INLA-MRA: A Bayesian method for large spatiotemporal datasets

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Abstract

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Large spatiotemporal datasets are a challenge for conventional Bayesian models, because of the cubic computational complexity of the algorithms for obtaining the Cholesky decomposition of the covariance matrix in the multivariate normal density. Moreover, standard numerical algorithms for posterior estimation, such as Markov Chain Monte Carlo (MCMC), are intractable in this context, as they require thousands, if not millions, of costly likelihood evaluations. To overcome those limitations, we propose INLA-MRA, a method that mixes an estimation algorithm inspired by INLA (Integrated Nested Laplace Approximation), and a model taking advantage of the sparse covariance structure produced by the Multi-Resolution Approximation (MRA) approach. INLA-MRA extends MRA to spatiotemporal data, while also facilitating the approximation of the hyperparameter marginal posterior distributions. We apply INLA-MRA to large MODIS Level 3 Land Surface Temperature (LST) datasets, sampled between May 18 and May 31, 2012 in the western part of the state of Maharashtra, India. We find that INLA-MRA can produce realistic prediction surfaces over regions where concentrated missingness, caused by sizable cloud cover, is observed. Through a validation analysis, we also find that predictions tend to be very accurate.

*Keywords:* Spatiotemporal regression, sparse matrices, scalable methods, MODIS, LST
1 Introduction

Automated data collection has resulted in spatiotemporal data being produced at a very quick pace. Gaussian Random Fields (GRF) are a core component of conventional models applied to such data, but tend to be cumbersome when the datasets are large. Indeed, likelihood evaluations involve the inverse of a covariance matrix whose size increases with the number of observations. The computational complexity of the algorithm for obtaining the Cholesky decomposition, involved in matrix inversion and computation of the determinant, is cubic in the number of rows or columns. It follows that it cannot handle large dense matrices. Algorithms that rely on a sizable number of likelihood evaluations, such as Markov Chain Monte Carlo (MCMC), also turn out to be impractical, as a single likelihood calculation can take up to several minutes.

This study proposes a new Bayesian method, called INLA-MRA, that helps overcome the computational limitations of conventional approaches for modeling spatiotemporal data. Computationally tractable algorithms for obtaining the Cholesky decomposition of large sparse matrices have been proposed (Guennebaud et al., 2010; Davis, 2006). INLA-MRA uses those algorithms to handle the sparse covariance structure of the Multi-Resolution Approximation (Katzfuss, 2017; Katzfuss and Gong, 2017) (MRA), which it extends to the spatiotemporal case. It also improves on the model’s original formulation by permitting the direct estimation of the marginal hyperparameter posterior distributions. It does so with the help of a novel importance sampling algorithm, and in this way, avoids reliance on costly numerical simulations.
1.1 Scalable spatial regression models

Scalable models in spatial statistics tend to rely on a combination of three strategies (Heaton et al., 2019). First, the low-rank approximation strategy involves a dimension-reduction scheme for the covariance matrix, achieved through decomposition of the GRF into a finite sum of orthogonal terms whose deterministic coefficients are obtained by computing the values of basis functions. The predictive process (Banerjee et al., 2008), LatticeKrig (Nychka et al., 2015), and fixed-rank Kriging (Cressie and Johannesson, 2008), for example, use that approach. A second strategy involves imposing sparsity on the covariance or precision matrix, i.e. the inverse of the covariance matrix. This can be done by assuming conditional independence between some of the observations, such as in the spatial partitioning (Heaton et al., 2017) and Stochastic Partial Differential Equation (SPDE) approaches (Lindgren et al., 2011), or through tapering, that is, multiplying the covariance function by a correlation function with compact support (Furrer et al., 2006). Finally, recent methodological development has focused on parallelisation. Meta-kriging (Guhaniyogi and Banerjee, 2018) and the parallel low-rank models by Katzfuss and Hammerling (2017) have used that approach.

The Multi-Resolution Approximation (MRA) (Katzfuss, 2017; Katzfuss and Gong, 2017) mixes all three strategies. Unlike other low-rank approaches, MRA does not produce overly smooth predictions. By imposing sparsity on the precision matrices, matrices of a much higher rank can be used without straining computational resources. MRA is formulated in such a way that core computations in the likelihood and posterior evaluations can be performed in parallel, with little communication required between processes. Its performance in terms of predictive accuracy has also been shown to be excellent (Heaton et al., 2019).
1.2 MODIS land surface temperature data

Figure 1: Land surface temperatures (in degrees Celsius) recorded on May 29, 2012 over a 389 km × 445 km region in the western part of Maharashtra, India. Also shown are district boundaries and markers for major cities.

