Multi-resolution Spatial Regression for Aggregated Data with an Application to Crop Yield Prediction

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Abstract

We develop a new methodology for spatial regression of aggregated outputs on multi-resolution covariates. Such problems often occur with spatial data, for example in crop yield prediction, where the output is spatially-aggregated over an area and the covariates may be observed at multiple resolutions. Building upon previous work on aggregated output regression, we propose a regression framework to synthesise the effects of the covariates at different resolutions on the output and provide uncertainty estimation. We show that, for a crop yield prediction problem, our approach is more scalable, via variational inference, than existing multi-resolution regression models. We also show that our framework yields good predictive performance, compared to existing multi-resolution crop yield models, whilst being able to provide estimation of the underlying spatial effects.

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1 Introduction

In spatial statistics, the widely-used technique of kriging is equivalent to what is known as Gaussian process (GP) regression (Rasmussen (2003)) in the machine learning community. This nonparametric technique has been successfully applied to crime (Flaxman et al. (2019)), air quality monitoring (Hamelijnck et al. (2019), remote sensing (Tou et al. (2018)) and epidemiology (Law et al. (2018a); Bhatt et al. (2017)). Although GP regression becomes computationally intractable for large datasets due to the $O(n^3)$ and $O(n^2)$ complexities of inverting and storing the kernel matrix, various approximation methods such as variational inference (Titsias (2009); Hensman et al. (2013, 2015a); Shi et al. (2020)) and the Integrated Nested Laplace Approximation (INLA) (Rue et al. (2016)) have been used to alleviate this.

We focus on performing inference in the case where the outputs are available at a lower spatial resolution than the covariates. Additionally, each of the covariates may have a different spatial resolution. For crop yield prediction, crop yields are only observed at the county level over an entire year due to the scarcity of agricultural census data (Burke et al. (2021)), whereas the covariates, such as satellite imagery, are abundantly available at daily temporal and pixel-level (e.g. 500m by 500m squares in space) spatial resolution. Similarly, in epidemiology, disease diagnostic data (Bhatt et al. (2017)) is also only available at the census (or aggregated) level due to privacy reasons. To accomplish prediction at the census level, a straightforward approach would be to spatially average the covariates within each census level in order to create a standard supervised learning dataset (Bhatt et al. (2017); Mateo-Sanchis et al. (2019)). The drawback of this approach is that it would result in a loss of within region-level variability and the ability for disaggregation modelling (Law et al. (2018a); Lucas et al. (2020)). For both problems of crop yield and epidemiology, high-resolution disaggregation can be very important for policy making as it would allow for interventions at a high precision. In this work we also present the first attempt, to the best of our knowledge, at disaggregation for crop yield modelling.

In the literature, this type of problem has recently been approached in many ways under the lens of regression with aggregated outputs (Gelfand (2010); Law et al. (2018a); Hamelijnck et al. (2019); Yousefi et al. (2019); Tanaka et al. (2019); Zhang et al. (2020)), distribution regression (Law et al. (2018b); Mateo-Sanchis et al. (2019); Adsuara et al. (2019); Lemercier et al. (2021)) and multiple instance learning (Maron and Lozano-Pérez (1998); Kim and De la Torre (2010)). Distribution regression has been widely used in the context of crop yield prediction (Thorns (2018); Mateo-Sanchis et al. (2019); Adsuara et al. (2019); Lemercier et al. (2021)) and the reason for this is partly because of its attractive theoretical properties (Szabó et al. (2016)) and ability to fuse together covariates at different resolutions (Thorns (2018); Adsuara et al. (2019)).

However, distribution regression is a computationally expensive procedure due to its $O(\sum_{i,j=1}^{n} N_i N_j)$ complexity of computing the kernel matrix, where $N_i$ and
$N_j$ are the number of covariate vectors for outputs $i$ and $j$. Typically, $N_i$ and $N_j$ may be of the order of $10^2$ or $10^3$, depending on the resolution of the labels, and it will become computationally intractable to perform hyperparameter search. Previous methods that proposed to reduce this complexity include the use of random Fourier features \cite{rahimi2008random}, radial basis function (RBF) networks and Bayesian distribution regression \cite{law2018b}, at a slight cost to the approximation error.

Using the framework of aggregated output regression, where Gaussian process priors are often used for an underlying regression function, performing inference is still an expensive procedure. Exact inference or Markov chain Monte Carlo (MCMC) methods would still involve the $O(\sum_{i,j=1}^{n} N_i N_j)$ complexity of computing the aggregated kernel matrix and would also prohibit hyperparameter tuning. \cite{law2018a} and \cite{yousefi2019variational} used variational inference to approximate the Gaussian process posterior, where one compresses all the information onto a set of $M$ inducing points, and thereby bypassing the need for the full aggregated kernel matrix computation, reducing the computational complexity to $O(M^3 + M^2 \sum_{i=1}^{n} N_i)$ and allowing for mini-batch training.

**Contributions:**

- We develop a new methodology of performing spatial regression with aggregated outputs and multi-resolution covariates by building upon VBAgg \cite{law2018a}. Our methodology could be interpreted as a generalisation of \cite{law2018a} in the context of using satellite imagery covariates and is an extension of spatial kriging to the aggregated output setting due to the addition of an extra spatial effects component.

