longer.

### 3.5.4 Convergence

For GPs as described in Section 2.1, the log-posterior in (1) is concave under appropriate parameterizations, and so the Newton-Raphson algorithm used in the Laplace approximation is theoretically guaranteed to converge to its mode (e.g., Boyd and Vandenberghe, 2004, Section 9.5.2). In our VL Algorithm 1, we apply a general Vecchia approximation within the Newton-Raphson procedure, which can be considered a quasi-Newton method that significantly improves the computational complexity by approximating the spatial dependency structure.

Unfortunately, it is difficult to prove that Algorithm 1 is guaranteed to converge, except in special cases. As discussed in Section 3.5.3, the VL updates at each iteration of Algorithm 1 are exact for $m \geq n - 1$, and virtually exact for sufficiently large $m$, so in those case convergence is (virtually) guaranteed. The case $m = 0$ is equivalent to assuming that
the \( y_i \) are independent, which also leads to a concave log-posterior and hence guaranteed convergence. However, for small \( m > 0 \) in between these special cases, it is difficult to theoretically guarantee convergence or even to determine what objective function is being optimized, because the approximate distribution \( \hat{p}(y) \) depends on pseudo-variances \( D_y^{(l)} \) that change at each iteration \( l \), except in the Gaussian case.

Fortunately, empirical testing of Algorithm 1 under different parameter and data settings, including small values of \( m \), showed that convergence can always be expected when machine precision is not an issue.

### 3.6 Other VL approaches

Our VL approach can be viewed as a way of combining the Laplace approximation with general Vecchia approximations for inference on large GGP data. Katzfuss and Guinness (2017) discussed that a variety of GP approximations can be viewed as special cases of general Vecchia by choosing appropriate ordering and conditioning schemes, including the modified predictive process (MPP, Banerjee et al., 2008; Finley et al., 2009), the full-scale approximation (FSA, Sang et al., 2011), the multi-resolution approximation (MRA, Katzfuss, 2017; Katzfuss and Gong, 2019), the nearest-neighbor Gaussian process (NNGP, Datta et al., 2016), and standard (response) Vecchia (Vecchia, 1988). Hence, our approach in principle allows for combination of Laplace with any of these GP approximations.

However, these approximations have drawbacks. MPP is a low-rank approach that is most suitable to capturing smooth latent functions. Standard Vecchia is expected to perform poorly for non-Gaussian likelihoods with large pseudo-noise (cf. Katzfuss and Guinness, 2017). NNGP does fully latent conditioning, in which case the Cholesky factor \( V \) generally cannot be computed in linear time. The MRA and its special cases have some useful properties (e.g., Jurek and Katzfuss, 2018), but predictions using the MRA are generally less accurate than those from Vecchia-RF (Katzfuss et al., 2018).

### 3.7 Vecchia-Laplace for log-Gaussian Cox processes

Point patterns are sets of points or locations \( s_1, \ldots, s_N \) in a domain \( D \). A popular model for point patterns is the log-Gaussian Cox process (LGCP), a doubly stochastic Poisson process whose intensity function \( \lambda(\cdot) \) is modeled as random, \( \log \lambda(\cdot) = y(\cdot) \sim GP(\mu, C) \). Inference for LGCPs is difficult due to stochastic integrals.

Figure 2 illustrates a commonly used approximation (e.g., Diggle et al., 2013) that fits the LGCP into the GGP framework. It relies on partitioning the domain \( D \) into \( n \) grid cells \( A_1, \ldots, A_n \) with center points \( a_1, \ldots, a_n \), respectively. Then, consider as the data \( z_i = z(A_i) = \sum_{j=1}^N 1_{s_j \in A_i} \), the number of observed points in \( A_i \). These gridded data conditionally follow a Poisson distribution, \( z_1, \ldots, z_n \mid y(\cdot) \sim ind. \mathcal{P}(\mu(A_i)) \), where

\[
\mu(A_i) = \int_{A_i} \lambda(s) ds \approx |A_i| \lambda(a_i) = |A_i| e^{y(a_i)}.
\]

The smaller the grid cells, the better the approximation, and so \( n \) is often much larger than the number of observed points, and many of the \( z_i \) are zero.
Thus, a point pattern modeled as an LGCP realization can be approximated as data from a GGP with Poisson likelihood observed on a grid. This allows us to apply our VL methods to obtain fast inference for point patterns even for very large grid sizes.