We will illustrate the use of INLA-MRA on MODIS (Moderate Resolution Imaging Spectroradiometer) Level-3 land surface temperature (LST) data [Wan et al., 2015b,a]. LST, also called land surface emissivity, is an indicator of ground temperature or brightness. LST does not correspond to air temperature, measured by weather stations, but is highly
correlated with it \cite{Mildrexler2011}. The MODIS imaging sensor has been loaded onto two satellites, Terra and Aqua, launched in 1999 and 2002, respectively. The raw spectroradiometry data collected by the spacecrafts is transformed into several gridded products, such as water vapor and aerosol levels, snow cover, and LST. The grid used for daily LST observations has a resolution of $1 \text{ km} \times 1 \text{ km}$. Missing values are however very common, as thick cloud formations may prevent the satellites from viewing the surface.

This paper considers MODIS LST data collected near the cities of Pune and Nashik, India, which are on a plateau overlooking the Konkan coast, where Mumbai is located. LST data from May 29 2012, a sunny day with relatively few missing values, is shown in Fig. 1. We do not have temperature data for larger water surfaces, such as the Arabian sea to the west. The correspondence between geopolitical borders and temperature patterns is mostly due to the presence of hills or rivers, which serve as convenient boundaries for splitting a territory. A large patch of missing data appears in the southeastern corner. Inferring missing values is a problem that can be well addressed by Bayesian methods for spatiotemporal inference such as INLA-MRA.

\section{Methods}

\subsection{Model}

Let the $i$’th observation, recorded at spatiotemporal coordinates $(s_i, t_i)$, be denoted $Y_i$, the set of all sampled responses be denoted $y$, and the corresponding matrix of covariates be denoted $X$. We assume that

$$Y_i \sim N[X(s_i, t_i)\beta + W(s_i, t_i), \sigma^2], \quad (1)$$
with $W(s_i, t_i)$ being a GRF with mean 0 and covariance function

$$\text{Cov}[W(s + u, t + v), W(s, t)] = \sigma_M^2 \text{Matérn}(|u|; \rho, \nu) \exp(-|v|/\phi), \quad (2)$$

$\phi$ being known as the temporal range parameter. The expression $\text{Matérn}(|u|; \rho, \nu)$ denotes the Matérn covariance function,

$$\text{Matérn}(|u|; \rho, \nu) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu |u|}}{\rho} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu |u|}}{\rho} \right), \quad \rho > 0, \nu > 0, \quad (3)$$

with $K_\nu(.)$ being the modified Bessel function of the second kind, $|u|$ being the norm of $u$, and $\rho$ and $\nu$ being known as the spatial range and differentiability parameters, respectively. We use the Haversine distance (or great circle distance, see Sinnott [1984]) formula to obtain $|u|$. We fix $\nu$ at 1.5, following the advice of Stein [2012]. The methodology developed here requires Gaussian priors for $\beta$, and we use independent Gaussian distributions with variance 100. Variance parameters, expressed on the logarithmic scale, are denoted $\Psi \equiv \{\log(\sigma_M), \log(\rho), \log(\phi), \log(\sigma_i)\}$ and also have independent Gaussian priors. Finally, writing $W^\top \equiv \{W(s_1, t_1), \ldots, W(s_n, t_n)\}$, the covariance matrix has entries $\Sigma_{ij} = \text{Cov}[W(s_i, t_i), W(s_j, t_j)]$.

### 2.2 The spatiotemporal Multi-Resolution Approximation

Under MRA [Katzfuss, 2017], the spatiotemporal domain is partitioned into $K$ levels of increasingly fine resolution. Write $R_0$ to refer to the entire domain, and $R_{1\ell}, \ell = 1 \ldots L_1$, to the level 1 regions, which together form a partition of $R_0$. Each deeper level $k$ has regions $R_{km}, m = 1, \ldots, L_k$, nested within $R_{k-1,\ell}$. We define sets of increasingly dense
knot positions $\mathcal{Q}_k$, $k = 1, \ldots, K$, as well as interpolants $\tau_k(s, t)$ and residuals $\delta_k(s, t)$, with

$$
\tau_0(s, t) = E[W(s, t) \mid W(u, v) : u, v \in \mathcal{Q}_0],
$$

$$
\delta_1(s, t) = W(s, t) - \tau_0(s, t),
$$

$$
\tau_k(s, t) = E[\delta_k(s, t) \mid \delta_k(u, v) : u, v \in \mathcal{Q}_k \cap R_{k\ell}], \quad (s, t) \in R_{k\ell},
$$

$$
\delta_{k+1}(s, t) = \delta_k(s, t) - \tau_k(s, t).
$$

We define approximation

$$
\tilde{W}(s, t) = \delta_K(s, t) + \sum_{k=0}^{K-1} \tau_k(s, t),
$$

which we re-write

$$
\tilde{W}(s, t) = \sum_k b_{k\ell_k}^\top(s, t) \eta_{k\ell_k}, \quad (s, t) \in R_{k\ell_k},
$$

where $\ell_k$ is such that $(s, t) \in R_{k\ell_k}$, and with basis functions and coefficients