- We formulate a model, Multi-resolution Variational Bayes with Aggregated Output Gaussian Processes (MVBAgg), that extends \cite{law2018a} by using multiple sets of inducing points for each resolution to perform variational inference. We thereby also inherit the attractive properties of computational tractability, ability for GPU-acceleration, uncertainty quantification and disaggregation of \cite{law2018a}. We then demonstrate that it gives good prediction performance relative to distribution regression, GPs trained on centroid covariates and VBAgg on a crop yield dataset located in the Corn Belt of the US \cite{adsuara2019domain, mateo2019combining}.

## 2 Background

### 2.1 Distribution Regression:

Distribution regression is a method for nonparametric regression \cite{szabo2016distribution}, which has been recently used for crop yield prediction \cite{thorns2018estimating, mateo2019combining, adsuara2019domain}. It assumes that the data
comes in the form of
\[
\{(\Pi_i, y_i)\}_{i=1}^n,
\]
where \(y_i \in \mathbb{R}\) is a label, \(\Pi_i\) is a distribution over covariates \(x \in \mathcal{X} \subseteq \mathbb{R}^d\), where \(d \in \mathbb{N}_+\). In practice, \(\Pi_i\) is replaced with the empirical measure \(\hat{\Pi}_i = N_i^{-1} \sum_{j=1}^{N_i} \delta_{x_{i,j}}\) for some observed covariates \(\{x_{i,j}\}_{j=1}^{N_i}\), where \(\delta_{x_{i,j}}\) is a Dirac measure centred at \(\{x_{i,j}\}\) and \(N_i \in \mathbb{N}_+\). Suppose that we want to find a predictive model \(\hat{f}\) that minimises the regularised empirical risk
\[
\hat{f} := \arg\min_{f \in \mathcal{H}_x} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\tilde{\mu}_i))^2 + \lambda \|f\|^2_{\mathcal{H}_x},
\]
where \(\tilde{\mu}_i := \int_{\mathcal{X}} k(\cdot, x) d\hat{\Pi}_i(x) = N_i^{-1} \sum_{j=1}^{N_i} k(\cdot, x_{i,j})\) is the empirical mean embedding of \(\hat{\Pi}_i\) into the reproducing kernel Hilbert space (RKHS) \(\mathcal{H}_k\) for some kernel \(k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}\). Solving \(\hat{f}\) corresponds to kernel ridge regression on the mean embeddings (KRR). Predictive functions \(f\) are taken from \(\mathcal{H}_x\), the RKHS of a second-level kernel \(\rho: \mathcal{H}_k \times \mathcal{H}_k \to \mathbb{R}\), and \(\lambda\) is a regularisation parameter. Given any set of covariates \(\{x_{*,j}\}_{j=1}^{N_*}\), where \(N_* \in \mathbb{N}_+\), and using the kernel trick, this yields a solution \(\hat{f}(\mu_*) = K_* \hat{\alpha}\), for \(\mu_* = N_*^{-1} \sum_{j=1}^{N_*} k(\cdot, x_{*,j})\), where
\[
K_* := \langle \rho(\tilde{\mu}_*, \tilde{\mu}_1), \ldots, \rho(\tilde{\mu}_*, \tilde{\mu}_n) \rangle,
\]
\[
\hat{\alpha} := (K + \lambda I_n)^{-1} y,
\]
with \((K)_{i,j} = \rho(\tilde{\mu}_i, \tilde{\mu}_j)\). Using the kernel trick again and with the linear kernel \(\rho(f, g) = \langle f, g \rangle_{\mathcal{H}_k}\), this recovers linear regression on the mean embeddings (LRe), in which \((K)_{i,j} = (N_*N_j)^{-1} \sum_{l=1}^{N_*} \sum_{r=1}^{N_j} k(x_{i,l}, x_{j,r})\) and \(I_n\) being the \(n\)-dimensional identity matrix. Note that the LRe also employs the kernel trick since mean embeddings are potentially infinite-dimensional, i.e. no explicit coefficients of the linear model are used. Similarly, one can also use a non-linear kernel \(\rho\), which we call kernel ridge regression on the mean embeddings (KRR), and this has been shown to improve its performance in certain scenarios (Muandet et al. (2012)).

A major disadvantage of distribution regression is the need to perform \(O(\sum_{i=1}^{n} \sum_{j=1}^{N_i} N_i N_j)\) number operations to compute the matrix \(K\), and a subsequent \(O(n^3)\) to invert \(K + \sigma^2 I_n\), therefore prohibiting the ability to efficiently tune the regularisation parameter \(\lambda\) and kernel hyperparameters of \(k\) (in contrast to the hyperparameters of \(\rho\), which can be tuned more efficiently). It is also possible to make use of RBF networks and Bayesian distribution regression (Law et al. (2018b)) by inducing points approximations, and RFF to approximate the kernel matrix (Rahimi and Recht (2008)) for improving the computational scalability.