4 Simulations and comparisons

We compared our VL approaches to other methods using simulated data. Throughout Section 4, unless specified otherwise, we simulated realizations $y$ on a grid of size $n$ on the unit square from a GP with mean zero and a Matérn covariance function with variance 1, smoothness $\nu$, and range $\lambda = 0.05$. The data were then generated conditional on $y$ using one of the four likelihoods in Table 1, with $a = 2$ in the Gamma case.

As low-rank approximations are very popular for large spatial data, we also considered a fully independent conditional or modified-predictive-process approximation to Laplace with $m$ knots (abbreviated as LowRank here), which is equivalent to VL-IW except that each conditioning set $Q_y(i) = (1, \ldots, m)$ simply consists of the first $m$ latent variables in maxmin ordering. This equivalence allowed us to run VL and LowRank using the same code base, thus avoiding differences solely due to programming.

Criteria used for comparison are the run time (on a 2017 MacBook Pro), the relative root mean square error (RRMSE) and the difference in log scores (dLS). The RRMSE is the root mean square error of the posterior mean of $y$ obtained by one of the approximation methods relative to the true simulated $y$, divided by the RMSE of the Laplace approximation. The log score is computed as the negative logarithm of the approximated posterior density of $y$ evaluated at the true $y$, with low values corresponding to well calibrated and sharp posterior distributions (e.g., Gneiting and Katzfuss, 2014, Sect. 3). The dLS is the log score of an approximation method minus the log score for the Laplace approximation. When averaged over a sufficient number of simulated data, the dLS can be shown to approximate the difference between the Kullback-Leibler (KL) divergence of the exact posterior distribution and the considered approximation, minus the KL divergence between the exact distribution and the Laplace approximation.
4.1 Comparison to MCMC

Non-Gaussian spatial models are often fitted using Markov-chain Monte Carlo (MCMC), which under mild regularity conditions is “exact approximate,” converging to the true posterior as the number of iterations approaches infinity. For finite computation time and large $n$, however, MCMC results can be very poor relative to the Laplace approximation. To demonstrate this, we simulated a single dataset consisting of $n = 625$ Bernoulli observations with $\nu = .5$, and compared Laplace and VL to Hamiltonian Monte Carlo (HMC; Neal et al., 2011), an MCMC method well suited to sampling correlated variables. As can be seen in Figure 3, VL quickly achieved the same accuracy as Laplace as $m$ increased, but at a fraction of the computing time. In contrast, HMC took orders of magnitude longer to achieve similar accuracy. We expect the relative performance of HMC to degrade further as $n$ increases. More details can be found in Section S3.1.

4.2 Computational scaling of Laplace approximations

While the Laplace approximation is very useful for moderate data sizes $n$, we now briefly illustrate the computational infeasibility for large $n$ due to its cubic scaling. In Figure 4, we show the average computation time for observations with smoothness $\nu = 0.5$. Clearly, Laplace using Newton-Raphson quickly became infeasibly slow as $n$ increased. In contrast, VL and LowRank scaled roughly linearly.

4.3 VL accuracy in one-dimensional space

We now compare the accuracy of the VL and LowRank approximations. Both approaches scale linearly in $n$ for fixed $m$, and both approaches converge to the Laplace approximation as $m$ increases, with equivalence guaranteed for $m = n - 1$.

Figure 5 shows the average results for 100 simulated datasets of size $n = 2,500$ each, on the unit interval. For the Gaussian likelihood, the noise variance was $\tau^2 = 0.1^2$. Clearly, VL-IW was extremely accurate and delivered essentially equivalent results to the Laplace
approximation, even for very small $m$. For exponential covariance (i.e., Matérn with smoothness $\nu = 0.5$), an exact screening effect holds in one-dimensional space, and so VL-IW is exactly equal to Laplace for any $m \geq 1$. LowRank required much larger $m$ to achieve equivalence to Laplace.

### 4.4 VL accuracy in two-dimensional space

Figure 6 shows results for the same simulation study as in Section 4.3, except that the data were simulated on the two-dimensional unit square, with noise variance $\tau^2 = 0.1$ for the Gaussian likelihood.

While all methods are again equivalent to Laplace for $m = n - 1$, the two-dimensional problem is considerably more difficult, and higher values of $m$ were required for accurate approximations. As we can see, the recommended VL-RF had roughly equivalent performance to Laplace once $m$ reached 20 to 40, and it was more accurate than VL-IW for $m > 10$. LowRank performed considerably worse than the VL methods, and further simulations (not shown) showed that in some cases LowRank approached the accuracy of Laplace only when $m$ was almost as large as $n$.