$$
b_{k\ell}(s, t) = \text{Cov}\{\delta_k(s, t), \Delta_{k\ell}\}, \quad (s, t) \in R_{k\ell},
$$

$$
\Delta_{k\ell} = \{\delta_k(u, v) : (u, v) \in \mathcal{Q}_k \cap R_{k\ell}\},
$$

$$
\eta_{k\ell} \sim N(0, \Gamma_{k\ell}),
$$

$$
\Gamma_{k\ell} = \text{Var}(\Delta_{k\ell})^{-1}.
$$

In INLA-MRA, we express the multivariate extension of Eq. 4

$$
\tilde{W} = F(\Psi_{ST}; \mathcal{Q}) \eta,
$$

with

- $\mathcal{Q}$ being the set of all knot positions,
• $\eta$ being the set of all $\eta_{k\ell}$ vectors,

• $\Psi_{ST} \equiv \{\log(\rho), \log(\phi), \log(\sigma_M)\}$.

It follows from the definition of $\Gamma_{k\ell}$ that $\eta$ has a block diagonal covariance structure, which we denote $\Gamma$, and we find that

$$\Sigma_{\tilde{W}} = F(\Psi_{ST}; \mathcal{Q}) \Gamma F(\Psi_{ST}; \mathcal{Q})^\top. \quad (6)$$

We stress that row $i$ of $F(\Psi_{ST}; \mathcal{Q})$ is

$$F_{[i, \cdot]}(\Psi_{ST}; \mathcal{Q}) = [b_{01}^\top(s_i, t_i), b_{11}^\top(s_i, t_i), \ldots, b_{1L_1}^\top(s_i, t_i), \ldots, b_{K_1}^\top(s_i, t_i), \ldots, b_{KL_K}^\top(s_i, t_i)],$$

and it follows that $F(\Psi_{ST}; \mathcal{Q})$ is sparse, as $b_{k\ell}^\top(s_i, t_i)$ is non-zero only when $\ell = \ell_k$ such that $(s_i, t_i) \in \mathcal{R}_{k\ell_k}$. Moreover, $F(\Psi_{ST}; \mathcal{Q})$ has number of rows and columns equal to the number of observations and number of knots across all regions, respectively. We can now see why $\tilde{W}$ is computationally tractable: its covariance matrix is sparse because of the compact support of each basis function.

### 2.3 Importance sampling for approximating hyperparameter posteriors

Based on MRA, we obtain approximation

$$\hat{Y} \sim N[X\beta + F(\Psi_{ST}; \mathcal{Q})\eta, \sigma^2]. \quad (7)$$

Let $v^\top = \{\beta^\top, \eta^\top\}$ denote the mean parameters. We then rewrite Eq. 7

$$\hat{Y} \sim N[H(\Psi_{ST}; \mathcal{Q})v, \sigma^2].$$
where

\[ H(\Psi_{ST}; Q) = \begin{bmatrix} X & F(\Psi_{ST}; Q) \end{bmatrix}. \]

The number of covariates is usually small compared to the total number of knots. As a result, although \( X \) is dense, \( H(\Psi_{ST}; Q) \) remains sparse.

The next steps are based on parts of the Integrated Nested Laplace Approximation (INLA) algorithm (Rue et al., 2009; Martins et al., 2013). Using Bayes law, we can show that

\[
p[\Psi | y] \propto \frac{p(\Psi)p(v | \Psi)p(y | v, \Psi)}{p[v | \Psi, y]}.
\]

(8)

Distribution \( p[\Psi | y] \) is used to obtain marginals \( p(\Psi_i | y), i = 1, \ldots, n_\Psi \), and \( p[v_i | y], i = 1, \ldots, n_v \).

We assume independence between the prior distributions of \( \beta \) and \( \eta \), and as a result, \( p(v | \Psi) \) is equal to their product. As noted in section 2.2, the prior for \( \eta \) is a multivariate normal distribution with mean \( 0 \) and covariance matrix \( \Gamma \). The likelihood \( p[y | v, \Psi] \) is multivariate normal, with mean and covariance \( H(\Psi_{ST}; Q)v \) and \( \sigma^2 I \), respectively.