### 2.2 Gaussian Process for Aggregated Output Regression

GPs can be used to tackle aggregated output regression (Law et al. (2018a); Hamelijnck et al. (2019); Tanaka et al. (2019); Yousefi et al. (2019)). This is a
common setting in spatial statistics, where each label is often associated with a set of observations within a region (areal unit). Again, suppose we have some covariate space \( \mathcal{X} \) and a response space \( \mathbb{R} \). The aggregated output regression model (Tanaka et al. (2019)) is defined as

\[
y_i = \int_{\mathcal{X}} f(x) d\Pi_i(x) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2),
\]

where \( \mathcal{X}_i \subseteq \mathcal{X} \) is an observation region with distribution \( \Pi_i \) with Lebesgue density \( \pi_i \) and \( \epsilon_i \) is an independently distributed Gaussian noise with \( \sigma > 0 \). We denote \( \mathcal{N}(a,b) \) and \( \mathcal{N}(a,b) \) as the distribution and density function of a Gaussian distribution with mean \( a \) and covariance \( b \).

In practice, we will want to approximate \( \int_{\mathcal{X}_i} f(x) d\Pi_i(x) \) using some available covariates \( \{x_{i,j}\}_{j=1}^{N_i} \) drawn from \( \Pi_i \). In general, this integral could be approximated by constructing quadrature weights \( w_{i,j} \) and states \( \{x_{i,j}\}_{j=1}^{N_i} \) such that \( \sum_{j=1}^{N_i} w_{i,j} = 1 \). Law et al. (2018a) used deterministic survey weights and Hamelijnck et al. (2019) constructed the weights using a Gaussian process regression network, but it is not clear how these will improve the estimation accuracy of \( \int_{\mathcal{X}_i} f(x) d\Pi_i(x) \) and so we will assume that \( w_{i,j} = N_i^{-1} \) for all \( j = 1, \ldots, N_i \). In the context of classification of images, alternative aggregation methods are max-aggregation or attention-aggregation (Kim and De la Torre (2010); Haussmann et al. (2017); Ilse et al. (2018)).

Using this setup, we thus work with the dataset

\[
\mathcal{Y}_i = \{(x_{i,j}, w_{i,j})_{j=1}^{N_i}, y_i\}_{i=1}^n.
\]

Using \( \hat{\Pi}_i \), Equation 2 becomes

\[
y_i = \sum_{j=1}^{N_i} w_{i,j} f(x_{i,j}) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2),
\]

where \( f \) is some underlying regression function and \( \sigma > 0 \). We can posit a GP prior \( f \sim \mathcal{GP}(m,k) \), where \( m \) and \( k \) are the mean and covariance functions, in order to infer \( f \). We will denote the likelihood function of \( (3) \) as \( p(y_i|f_i) \), where \( f_i := (f(x_{i,1}), \ldots, f(x_{i,N_i}))^\top \), and denote the weights \( w_i := (w_{i,1}, \ldots, w_{i,N_i})^\top \). Similarly, denote \( f_* := (f_{*,1}, \ldots, f_{*,N_*})^\top \) for prediction points \( \{x_{*,j}, w_{*,j}\}_{j=1}^{N_*} \) with true label \( y_* \). Suppose further that \( X_i := (x_{i,1}, \ldots, x_{i,N_i})^\top \), \( X_* := (x_{*,1}, \ldots, x_{*,N_*})^\top \) and \( k_{X_i,X_j} := (k(x_{i,1}, x_{j,1}), \ldots, k(x_{i,N_i}, x_{j,N_j}))_{l,m} \) for pairs \( i, j \), and \( l = 1, \ldots, N_i \) and \( m = 1, \ldots, N_j \).

The log-likelihood is \( \log p(y_i|f_i) \) is

\[
\log p(y_i|f_i) = \frac{1}{2\sigma^2} (y_i - w_i^\top f_i)^2 - \frac{1}{2} \log (2\pi\sigma^2) .
\]

Since we have

\[
\begin{pmatrix}
y_1 \\
\vdots \\
y_n \\
w_i^\top f_*
\end{pmatrix} = \mathcal{N}
\begin{pmatrix}
w_i^\top m_{X_1} \\
\vdots \\
w_i^\top m_{X_n} \\
w_i^\top m_{X_*}
\end{pmatrix},
\begin{pmatrix}
K + \sigma^2 I_n & K_* \\
K^\top_* & K_{*,*}
\end{pmatrix},
\]

5
With a zero mean function, the posterior mean obtained here is the exact
although kernel ridge and exact Gaussian process regression provide elegant
inference procedures for learning from aggregated outputs, the computational
burden in the kernel matrix operations.

With a zero mean function, the posterior mean obtained here is the exact
expression from LRe, similar to the connection between standard, non-aggregated
GP regression and kernel ridge regression (Kanagawa et al. (2018)). With this,
we are still prohibited by the large computational burden in the kernel matrix
operations.