The relative performance of the methods was similar in higher dimensions; plots for 3 and 4 dimensions are shown in Section S4.

For larger $n$, the differences between LowRank and VL become even more pronounced. Figure 7 shows the RMSE for simulations with increasing sample size $n$ but fixed $m$. VL-RF improved in accuracy under this asymptotic in-fill scenario almost as fast as Laplace, while LowRank failed to improve.

### 4.5 Analysis of LGCP point patterns

Consider an LGCP (Section 3.7) whose log-intensity is modeled as a GP with Matérn covariance with range parameter 2.5 on a spatial domain $D = [0, 50]^2$, discretized into $n = 2,500 = 50 \times 50$ unit-square grid cells, as illustrated in Figure 2. This is equivalent to the simulation in Section 4.4, as the domain can be scaled to a unit-square domain with
Figure 5: Simulation results for $n = 2,500$ observations on a **one-dimensional** spatial domain
Figure 6: Simulation results for $n = 2,500$ observations on a two-dimensional spatial domain.
4.6 Parameter estimation

We also compared integrated-likelihood approximations for a single dataset of size $n = 625$ with a Poisson likelihood and true smoothness $\nu = 0.5$. Holding the variance fixed at the true value of one, we sequentially evaluated the integrated likelihood on a grid of values for the range and smoothness parameters, using the Laplace approximation in (9), and the VL-RF approximation with $m = 20$ in (10). The exact integrated likelihood is intractable.

As shown in Figure 8, the integrated likelihoods as approximated by Laplace and by VL were almost identical, while the LowRank approximation was quite poor. Note that these
likelihood approximations are equivalent to approximations to the posterior distribution \( p(\theta | z) \) assuming flat priors for \( \theta \). This indicates that likelihood-based parameter inference (e.g., maximum-likelihood estimation or Metropolis-Hastings) using the VL approximation will be very similar to the inference obtained using the Laplace approximation, except that VL will be considerably faster for large \( n \).

4.7 Interpretation of simulation results

In our simulations, VL provided similar accuracy as Laplace with a considerably smaller number \( m \) of conditioning points compared to LowRank. The time required per iteration for VL approaches is \( O(nm^3) \). At the expense of fully parallel computation, LowRank can be carried out in \( O(nm^2) \) time by computing the decomposition of the covariance of the conditioning set once at the beginning of the procedure. However, as VL with any given \( m \), say \( m = \tilde{m} \), was substantially more accurate than LowRank with \( m = \tilde{m}^{3/2} \), we conclude that VL is more computationally efficient than LowRank for a given approximation accuracy. The improvement in accuracy for VL relative to LowRank became even more pronounced as we increased the sample size under in-fill asymptotics.

5 Application to satellite data

We applied our methodology to a large, spatially correlated, non-Gaussian dataset of column water vapor. These data were collected by NASA’s Moderate Resolution Imaging Spectroradiometer (MODIS), which is mounted on the NASA Aqua satellite (Borbas et al., 2017). We considered a Level-2 near-infrared dataset of total precipitable water at a \( 1354 \times 2030 = 2,746,820 \) grid of 1km pixels. We used up to 500,000 of these data points for our demonstration. Our dataset was observed between 13:45 and 13:50 on March 28, 2019 over a rectangular region off the coast of west Africa with west, north, east, and south bounding coordinates \(-42.707, 67.476, 4.443, \) and \( 45.126 \), respectively and was found on the NASA Earthdata website, [https://earthdata.nasa.gov](https://earthdata.nasa.gov).

Precipitable water amounts are continuous and strictly positive, with values near 0 corresponding to clear skies and larger values implying more water. Exploratory plots showed a right-skewed density, so we assumed that the data can be modeled using a spatial generalized GP with a Gamma likelihood:

\[
   z(s_i) | y(s_i) \sim \mathcal{G}(a, ae^{-y(s_i)}), \quad y(\cdot) \sim \mathcal{N}(\mu, K),
\]

where \( E(z(s) | y(s)) = \exp(y(s)), \mu(s) = \beta_1 + \beta_2 \text{lat}(s) \) is a linear trend consisting of an intercept and a latitudinal gradient, and \( K \) is an isotropic Matérn covariance function with variance \( \sigma^2 \), smoothness \( \nu \), and range parameter \( \rho \). We estimated the parameter values \( \beta_1 = -1.515, \beta_2 = 0.000766, a = 0.89, \sigma^2 = .25, \rho = 31 \text{ km}, \) and \( \nu = 3 \) as described in Section S6.