The distribution \( p[v | \Psi, y] \) is known as the full conditional. It can be shown that when the likelihood is normal, the full conditional is also normal, with precision matrix (Eidsvik et al., 2012)

\[
Q = \begin{bmatrix} \Sigma_\beta & \Sigma_\eta \\ \end{bmatrix}^{-1} + \frac{1}{\sigma^2} H(\Psi_{ST}; Q)^T H(\Psi_{ST}; Q).
\]

(9)

The full conditional mean is equal to \( Q^{-1} \xi \), with \( \xi = (1/\sigma^2) H(\Psi_{ST}; Q)^T y \) (Eidsvik et al., 2012). The precision matrix is therefore sparse. This results in a reasonable computational burden that can be controlled by adjusting the total number of knots and \( K \), the depth of the decomposition of the spatiotemporal domain.
We cannot use Eq. 8 directly to derive posteriors, as it is not standardised. We can however circumvent the issue with an importance sampling (IS) scheme. It involves obtaining $N_{IS}$ draws from a Gaussian proposal distribution denoted $p'(\cdot)$, with mean equal to the mode of $p[\Psi | y]$, and covariance matrix equal to the inverse of the Hessian matrix computed numerically at the mode (Rue et al. 2009). Optimisation relies on the L-BFGS algorithm (Liu and Nocedal 1989), with the gradient being estimated numerically by using a finite difference approximation.

Let,

$$p[\Psi | y] = \frac{\tilde{p}[\Psi | y]}{c_I},$$

where $c_I$ is the unknown standardisation constant and $\tilde{p}[\Psi | y]$ is the non-standardised distribution given in Eq. 8. We note that

$$\int_\Psi p[\Psi | y] d\Psi = 1$$

$$= \int_\Psi \frac{p[\Psi | y]}{p'(\Psi)} p'(\Psi) d\Psi$$

$$= \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} \frac{p[\Psi'_i | y]}{p'(\Psi'_i)}$$

$$= \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} \frac{\tilde{p}[\Psi'_i | y]}{c_I p'(\Psi'_i)}$$

where $\Psi'_i$ are values sampled from proposal distribution $p'(\Psi)$. It follows that,

$$c_I \approx \sum_{i=1}^{N_{IS}} \frac{\tilde{p}[\Psi'_i | y]}{N_{IS} p'(\Psi'_i)}.$$

The IS weight for the $i$’th draw from the proposal is therefore,

$$\omega_i = \frac{\tilde{p}[\Psi'_i | y]}{c_I p'(\Psi'_i)}.$$
We obtain an empirical estimate of $p[\Psi_j \mid y]$, $j = 1, \ldots, n$, by integrating $p[\Psi \mid y]$ based on the values sampled from the proposal distribution, that is,
\[
p[\Psi_j \mid y] \approx \delta(\Psi_j = \Psi'_{i,j})c_I\tilde{p}[\Psi = \Psi'_i \mid y], \quad i = 1, \ldots, N_{IS},
\]
where $\delta(.)$ is the delta function. We also have that,
\[
p[v_j \mid y] \approx \sum_{i=1}^{N_{IS}} p[v_j \mid \Psi'_i, y]\omega_i.
\]
Note that since the full conditional is multivariate normal, $p[v_j \mid \Psi, y]$ can be readily obtained.

### 2.4 Spatiotemporal prediction

Let $y^P_k$ denote the predicted responses at coordinate $(s^P_k, t^P_k)$. We aim to obtain moments of the posterior predictive distribution $p[y^P \mid y]$. The posterior predictive distributions themselves are computationally intractable, as they involve the dense covariance matrix of $W$.

We define $F_P(\Psi_{ST}; Q)$ similarly to $F(\Psi_{ST}; Q)$, but with the spatiotemporal coordinates $(s^P_k, t^P_k)$ in place of $(s_i, t_i)$, and
\[
H_P(\Psi_{ST}; Q) = \begin{bmatrix} X^P & F_P(\Psi_{ST}; Q) \end{bmatrix},
\]
where $X^P$ has row $k$ with covariates at $(s^P_k, t^P_k)$. We note that
\[
E[Y^P \mid y] = E\{E[Y^P \mid y, \Psi]\}
\approx \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} E[Y^P \mid y, \Psi = \Psi'_i]\omega_i,
\]
where we re-use the hyperparameter values $\Psi_i'$ and IS weights obtained previously. It follows that

$$
E[Y^P | y] \approx \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} E[H_P(\Psi_i'; Q) v | y, \Psi = \Psi_i'] \omega_i
$$

$$
= \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} H_P(\Psi_i'; Q) Q_i^{-1} \xi_i \omega_i,
$$

where $Q_i$, and $\xi_i$ are the $Q$ matrix and $\xi$ vector obtained conditional on $\Psi = \Psi_i'$. To obtain marginal variances $\text{Var}[Y^P_j | y]$, $j = 1, \ldots, n_P$, we first note that

$$
\text{Var}[Y^P_j | y] = \text{Var}\{E[Y^P_j | \Psi, y]\} + E\{\text{Var}[Y^P_j | \Psi, y]\}.
$$