On the other hand, if \( \Pi_i \) is known, then we would obtain

\[
\begin{pmatrix}
y_1 \\
\vdots \\
y_n \\
\int_{X_i} f_*(u) \pi_*(x) \, dx
\end{pmatrix} = \mathcal{N}
\begin{pmatrix}
\int_{X_i} m(x) \pi_1(x) \, dx \\
\vdots \\
\int_{X_n} m(x) \pi_n(x) \, dx \\
\int_{X_\ast} m(x) \pi_*(x) \, dx
\end{pmatrix}, \begin{pmatrix}
K + \sigma^2 I_n & K_* \\
K_\ast & K_\ast\ast
\end{pmatrix},
\]

where

\[
(K)_{ij} := \int_{X_i} \int_{X_j} k(u,v) \pi_i(u) \pi_j(v) \, du \, dv,
\]

\[
(K_*) := \int_{X_i} \int_{X_\ast} \int_{X_\ast} k(u,v) \pi_*(u) \pi_*(v) \, du \, dv,
\]

\[
(K_{\ast\ast}) := \int_{X_i} \int_{X_i} k(u,v) \pi_*(u) \pi_*(v) \, du \, dv.
\]

The posterior distribution over the integral \( \int_{X_i} f(x) \, d\Pi_i(x) \) would thus be

\[
\int_{X_\ast} f(x) \, d\Pi_\ast(x) \, dx \sim \mathcal{N}(\bar{m}, \bar{k}),
\]

with

\[
\bar{m} := \int_{X_\ast} m(x) \pi_*(x) \, dx + K_\ast \ast (K + \sigma^2 I_n)^{-1} (y - m_X),
\]

\[
\bar{k} := K_{\ast\ast} - K_\ast \ast (K + \sigma^2 I_n)^{-1} K_*.
\]

Having learned the posterior distribution of \( f \), it is then possible to make
predictions and provide statistical insights at the individual covariate level (Law et al. (2018a)).

2.3 Variational Bayes with Gaussian Processes (VBAgg)

Although kernel ridge and exact Gaussian process regression provide elegant
inference procedures for learning from aggregated outputs, the computational
we may only observe a noisy version of

This thus allows the lower bound to be written down explicitly as

where

variational approximation

In spatial statistics, we often make use of spatially-resolved covariates, where we implicitly assume that they are a function of the spatial coordinates. Suppose that \( S \subseteq \mathbb{R}^2 \) represents a spatial domain and \( q : S \to \mathbb{R}^d \), where \( d > 0 \), is an unknown function that represents a covariate. Then \( q \), for example, could be the solution of the heat equation if it represents temperature, although in reality we may only observe a noisy version of \( q \) collected via remote sensing methods.

3 Aggregated Output Spatial Regression

In spatial statistics, we often make use of spatially-resolved covariates, where we implicitly assume that they are a function of the spatial coordinates. Suppose that \( S \subseteq \mathbb{R}^2 \) represents a spatial domain and \( q : S \to \mathbb{R}^d \), where \( d > 0 \), is an unknown function that represents a covariate. Then \( q \), for example, could be the solution of the heat equation if it represents temperature, although in reality we may only observe a noisy version of \( q \) collected via remote sensing methods,
such as satellite sensors and cameras. We can thus formulate aggregated output spatial regression as

\[ y_i = \frac{1}{|S_i|} \int_{S_i} f^1(g(s))ds + \frac{1}{|S_i|} \int_{S_i} f^0(s)ds + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2), \quad (4) \]

where \( S_i \subseteq S \), and \( f^1 \) and \( f^2 \) are functions indicating effects from remote sensing covariates and additional spatial variability. Note that the first integral can also be written as \( \frac{1}{|S_i|} \int_{T_i} f^1(t)d(g_\sharp \lambda)(t) \), where \( \lambda \) is the Lebesgue measure, \( g_\sharp \lambda \) is the push-forward measure and \( g^{-1}(T_i) = S_i \), meaning that we can use the aggregated output models as previously discussed. It is interesting to note that \( \lambda \) could also be other measures, such as the spherical measure, a generalisation of the Lebesgue measure on the sphere \( \mathbb{S}^2 \subset \mathbb{R}^3 \) and may be a more realistic measure for modelling Earth observations.

In the context of images, such as ones obtained via satellites, each datapoint represents a pixel, which is a square over space, as shown in Figure 1. It should be noted that this limits the number of points that one can use for performing numerical integration as it would depend on the spatial resolution of the covariates. For each pixel, suppose we have a representative latitude-longitude pair \( [s] \). For a subset with latitude and longitude \( S \subseteq \mathbb{R}^2 \) and Lebesgue measure \( \lambda \), this means that we have to discretise the domains \( S \) into a discrete measure space \( \mathcal{S} \) of the representatives \( [s] \), with measure \( \hat{\lambda}(S) = \frac{1}{|S_i|} \sum_{s \in S} \mathbf{1}_{S_i}(s) \) for any \( S \subseteq S_i \). This changes Equation (4) to

\[ y_i = \frac{1}{|S_i|} \sum_{s \in S_i} f^1(g(s)) + \frac{1}{|S_i|} \int_{S_i} f^0(s)ds + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2), \quad (5) \]

where we note that we can still approximate the second integral with arbitrarily many points in space without discretisation as the spatial covariates have infinite resolution. In contrast, Law et al. (2018a) only allows for a single integral and the number of spatial points must match the number of pixels for the spatially-resolved covariates.