We again compared our VL approach to a LowRank method. We randomly sampled \( n = 250,000 \) observations \( z \) of the full dataset as training data, and 250,000 of the remaining observations as test data \( z^* \) at locations \( S^* \). For VL, we set \( m = 20 \) following our recommendations in Section 4.4 and further justified in Section S6. For LowRank, we used
Table 2: For the MODIS data, comparison of prediction scores (lower is better) between VL and LowRank

| Method  | MSE   | CRPS  |
|---------|-------|-------|
| VL      | 0.0149| 0.144 |
| LowRank | 0.0528| 0.170 |
| Ratio   | 3.54x | 1.18x |

Table 2: For the MODIS data, comparison of prediction scores (lower is better) between VL and LowRank.

$m = 89 \approx (20)^{3/2}$ for a computationally fair comparison. On an Intel Xeon E5-2690 CPU with 64GB RAM, Algorithm 1 for VL required 10 iterations with a total run time of about 18 minutes (1.8 minutes per iteration). Taking advantage of an implementation that achieves the $O(nm^2)$ scaling, each iteration for LowRank required 1.3 minutes on average across 6 iterations. Note that, based on our numerical experiments, we estimate that Laplace without further approximation would take months of computing time, while HMC-based approaches would take years to achieve the same accuracy as VL.

Figure 9a shows prediction maps of the posterior mean $E(z^*|z) = E(\exp(y^*)|z)$ with $i$th entry $\exp(E(y^*_i|z) + \text{var}(y^*_i|z)/2)$. Clearly, much of the fine-scale structure was lost when using LowRank. To further illustrate this issue, we made predictions on a $200 \times 200$ grid over a small subregion. As shown in Figure 9b, the LowRank predictions were virtually useless at this scale, while VL was able to recover much of the important spatial structure from the noisy and incomplete training data.

Table 2 quantifies the improvement in predictions using VL over LowRank. We computed the MSE based on the posterior mean $E(z^*|z)$. To compare the accuracy of the uncertainty quantification, we also computed the continuous ranked probability score (CRPS; e.g., Gneiting and Katzfuss, 2014), which encourages well calibrated and sharp predictive distributions. Table 2 shows that VL strongly outperformed LowRank for comparable computational complexity.

6 Conclusions and future work

In this work, we presented a novel combination of techniques that allow for efficient analysis of large, spatially correlated, non-Gaussian datasets or point patterns. The key idea is to apply a Vecchia approximation to the Gaussian (and hence tractable) joint distribution of GP realizations and pseudo-data at each iteration of the Laplace algorithm. Our Vecchia-Laplace (VL) techniques guarantee linear complexity in the sample size while capturing spatial dependence at all scales. Compared to alternative methods such as low-rank approximations or sampling-based approaches, our VL approximations can achieve higher accuracy at a fraction of the computation time.

Vecchia approximations require specification of an ordering of the model variables and of a conditioning set for each variable, and these two issues also play a critical role in the performance of our VL approaches. Through simulation studies, we showed that, in one-dimensional space, interweaving the GP realizations and the pseudo-data (Katzfuss and Guinness, 2017) can provide results that are virtually indistinguishable from Laplace, even for very small conditioning sets. For two-dimensional space, we recommend the response-first Vecchia approximation (Katzfuss et al., 2018). Due to the computational efficiency of
Figure 9: Prediction maps for MODIS data using VL and LowRank (LR)
our approach, it is also possible to use a VL approximation of the integrated likelihood for parameter inference, for which we recommend the interweaved ordering in any dimension.

The methods and algorithms proposed here are implemented in the freely available R package GPvecchia available at https://github.com/katzfuss-group/GPvecchia. The default settings of the package functions reflect the recommendations in the previous paragraph. Our methods and the code are applicable in more than two dimensions, but a thorough investigation of their properties in this context will be carried out in future work.