We then have that

$$
\text{Var}\{E[y^P_j(s^P_j, t^P_j) | \Psi, y]\} = E\{E[y^P_j(s^P_j, t^P_j) | y, \Psi] \}^2 - E[y^P_j | y]^2
$$

$$
= E\{[H_P(\Psi_{ST}; Q)_{[j,i]} Q^{-1} \xi_i]^2\} - E[y^P_j | y]^2
$$

$$
\approx \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} [H_P(\Psi_i'; Q)_{[j,i]} Q_i^{-1} \xi_i]^2 \omega_i - E[y^P_j | y]^2,
$$

where $H_P(.)_{[j,i]}$ is the $j$'th row of matrix $H_P(.)$, and,

$$
E\{\text{Var}[Y^P_j | \Psi, y]\} = E\{\text{Var}[H_P(\Psi_{ST}; Q)_{[j,i]} v + \epsilon^P_j | \Psi, y]\}
$$

$$
= E\{[H_P(\Psi_{ST}; Q)_{[j,i]} \text{Var}[v | \Psi, y][H_P(\Psi_{ST}; Q)_{[j,i]}]^T + \sigma_v^2]\}
$$

$$
= E\{H_P(\Psi_{ST}; Q)_{[j,i]} Q^{-1} [H_P(\Psi_{ST}; Q)_{[j,i]}]^T + \sigma_v^2\}
$$

$$
\approx \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} \{H_P(\Psi_i'; Q)_{[j,i]} Q_i^{-1} [H_P(\Psi_i'; Q)_{[j,i]}]^T + [(\sigma_i')]^2\} \omega_i.
$$

We provide additional details in Appendix A.
2.5 Software

The R package used to fit INLA-MRA is available at [https://github.com/villandre/MRAinla/](https://github.com/villandre/MRAinla/). The software is written in R and C++, with the interface between the two relying on the Rcpp (Eddelbuettel and François, 2011; Eddelbuettel 2013; Eddelbuettel and Balamuta, 2017) and RcppEigen (Bates and Eddelbuettel, 2013) libraries. RcppEigen relies on the Eigen library (Guennebaud et al., 2010).

The main computational challenge results from expressions like $Q^{-1}x$, which appear, for example, in the full conditional mean, and the posterior predictive means and variances. Since the $Q$ matrix is sparse, its Cholesky ($LDL^T$) decomposition can be obtained. Moreover, the constant sparsity structure of $Q$ allows for additional computational benefits. Indeed, the positions of non-zero values in $Q$ depend strictly on the structure of $H(\Psi_{ST}; Q)$, which is itself determined strictly by the observation locations. Obtaining the permutation order can take a considerable amount of time, but it is only computed once. The creation of large sparse matrices is also time-consuming. After initialisation, $H(\Psi_{ST}; Q)$ is updated by iterating through its non-zero elements only. The computation of the posterior predictive variances is also fairly demanding, as it involves solving as many linear systems as observations in the sample. Thanks to openMP parallelisation, we are able to complete that step reasonably quick. For this reason, we strongly recommend running the software on a machine with openMP support enabled. We provide additional information on the software in Appendix A.
3 Illustrative example

The main analysis focuses on a dataset consisting of 1,116,319 daytime LST observations, derived from MODIS spectroradiometry data collected between May 25 and May 31, 2012 in the western part of the state of Maharashtra, India. On each day, we have two LST datasets, one from Terra and one from Aqua, which fly over the region around 11AM and 1PM, respectively. Of the two, we keep the one with the fewest missing values. The main objective is to impute the 81,574 LSTs missing over non-oceanic tiles on May 28. We consider four covariates: land cover, elevation, satellite, i.e. Terra or Aqua, and day of observation. We obtained land cover values from the Terra and Aqua combined MODIS Land Cover Type (MCD12Q1) Version 6 data product [Friedl and Sulla-Menashe (2019)], and we used elevation estimates from the ASTER Global Digital Elevation Model Version 3 [NASA/METI/AIST/Japan Spacesystems and U.S./Japan ASTER Science Team (2019)]. We include the satellite covariate to reflect a potential discrepancy in temperatures recorded by Terra and Aqua, due to the different fly over times. Finally, we create a day-of-observation covariate using dummy variables. It is analogous to a “cluster-specific intercept”, that is, it provides a region-wide adjustment to the mean temperature observed on any given day.