As it is the case that the covariate effects from \( g(s) \) and spatial effects from \( s \) do not need to be treated at the same resolution, various spatially-resolved covariates may also correspond to different resolutions. In previous aggregated output modelling works, the covariates are usually preprocessed to the same resolution (Mateo-Sanchis et al. (2019)). This means that when using aggregate output methods, the integrals of the mean and covariance functions will be integrated over a discrete measure with fewer points, giving less accurate and higher variance approximations. On the other hand, up-sampling may result in errors from the approximation algorithms used, introducing bias into the integrals. This thus motivates the use of multi-resolution models, where the integrals for different resolution are separated without up-sampling or down-sampling by assuming an additive structure. Suppose we have \( D \) covariates, each with a different spatial resolution. By treating each resolution separately, we can modify Equation (5) and obtain

\[ y_i = \sum_{l=1}^{D} \frac{1}{|S_{i,l}|} \sum_{s \in \hat{S}_{i,l}} f^k(g_l(s)) + \frac{1}{|S_i|} \int_{S_i} f^0(s)ds + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2), \]

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Figure 1: Pixel squares of the MCD12C1 land cover mask (Friedl and Sulla-Menashe, 2015) over Adams county, Illinois, USA. Note that some of the data is missing, as represented by the white squares.

for resolutions $l = 1, \ldots, D$ and $g_l : S \rightarrow \mathbb{R}^{d_l}$ for $d_l > 0$. Note that we here consider an additive model across covariates corresponding to different resolutions. This results in the additive covariance kernel structure. It is also possible to formulate a product covariance kernel structure, but we do not pursue it further in this work.

3.1 Multi-resolution Variational Bayes with Aggregated Output Gaussian Processes (MVBAgg)

A natural extension to VBAgg is to include covariates of multiple sets and hence observing the dataset

$$
\left\{\left\{\{x_{i,j,l}, w_{i,j,l}\}_{j=1}^{N_i,l}\right\}_{l=1}^{D}, y_i\right\}_{i=1}^{n},
$$

where $l = 1, \ldots, D$ is the index of the covariates. Adsuara et al. (2019) proposes incorporating sets of covariates at different resolutions, in the context of LRe, by considering kernel regression functions in the space equal to the direct sum of RKHSs with kernels $\rho_1, \ldots, \rho_D$, where $\rho_l : \mathcal{H}_{k_l} \times \mathcal{H}_{k_l} \rightarrow \mathbb{R}$. From a GP point of view, we may learn similar functions by modifying Equation 3 to

$$
y_i | \left\{\{x_{i,j,l}, w_{i,j,l}\}_{j=1}^{N_i,l}\right\}_{l=1}^{D} \sim \mathcal{N}\left(\sum_{l=1}^{D} \sum_{j=1}^{N_i,l} w_{i,j,l} f^l(x_{i,j,l}), \left(\sum_{l=1}^{D} \sum_{j=1}^{N_i,l} w_{i,j,l}^2\right) \sigma^2\right),
$$
where \( f^i \) is a function induced with a \( \mathcal{GP}(0, k_i) \) with kernel \( k_i : \mathcal{X}_i \times \mathcal{X}_i \to \mathbb{R} \), where \( \mathcal{X}_i \) is the covariate space for the \( i \)th resolution in the region indexed by \( i \). We assume that the \( f^i \)'s are mutually independent. To use a VBAgg approximation framework, we pose the variational distribution \( q(f^1, \ldots, f^D, u_1, \ldots, u_D) := \prod_{i=1}^D p(f^i|u_i)q(u_i) \) with different inducing points \( u_i = (f^1(z_{i,1}), \ldots, f^D(z_{i,L_i}))^T \) at each sets of locations \( Z_i = (z_{i,1}, \ldots, z_{i,L_i})^T \). We can thus obtain the approximate posterior \( q(f^i) \) for each \( i \) as \( q(f^i) = N(f^i_l; \tilde{m}_{X_{i}}, \tilde{k}_{X_{i}}) \)

\[
\tilde{m}_{X_{i,l}} = m_{X_{i,l}} + k_{X_{i,l},Z_l}k_{Z_l,Z_l}^{-1}(\eta_{Z_l} - m_{Z_l}),
\]

\[
\tilde{k}_{X_{i,l},X_{i,l}} = k_{X_{i,l},X_{i,l}} - k_{X_{i,l},Z_l}k_{Z_l,Z_l}^{-1}k_{Z_l,X_{i,l}}k_{Z_l,Z_l}^{-1}k_{Z_l,X_{i,l}},
\]

where \( X_{i,l} := (x_{i,1,l}, \ldots, x_{i,N_{i,l},l})^T \). The lower bound can then be written as