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**A Newton-Raphson update using pseudo-data**

The desired Newton-Raphson update has the form

\[
\mathbf{h}(\mathbf{y}) = \mathbf{y} - \left( \frac{\partial^2}{\partial \mathbf{y}^2} \log p(\mathbf{y}|\mathbf{z}) \right)^{-1} \left( \frac{\partial}{\partial \mathbf{y}} \log p(\mathbf{y}|\mathbf{z}) \right).
\]

(11)

As shown in Section 2.2, we have \( \frac{\partial}{\partial \mathbf{y}} \log p(\mathbf{y}|\mathbf{z}) = \mathbf{K}^{-1}(\mathbf{\mu} - \mathbf{y}) + \mathbf{u} \) and \( -\frac{\partial^2}{\partial \mathbf{y}^2} \log p(\mathbf{y}|\mathbf{z}) = \mathbf{K}^{-1} + \mathbf{D}^{-1} = \mathbf{W} \).

Using an idea similar to iterative weighted least squares (Section 2.5, McCullagh and Nelder, 1989), we can premultiply the variable \( \mathbf{y} \) by the Hessian to combine terms, and then rearrange and pull out the prior mean. Dropping the iteration subscript of \( \mathbf{y} \) for ease of notation, we can write (11) as

\[
\mathbf{h}(\mathbf{y}) = \mathbf{y} + \mathbf{W}^{-1}(\mathbf{K}^{-1}(\mathbf{\mu} - \mathbf{y}) + \mathbf{u})
\]

\[
= \mathbf{W}^{-1}(\mathbf{K}^{-1} + \mathbf{D}^{-1})\mathbf{y} - \mathbf{K}^{-1}\mathbf{y} + (\mathbf{K}^{-1}\mathbf{\mu} + \mathbf{D}^{-1}\mathbf{\mu}) - \mathbf{D}^{-1}\mathbf{\mu} + \mathbf{D}^{-1}\mathbf{Wu}
\]

\[
= \mathbf{\mu} + \mathbf{W}^{-1}(\mathbf{D}^{-1}(\mathbf{y} + \mathbf{Wu} - \mathbf{\mu}))
\]

\[
= \mathbf{\mu} + \mathbf{W}^{-1}\mathbf{D}^{-1}(\mathbf{t} - \mathbf{\mu}),
\]

where \( \mathbf{t} = \mathbf{y} + \mathbf{Wu} \).

Now consider the posterior mean in the case of a Gaussian likelihood \( \mathbf{t}|\mathbf{y} \sim \mathcal{N}_n(\mathbf{y}, \mathbf{D}) \) with a conjugate Gaussian prior, \( \mathbf{y} \sim \mathcal{N}_n(\mathbf{\mu}, \mathbf{K}) \). Employing a well-known formula, we have

\[
E(\mathbf{y}|\mathbf{t}) = (\mathbf{K}^{-1} + \mathbf{D}^{-1})^{-1}(\mathbf{K}^{-1}\mathbf{\mu} + \mathbf{D}^{-1}\mathbf{t}) = \mathbf{\mu} + \mathbf{W}^{-1}\mathbf{D}^{-1}(\mathbf{t} - \mathbf{\mu}).
\]

Thus, we have \( \mathbf{h}(\mathbf{y}) = E(\mathbf{y}|\mathbf{t}) \), the posterior mean under the assumption of Gaussian pseudo-data \( \mathbf{t} \).

**B Computing U**

Consider a general Vecchia approximation of the form (6). To obtain \( \mathbf{U} \), define \( C(x_i, x_j) \) as the covariance between \( x_i \) and \( x_j \) implied by the true model; that is, \( C(y_i, y_j) = C(t_i, t_j) = K(s_i, s_j) \) and \( C(t_i, t_j) = K(s_i, s_j) + \mathbb{I}_{i=j}d_i \). Then, the \( (j, i) \)th element of \( \mathbf{U} \) can be calculated as

\[
U_{ji} = \begin{cases} r_i^{-1/2}, & i = j, \\ -b_i^{(j)}r_i^{-1/2}, & j \in c(i), \\ 0, & \text{otherwise}, \end{cases}
\]

where \( b_i = C(x_i, x_{c(i)})C(x_{c(i)}, x_{c(i)})^{-1}r_i = C(x_i, x_i) - b_iC(x_{c(i)}, x_i) \), and \( b_i^{(j)} \) denotes the \( k \)th element of \( b_i \) if \( j \) is the \( k \)th element in \( c(i) \) (i.e., \( b_i^{(j)} \) is the element of \( b_i \) corresponding to \( x_j \)).
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