We ran all computations on a machine equipped with an Intel(R) Xeon(R) W-2145 CPU @ 3.70GHz CPU and 188GB of memory. Datasets, output files, and scripts used to produce the results can be found at https://github.com/villandre/dataFilesForAnalyses.
| Parameter name | Mean  | StdDev | CI-2.5% | CI-97.5% |
|----------------|-------|--------|---------|----------|
| Elevation, satellite |       |        |         |          |
| Elevation       | -0.001| < 0.001| -0.001  | -0.001   |
| Satellite: Aqua | 0.793 | 4.472  | -7.965  | 9.490    |
| Land cover      |       |        |         |          |
| Evergreen Needleleaf Forests | 1.000 | 0.168  | 0.880   | 1.301    |
| Evergreen Broadleaf Forests  | 0.979 | 0.025  | 0.931   | 1.026    |
| Deciduous Broadleaf Forests  | 1.181 | 0.022  | 1.130   | 1.230    |
| Mixed Forests   | 1.087 | 0.022  | 1.044   | 1.130    |
| Closed Shrublands | 2.097 | 0.129  | 1.846   | 2.347    |
| Open Shrublands | 1.448 | 0.060  | 1.332   | 1.565    |
| Woody Savannas  | 1.329 | 0.028  | 1.276   | 1.383    |
| Savannas        | 1.303 | 0.018  | 1.255   | 1.427    |
| Graslands       | 1.506 | 0.018  | 1.474   | 1.540    |
| Permanent Wetlands | 0.705 | 0.020  | 0.666   | 0.744    |
| Croplands       | 1.588 | 0.018  | 1.554   | 1.623    |
| Urban and Built-up Lands | 1.623 | 0.019  | 1.578   | 1.659    |
| Cropland/Natural Vegetation Mosaics | 1.430 | 0.021  | 1.389   | 1.470    |
| Non-Vegetated Lands | 0.667 | 0.028  | 0.612   | 0.721    |
| Time            |       |        |         |          |
| May 26          | -2.980| 4.472  | -11.677 | 5.717    |
| May 27          | -0.031| 4.472  | -8.731  | 8.664    |
| May 28          | -6.319| 0.071  | -6.458  | -6.180   |
| May 29          | 1.155 | 4.472  | -7.542  | 9.853    |
| May 30          | -3.438| 0.078  | -3.590  | -3.286   |
| May 31          | 2.650 | 4.472  | -6.047  | 11.348   |
| Hyperparameters  |       |        |         |          |
| $\rho$          | 5.660 | 0.014  | 5.632   | 5.688    |
| $\phi$          | 3.601 | 0.018  | 3.567   | 3.635    |
| $\sigma_M$      | 4.140 | 0.013  | 4.114   | 4.166    |

Table 1: **Mean and standard deviation of posteriors with credible intervals.** Water (land cover = 0 in UMD classification) is the reference category for land cover. “Time = May 25” is the reference category for the time parameters, and “Terra” is the reference for the “Satellite: Aqua” parameter. We used the Delta method to get untransformed mean and standard deviations for hyperparameters.
3.1 Results

Mean, standard deviations, and credible intervals for the fixed effects and log-hyperparameter posteriors are given in Table 1. The spatial range hyperparameter translates to correlations of 0.962 at one kilometer, and 0.19 at ten kilometers. For time, we have instead a correlation of 0.758 after one day, and 0.143 after a week. We found that the effect of land cover was usually modest, but supported by narrow credible intervals. We observed the most compelling effects for closed shrublands (Mean = 2.097, SD = 0.129) and urban and built up environments (Mean = 1.623, SD = 0.019). We found the day of observation covariate however to be fairly influential. For example, the decrease in the posterior means due to time on May 28 was 6.319 degrees Celsius (SD = 0.071), with May 25 serving as the reference. When the model could not reliably identify a mean difference, it produced a fairly high standard deviation for the associated posterior, around 4.472.

Fig. 2 shows the observed data for May 28, as well as the prediction surface from INLA-MRA. The predictions form a realistic pattern overall, with lower predicted temperatures near the coast even though there are few observed data. The surface is not uniformly smooth: several small vertical breaks are present in the lower-middle section of the prediction and standard deviation maps. Those breaks result from the partitioning of the domain (Katzfuss and Gong, 2017). Further, we observe lower standard deviations in posterior predictive distributions for locations closer to where data were available on May 28. This is due to the higher spatial correlation inherent to LST data. The largest standard deviations, taking values slightly under 7 degrees Celsius, are found along the breaks mentioned previously. This effect can however be offset by the proximity of observed data, if they are located in the same subregion at the finest resolution. Closer to the middle of these subregions, standard deviations are usually between 3 and 4 degrees Celsius.
Figure 2: Observed LST data, predictions, and standard distributions of predictions.
The method did output a small number of more extreme values. Out of the 81,574 predicted values, 77 are below the range of the sampled LSTs by at least one degree, while none are above it. The lowest prediction is 4.41 degrees Celsius, and is for a coastal tile whose center is located at (18.888, 72.905), just south of Mumbai. The second most extreme prediction, at 14.76 degrees Celsius, is for another coastal tile, located immediately north of the first one (18.896, 72.908).

3.2 Validation

We validate model predictions with a second dataset, whose observations were collected between May 18, 2012 and May 24, 2012 across a subset of the region considered in the main analysis. We split that dataset into training and test sets, comprising 108,079 and 13,234 observations, respectively. We create the test set by holding out observations falling under a simulated cloud cover on May 21. To obtain a realistic missingness pattern, we reproduce the cloud cover recorded on May 28. Assuming the same model as before, we then use INLA-MRA to estimate the posterior predictive means, and we finally compute prediction errors. We provide more information regarding tuning parameters, priors, hyperpriors, and the recursive domain splitting scheme in Appendix B.