\[
\mathcal{L} := \sum_{i=1}^D KL(q(u_i)||p(u_i)) - \frac{1}{2} \sum_{i=1}^D \left( \frac{1}{\pi} - 2y_i \sum_{l=1}^{D} w_{i,l}^T \tilde{m}_{X_{i,l}} + \sum_{l=1}^{D} w_{i,l}^T (\tilde{k}_{X_{i,l},X_{i,l}} + \tilde{m}_{X_{i,l}} \tilde{m}_{X_{i,l}}^T)w_{i,l} \right) - \log(2\pi\sigma^2),
\]

where \( w_{i,l} := (w_{i,1,l}, \ldots, w_{i,N_{i,l},l})^T \). Similarly, the predictive distribution for \( y_* \) would be

\[
q(\sum_{i=1}^{D} w_{i,l}^T f^i_l) = N(\sum_{i=1}^{D} w_{i,l}^T \tilde{m}_{X_{i,l}}, \sum_{i=1}^{D} w_{i,l}^T \tilde{k}_{X_{i,l},X_{i,l}} w_{i,l}^T).
\]

To initialise the inducing points \( Z_i \)'s, we follow the setup in VBagg (Law et al. (2018a)) and pick 1 point from each region \( i \) using the cluster centres with KMeans. We can also set the inducing points to be trainable or fixed. Inheriting the nice properties of VBAgg, we can attain \( \mathcal{O}(\sum_{i=1}^{D} L_i^3 + L_i^2 \sum_{i=1}^{D} N_{i,l}) \) complexity in time, can performing mini-batch training and make use of GPU-acceleration. In comparison, (Adsuara et al. (2019)) gives \( \mathcal{O}(\sum_{i=1}^{D} \sum_{j=1}^{N_{i,l} N_{j,l}}) \) complexity. Although it is possible to employ RFF to give a reduction to \( \mathcal{O}(\sum_{i=1}^{D} L_i^3 + L_i^2 \sum_{i=1}^{D} N_{i,l}) \), where \( L_i \) is now the dimension of the RFF map, it still cannot perform kernel parameter tuning without cross-validation, whereas we propose to tune the parameters in a data-driven way via the variational lower bound. The full inference scheme is detailed in Algorithm 1.

Returning to the context of aggregated outputs in the spatial context, alongside sets of remote sensing covariates, we would also include a set of latitude and longitude coordinates that we can sample uniformly on the continuous spatial domain. This yields the spatial GP \( f^0 \) and the covariate GPs \( f^1, \ldots, f^D \). As motivated in (Law et al. (2018a)), the VBAgg model is also capable of performing disaggregation by learning an analytic form of the approximate posterior distribution on the underlying function \( f \). In a similar manner, with MVBAgg we can also study each of the GPs at the pixel level using the posterior distribution of each \( f^i \).
Algorithm 1 Training of Multi-resolution Variational Bayes with Aggregated Output Gaussian Processes (MVBAgg)

**Input** \{\{x_{i,j,l}, w_{i,j,l}\}_{j=1}^{N_i,l} \}_{i,l=1}^{D} \text{(dataset), } \{z_i\}_{i=1}^{D} \text{(landmark points), } \{\eta_{Z_l}\}_{l=1}^{D}, \{\Sigma_{Z_l}\}_{l=1}^{D} \text{(variational distribution parameters), kernels } \{k_l\}_{l=1}^{D}, \text{noise } \sigma, \text{total iterations } L, \text{batch size } B

1: Initialise ELBO \( \mathcal{L} \leftarrow 0 \)
2: for \( i = 1, \ldots, L \) do
3: Take a mini-batch \( \{\{x_{i,j,l}, w_{i,j,l}\}_{j=1}^{N_i,l} \}_{i,l=1}^{D}, y_i\}_{i \in B} \) with indexing set \( B \subset \{1, \ldots, n\} \)
4: Compute lower bound \( \mathcal{L}_B \) with this batch
5: \( \mathcal{L} \leftarrow \mathcal{L} + \frac{n}{B} \mathcal{L}_B \)
6: if \( i \mod n/B = 0 \) then
7: Backpropagate \( \mathcal{L} \) and update model parameters
8: end if
9: end for
10: return \( \{k_l\}_{l=1}^{D}, \sigma, \{\eta_{Z_l}\}_{l=1}^{D}, \{\Sigma_{Z_l}\}_{l=1}^{D} \)

4 Application to Crop Yield prediction

The task of crop yield prediction has recently been attempted by scientists using a variety of methods ([Bolton and Friedl (2013); Kuwata and Shibasaki (2015); Lobell et al. (2015); You et al. (2017); Thorns (2018); Mateo-Sanchis et al. (2019); Adsuara et al. (2019); Yang et al. (2019); Lemercier et al. (2021)]). The wide availability of remote sensing and geophysical data from NASA programmes such as Moderate Resolution Imaging Spectroradiometer (MODIS) ([Didan (2015)]), and Soil Moisture Active Passive (SMAP) ([Entekhabi et al. (2010)]), have also helped with this effort by providing modellers with pixel-resolution information on croplands. By utilising the vast amount of data, such as vegetation indices, that have biological links to crop health and hence to yield ([Mateo-Sanchis et al. (2019)]), as covariates of the croplands, modellers can formulate crop yield prediction as a supervised learning problem. However, existing works on crop yield modelling using aggregated output/distribution regression methods ([You et al. (2017); Thorns (2018); Mateo-Sanchis et al. (2019); Adsuara et al. (2019)]) do not consider the model uncertainty and interpretability, which is arguably as important as performing crop yield prediction itself.

Our work is most closely related to kernel methods for crop yield modelling, notably multi-source kernel ridge regression (on the mean embeddings) ([Adsuara et al. (2019)]), kernel ridge regression ([Mateo-Sanchis et al. (2019)]) and Bayesian distribution regression ([Thorns (2018)]). Another very popular approach is to extract signals from the image histograms of the pixel values using convolutional neural networks, as attempted in the Deep Gaussian process for crop yield prediction work ([You et al. (2017)]). However, this approach is not suitable for accounting for the underlying spatial structure and variability due to the the use
of image histograms, whereas our method keeps the pixel-level spatial structure. Our aim is to both predict the crop yield at the county-level and disaggregate the underlying spatial random surface at the pixel-level.

4.1 Data

We use a county-level crop yield dataset from Mateo-Sanchis et al. (2019), with yield in the U.S. Corn Belt in 2015, vegetation optical depth (VOD) (Konings et al. (2017)) derived from the SMAP products (Entekhabi et al. (2010)) and Enhanced Vegetation Index (EVI) from MODIS (Didan (2015)). Unfortunately, the covariates in this study are in the same spatial resolution due to the downsampling of the EVI covariates and the data processing procedure is non-trivial, but we can nonetheless obtain a multi-resolution dataset by adding sets of 100 spatial covariates (latitude + longitude in EPSG:4326 projection format) per county. Following Sanchis et al. (2019), we use only use covariates during the period April 2015 - October 2015, which covers the period from growth to just before harvest. For VOD and EVI respectively, this gives 213 and 13 observations for each spatial location respectively. We filter out regions where the geometry of the yield has not been provided, giving 375 outputs as shown in Figure 2.

4.2 Experimental Setup

For our experiments, we will assess the performance of the predictive models via 5-fold cross-validation, reporting the Root Mean Squared Error (RMSE) $\sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$ and Mean Average Percentage Error (MAPE) $\frac{1}{n} \sum_{i=1}^{n} |(y_i - \hat{y}_i)/y_i|$, averaged over 5 validation sets, with 300 and 75 training and test labels respectively per fold. Our benchmarks are Linear Regression (LR), Gaussian process (GP) regression, linear regression on the mean embeddings (LRe), kernel ridge regression on the mean embeddings (KRRe) and VBAgg. We compare these to MVBagg. For LR and GP, we use the centroid covariates, where we spatially average the covariates to obtain a standard supervised learning dataset. For all other models, we use the “stacked covariates” (Thorns (2018); Mateo-Sanchis et al. (2019); Adsuara et al. (2019)), where each column represents an observation at a certain time during the year and each row presents an observation at a certain spatial location. For MVBAgg, VBAgg and GP, the VOD and EVI covariates are treated in the same resolution with additive RBF kernels, defined as:

$$k(x, y) = \sigma^2 \exp \left(-\frac{||x-y||_2^2}{2\ell^2}\right), \quad \forall x, y \in \mathcal{X},$$

where $\sigma > 0$ is the scale, $\ell > 0$ is the lengthscale and $||\cdot||_2$ denotes the Euclidean norm. Similarly, the spatial components are specified with a Matérn-3/2 kernel:

$$k(x, y) = \sigma^2 \left(1 + \frac{\sqrt{3}||x-y||_2}{\ell} \right) \exp \left(-\frac{\sqrt{3}||x-y||_2}{\ell}\right).$$
We fit LR and GP using maximum likelihood estimation, and LRe and KRRe using the median heuristic for the lengthscale (Garreau et al. (2018)) and the scale $\sigma = 1$, with a regularisation parameter of $\lambda = 0.1$. In addition, LRe and KRRe use the linear and RBF second-level kernel respectively, in which for the latter we tune the lengthscale also using the median heuristic (of the difference of the mean embedding norms $||\hat{\mu}_i - \hat{\mu}_j||_{H^\rho}$ for counties $i, j$) and set $\sigma = 1$. We use the Adam optimiser with a learning rate of 0.001, 20,000 training iterations and the inducing points chosen by taking the centre of a K-Means algorithm (Oglic and Gärtner (2017)) in each county for MVBAgg and VBAgg. We relied on GPFlow (De G. Matthews et al. (2017)) and NumPy (Harris et al. (2020)) to implement our models. The code is available at https://github.com/ImperialCollegeLondon/MVBAgg. For VBAgg and MVBAgg, we used 2 Nvidia RTX 2080 GPUs, and for all the other methods, we used Intel(R) Xeon(R) Gold 6242 CPU @ 2.80GHz CPUs, both on the NVIDIA4 GPU Compute Server provided by the Department of Mathematics, Imperial College London.