Fig. 3a displays the LST measurements recorded on May 21, and Fig. 3b the values we subtracted to reproduce the cloud cover observed on May 28. Fig. 3c shows the errors obtained by subtracting the observed values from the corresponding posterior predictive means. As expected, there is visible spatial structure in the errors we obtained, which stretch from −9.96 to 5.38 degrees Celsius. The largest absolute difference is for a water tile on the Morbe lake (73.250, 18.913). The mean squared prediction error (MSPE) and median squared prediction error (MedSPE) are 2.94 and 1.13, respectively, which indicates
Figure 3: Validation results comparing INLA-MRA and INLA-SPDE from Lindgren et al. The training data on May 21 is obtained by masking the observed data with the cloud pattern on May 28. Prediction errors for INLA-MRA and INLA-SPDE are equal to observed values minus posterior means.
that the available data were reasonably informative. Further, 90% of absolute errors are under 2.83. We suspect the more extreme values result from the selected model’s difficulties in predicting accurately on or next to water bodies.

We briefly compared INLA-MRA to the INLA-SPDE approach [Lindgren et al., 2011], which also makes use of a convenient basis representation for the Gaussian field to propose a sparse covariance structure. We used functions in the INLA package [www.rinla.org] to fit the SPDE. As expected, INLA-SPDE did also well, with MSPE and MedSPE equal to 4.94 and 2.02, respectively. We map prediction errors in Fig. 3d on the same scale as in Fig. 3c to facilitate comparison. The figure highlights that INLA-SPDE had a tendency to overestimate observed LSTs, while INLA-MRA had a tendency to underestimate instead. Both approaches had comparable computational requirements in time and memory, with computational times depending strongly on the number of basis functions used.

4 Discussion

The algorithm we devised, INLA-MRA, allows computationally tractable Bayesian inference for large spatiotemporal datasets. It innovates by extending the MRA to spatiotemporal data, and by considerably simplifying hyperparameter posterior inference. Further, the estimation method, involving elements of INLA combined with an importance sampling scheme, is easily parallelisable. The analyses further revealed that INLA-MRA can produce realistic and accurate land surface temperature predictions.

Currently, the memory footprint of the algorithms used for obtaining the Cholesky decomposition of sparse matrices remains the greatest computational hurdle. A strategy that leverages the sparsity structure of the different precision matrices could help resolve that is-
sue, and help scale INLA-MRA to datasets comprising tens of millions of observations. An extension to non-Gaussian likelihoods, point processes or categorical outcomes for example, would also be a welcome improvement. Further, we would need to refine the strategies for knot placement and partitioning the study region. Altering the MRA smoothing scheme for eliminating breaks in prediction surfaces would also be desirable.

Massive datasets remain a considerable challenge for Bayesian inference methods. Nevertheless, their capacity to intuitively quantify uncertainty in parameter estimates or predictions and to account for measurement error in observations can be very valuable in practice. INLA-MRA represents a worthy step towards scaling Bayesian inference to much larger spatiotemporal datasets. The proposed improvements will help make the algorithm more flexible, and ultimately, applicable to data of a scale comparable to that of the MODIS land surface temperature database.

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SUPPLEMENTARY MATERIAL
Appendix A: Additional notes on the implementation of INLA-MRA

The importance sampling strategy we described involves running a short optimisation procedure to estimate the mode of \( p(\Psi \mid y) \). The software completes that step with the low-memory BFGS algorithm (Liu and Nocedal, 1989). Since there is no closed-form expression for the gradient, we rely on numerical differentiation instead. From the user-provided starting values, the software performs by default 25 iterations.

Two knot placement strategies have been implemented. The simplest one involves placing knots uniformly at random within each spatiotemporal block at resolutions \( 0, \ldots, K - 1 \). Knots at resolution \( K \) are placed at observation locations. The second scheme, that the software uses by default, is in two stages. In the first stage, we obtain knot positions by sampling prediction locations uniformly at random without replacement. We suspected this would help improve predictions, as they are based on an interpolation strategy that involves values computed at knot positions. Knot placement begins at resolution 0, and then, the algorithm moves to resolution 1, 2, and so on, repeating the scheme. Once all prediction locations have been selected, the algorithm starts the second stage, which involves placing knots on the edges of a cube nested within each subregion. This is based on a recommendation in Katzfuss (2017), which stated that placing knots close to the subregion boundaries might be preferable.

The software allows the user to specify the number of longitude, latitude, and time splits required. Longitude splits are processed first, followed by latitude splits, and finally, time splits. For example, if we require one longitude, one latitude, and one time split, we’ll have \( K = 3 \). The algorithm first splits the entire spatiotemporal domain in two,
based on observation longitudes, creating resolution 1. Then, the algorithm splits each of the resulting two subregions in two, based on observation latitudes, creating resolution 2. Finally, it splits all subregions in resolution 2 based on the observations’ temporal coordinates, resulting in resolution 3.