![Crop yield](https://github.com/ImperialCollegeLondon/MVBAgg)

**Figure 2**: Crop yield ($kg/m^2$) in the corn belt of the United States.

### 4.3 Results

We can see from Table 1 that the out-of-sample predictive performance for MVBAgg is slightly better than GP, LRe and KRRe in terms of RMSE and MAPE. Due to the larger difference in MAPE, we can interpret this as MVBAgg giving better individual county predictions on average. In many applications,

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1As there are over 20,000 covariate values, we take a maximum of 10 values per county, which reduces this number to around 3,000, and then compute the subsequent median lengthscale.
GP with centroid covariates is the commonly-used approach (Bhatt et al. (2017); Mateo-Sanchis et al. (2019); Martinez-Ferrer et al. (2020)) and our results suggest that there are gains in both predictive performance and reduction in uncertainty when using aggregated output methods.

![Figure 3: Prediction versus Observed Outputs with 95% posterior credible intervals on a test set of 20% of the points. 86.7% and 65.3% of the observations lie in the 95% and 80% credible intervals respectively.](image)

**Table 1**: Cross-validated predictive and average run-time performance of the models on the crop yield data. We also report the standard error over 5-fold cross-validation of the RMSE and MAPE, as indicated as se-RMSE and se-MAPE respectively, and well as the standard error over the run-time.

| Method | Covariates                  | RMSE       | MAPE       | Runtime (s)  |
|--------|-----------------------------|------------|------------|--------------|
| LR     | Centroid VOD + EVI         | 0.321±0.0446 | 0.411±0.0589 | 0.0457±0.0082 |
| GP     | Centroid VOD + EVI + space | 0.0766±0.00762 | 0.0891±0.0113 | 1.26±0.0097  |
| LRe    | Stacked VOD + EVI          | 0.0752±0.00457 | 0.0836±0.00732 | 36±1.14      |
| LRe    | Stacked VOD + EVI + space  | 0.0726±0.00478 | 0.0798±0.00695 | 598±2.81     |
| KRRRe  | Stacked VOD + EVI          | 0.0792±0.00514 | 0.0888±0.00828 | 1140±5.46    |
| KRRRe  | Stacked VOD + EVI + space  | 0.0726±0.00554 | 0.0806±0.00826 | 1750±14.9    |
| VBAgg  | Stacked VOD + EVI          | 0.0758±0.00411 | 0.0850±0.00647 | 28±1.14      |
| MVBAgg | Stacked VOD + EVI + space  | 0.0722±0.00454 | 0.0763±0.00619 | 478±0.485    |

LRe, the existing benchmark, requires hyperparameter tuning via cross-validation over a grid of configurations without the median heuristic. We also find that with our computational hardware, a full inference with VBAgg and MVBAgg is
Figure 4: Absolute prediction error (kg/m²) of MVBAgg on 75 counties that were held out as test set.

Figure 5: The spatial effects component of MVBAgg at the individual level after using the whole dataset for training.

faster than (See Table 1) fitting LRe or KRRe on a single set of hyperparameters, which confirms that our method is indeed more scalable.

As shown in Figure 4 of the prediction on 75 counties held out as test set, our model is unable predict well on Lincoln County, Minnesota which is an outlier as
can be seen in Figure 2. However, in Figure 3, we can see that most of the 95% posterior credible intervals for the test points contain the true crop yield. Finally, by looking at the posterior mean of the spatial component at the pixel-level in Figure 5, it is also interesting to see that we are able to uncover the additional spatial heterogeneity: for example, regions in Nebraska exhibit within-county variability as seen via the colour gradient within each county. This type of disaggregated information could be useful for agricultural policy makers to study where to impose interventions to improve productivity.

5 Conclusion

We developed a framework for spatial regression of aggregated outputs on multi-resolution covariates. Using Gaussian processes, we derived a multi-resolution version of VBAgg ([Law et al. (2018a)]), giving at least as good performance on a real world crop yield dataset as existing multi-resolution crop yield prediction models. In addition, our model is capable of performing inference on its model hyperparameters at scale and in a data-driven manner due to the variational formulation and the ability for GPU-acceleration, whereas kernel ridge regression requires tuning via cross-validation or the median-heuristic. We were also able to reconstruct the underlying fine-grained spatial effects by looking at the spatial component of MVBAgg and prediction uncertainty and we believe that this information would be particularly useful for organisations making policy interventions. We hope that this model could be useful for agriculture domain-experts who have access to other interesting crop yield datasets.

For future work, it would be interesting to consider our model for other problems such as disease mapping, as attempted previously by [Law et al. (2018a)] with VBAgg and [Lucas et al. (2020)]. For improved performance with fewer observations of covariates in each county, it may be interesting to use control variates to give estimators with lower variance for the required integrals ([Hammersley and Handscomb (1964)]). Our model also makes the assumption that data for different resolutions are not dependent on each other, which may not be the case, and it would be useful to explore methods that can account for dependence without data up-sampling or down-sampling. It also may be of interest to explore alternative stochastic process priors for the underlying function other than GPs. Lastly, while our modelling approach is flexible for aggregation spatially, the dimensionality of the covariate space at each spatial location may be high and so it may be useful to consider learning low-dimensional projections within the model ([Guhaniyogi and Dunson (2016); Delbridge et al. (2020)]).

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