To ensure a good balance in the distribution of observations among subregions, the software places the new boundary for each split at the median value for the dimension to be split. Boundaries are left-continuous, that is, an observation on a boundary is assigned to the subregion on its left ($\leq$). The total number of knots at each resolution grows by a multiplicative constant. By default, the software sets the number of knots at 20 at resolution 0, and multiplies it by a factor of $J = 2$ at each resolution until $M - 1$. In practice, more knots may reduce MSPE, but especially at high resolutions, adding knots tends to sizably increase the computational burden. That is why we also included a tuning parameter called the tip knots thinning rate, comprised between 0 and 1. If we set this tuning parameter at 0.5, for example, the software will only retain 50% of knots in each subregion at the finest resolution, the selection of which is uniform at random. By selecting a suitable thinning rate, we can keep the full conditional precision matrix $Q$ at a size that can be handled by the LDLT decomposition algorithm offered in the Eigen library. We stress that configuring the algorithm to respect memory constraints requires mainly limiting the number of knots, and the thinning rate is an important feature for that purpose.

Under certain hyperparameter values, the covariance matrices computed for the $\eta$ parameter vectors in the MRA can be computationally singular. To prevent the issue, we apply by default a nugget effect of $1e - 5$ to both the spatial and temporal covariance functions. Further, the software assumes that all hyperparameters have a gamma distribution, with the parametrisation in which the mean corresponds to $\alpha/\beta$ and the variance, $\alpha/\beta^2$. 24
In order to minimise the number of evaluations of $p(\Psi \mid y)$, instead of obtaining the hyperparameter marginal posteriors themselves, the software estimates their first three moments. It then approximates them with a skew normal distribution whose parameters are computed with moment matching.

### Appendix B: Notes on the analyses

The priors for all fixed effects $\mathbf{\beta}$ are normal with mean $\mathbf{0}$ and covariance $100 \mathbf{I}$, a large variance with respect to the scale of the fixed effects considered. All hyperparameters are expressed on the logarithmic scale, and have normal hyperpriors with mean 0 and standard deviation 2. We deemed that such a standard deviation would allow for a suitable range of probable values, since $[\exp(-4), \exp(4)] \approx [0.02, 54.60]$. We are very confident those bounds encompass the range or scaling values one would expect in LST data. In other words, those values were selected arbitrarily to make the priors reasonably uninformative. The standard deviation for the measurement error term, $\log(\sigma_\epsilon)$, known from validation studies (Wan, 2014), is fixed at $\log(0.5)$. We therefore have only three variable hyperparameters: the spatial and temporal range log-parameters, $\log(\rho)$ and $\log(\phi)$, and the scale log-parameter $\log(\sigma_M)$. We center all continuous covariates.

In the main analysis, we create six longitude splits, five latitude splits, and one time split, which results in $M = 12$. We place 8 knots in each region from resolutions 0 to 11 ($= M - 1$) based on the default placement scheme. We sample 100 values in the importance sampling step. We let the optimizer, used to identify the mode of the joint marginal hyperparameters posterior distribution, run for 20 iterations. We impose a tip knots thinning rate of one third. All those tuning parameters control the computational burden of the algorithm.
The total number of splits, $M$, should be set as small as possible, keeping in mind however that a smaller $M$ results in larger matrices to invert in the computation of the $\Gamma$ matrices, and affects the sparsity of $H(\Psi_{ST}; Q)$. Setting $M = 12$ ensured that the algorithm would run fairly quickly, and not use more than the available memory. Setting it lower would have greatly increased running time. Since we only had seven days of data, we deemed that we should not have more than one time split. We divided the remaining splits, 11, in two, resulting in the six longitude and five latitude splits mentioned. Because the default knot placement scheme, described in Appendix A, starts by placing knots on the eight vertices of a rectangular prism, we thought that 8 would be the minimum number of knots recommended. That choice ensures that prediction locations are always close to the selected knots at any resolution, and results in a smaller $H(\Psi_{ST}; Q)$ matrix. Finally, the thinning rate of one third eliminated 733,334 columns in $H(\Psi_{ST}; Q)$. With that choice, we made sure that the algorithm would not request more memory than was available. The re-ordering scheme implemented in the SimplicialLDLT solver in Eigen (cf. `analyzePattern`) is especially memory-intensive, and so, we found it best to keep $H(\Psi_{ST}; Q)$ below 700,000 columns.

In the validation analysis, as the region surveyed is smaller, we consider instead four longitude splits, five latitude splits, and no time split, which results in $M = 9$. We apply a tip knots thinning rate of 0.5, and all other tuning parameters are the same. Once again, those tuning parameters were selected for computational reasons: we found that they offered a reasonable trade-off between computational and predictive performance.
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