

Spatial Statistics

A comparison of geostatistical and non-spatial machine learning methods in NO₂ modelling: prediction accuracy, uncertainty quantification, and model interpretation

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Abstract:	NO ₂ is a traffic-related air pollutant that is strongly associated with cardiovascular and respiratory diseases. Ground NO ₂ monitoring stations measure NO ₂ concentrations at certain locations and statistical predictive methods have been developed to predict NO ₂ as a continuous surface to inform decision-making. Among them, machine learning methods are the most powerful in capturing non-linear relationships between NO ₂ measurements and geospatial predictors, but it is unclear if the spatial structure of NO ₂ is also captured in the response-covariates relationships. In addition, most model comparison studies only compare accuracy in the prediction mean at ground stations, but do not consider prediction intervals and model interpretation and the effects of different model evaluation methods. In this study, we dive into the comparison between spatial and non-spatial data models accounting for the above-mentioned aspects. Moreover, we implemented a spatial and a non-spatial methods that have not been applied to air pollution mapping before and evaluated stack learning methods with and without modelling the spatial process. We implemented our study using national ground station measurements of NO ₂ in Germany and Netherlands of the year 2017, predicting NO ₂ to 100 m resolution grid. Our results indicate the importance of modelling the spatial process especially in areas close to traffic. The prediction intervals predicted with ensemble tree-based methods are satisfactory but too narrow with the geostatistical methods. Compared to ensemble tree-based methods, the geostatistical methods provide important spatial information for analysing emission sources and the spatial process of observations.
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Dear Prof. Alfred Stein,

Please find attached to this letter our research paper

"A comparison of geostatistical and non-spatial machine learning methods in NO₂ modelling: prediction accuracy, uncertainty quantification, and model interpretation,

to be considered for publication in *spatial statistics*.

Machine learning (ML) methods have shown to be powerful in capturing non-linear relationships between NO₂ measurements and geospatial predictors but it is unclear if the spatial structure of NO₂ is sufficiently captured in the response-covariates relationships and how prediction intervals and model interpretation derived from ML models compare with geostatistical models. In addition, it is commonly not evaluated how different models behave in different geographical areas.

In this study, we compared geostatistical methods with ML methods in the spatial prediction of NO₂. We developed a comparison process that comprehensively compare the predicted mean, prediction intervals, and model interpretation of different spatial and non-spatial models. Spatial and non-spatial CV strategies are used to reveal prediction accuracy in different aspects. We also implemented two methods that to our knowledge have not been applied in air pollution mapping, one post-processes quantile random forest with L1-norm shrinkage (Lasso) regression and the other geostatistical stacked learning. These two methods considerably improve from the original (quantile) random forest and stacked learning methods, respectively.

With geospatial predictors and ground observations becoming increasingly available, many statistical methods have been developed in NO₂ mapping, but a study that comprehensively dive into models with different structures and complexity to understand the strength and limitations of each is lacking in air pollution mapping. Our comparison study is important in understanding different model behaviours and pointing out good practices in spatial prediction of air pollution and future directions for improvements. We also paid full attention to computational efficiency in the methods applied, all the methods we applied are highly scalable and the Lasso post-processing further reduces model redundancy. We therefore strongly believe our study is highly relevant to the domain of applied mathematics in *spatial statistics* .

Thank you very much for your consideration,

Dr. Meng Lu,
On behalf of Joaquin Cavieres and Dr. Paula Moraga

Highlight

- Geostatistical and machine learning methods show different strength and limitations.
- The model comparison concerns prediction intervals and model interpretation.
- Post-processing random forest with Lasso regression outperforms random forest.
- Geostatistical stacked learning outperforms stacked learning methods.
- It is important to model spatial structure in national NO₂ mapping.
- Non-spatial machine learning methods may not fully capture the spatial process.
- Spatial and non-spatial CV strategies affect model comparison.

¹ A comparison of geostatistical and non-spatial machine
² learning methods in NO_2 modelling: prediction accuracy,
³ uncertainty quantification, and model interpretation

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Abstract

NO₂ is a traffic-related air pollutant that is strongly associated with cardiovascular and respiratory diseases. Ground NO₂ monitoring stations measure NO₂ concentrations at certain locations and statistical predictive methods have been developed to predict NO₂ as a continuous surface to inform decision-making. Among them, machine learning methods are the most powerful in capturing non-linear relationships between NO₂ measurements and geospatial predictors, but it is unclear if the spatial structure of NO₂ is also captured in the response-covariates relationships. In addition, most model comparison studies only compare accuracy in the prediction mean at ground stations, but do not consider prediction intervals and model interpretation and the effects of different model evaluation methods. In this study, we dive into the comparison between spatial and non-spatial data models accounting for the above-mentioned aspects. Moreover, we implemented a spatial and a non-spatial methods that have not been applied to air pollution mapping before and evaluated stack learning methods with and without modelling the spatial process. We implemented our study using national ground station measurements of NO₂ in Germany and Netherlands of the year 2017, predicting NO₂ to 100 m resolution grid. Our results indicate the importance of modelling the spatial process especially in areas close to traffic. The prediction intervals predicted with ensemble tree-based methods are satisfactory but too narrow with the geostatistical methods. Compared to ensemble tree-based methods, the geostatistical methods provide important spatial information for analysing emission sources and the spatial process of observations.

Keywords: geostatistics; machine learning; spatial prediction; model comparison; prediction interval; model interpretation

30 1 Introduction

31 NO_2 is a traffic-related air pollutant and has been found in epidemiological time series analysis
32 to highly associated with respiratory (Luo et al., 2016) and cardiovascular (Chiusolo et al., 2011)
33 diseases. NO_2 values are measured using monitoring stations at certain locations (e.g. close to traffic)
34 and most of the epidemiological studies identified the relationships between NO_2 and diseases or
35 hospital admission using a single NO_2 monitoring station to represent the entire district. However,
36 NO_2 is highly dynamic over the district and the difference in NO_2 concentrations will reflect on
37 personal exposures to NO_2 . Detailed spatial mapping of NO_2 is therefore required for more accurate
38 quantification of the relationships between NO_2 and health effects. In addition, detailed NO_2 maps
39 are necessary for scientific recommendations to be provided to policymakers and city planners.

40 Statistical methods for NO_2 mapping have attracted a lot of attention with the burgeoning Ma-
41 chine Learning (ML)¹ methods and availability of ground monitoring station networks, atmospheric
42 satellite products, and geospatial predictors. Geospatial predictors are variables that are included
43 as covariates in a statistical air pollution model. Commonly used geospatial predictors are air
44 emission- (e.g. road networks) and dispersion-related (e.g. wind speed) variables, numerical mod-
45 elling (e.g. with chemistry transport model) output, and atmospheric remote sensing measurements
46 or products. A most recent (data available from Jan-2018) atmosphere sensing instrument, Tropomi

¹list of abbreviations: CRPS: Continuous Ranked Probability Score; CV: Cross Validation; DF: Distributional Forest; GRF: Gaussian Random Field; GMRF: Gaussian Markov Random Field; GAMLS: Generalised Additive Models for Location Scale and Shape; INLA: Integrated Nested Laplace Approximation; IQR: Interquartile range; GWR: Geographic Weighted Regression; KED: Kriging with external drift; LUR: Land Use Regression; MAE: Mean Absolute Error; ML: Machine Learning; RF: Random Forest; OMI: Ozone Monitoring Instrument; Quantile Random Forest; RMSE: Root Mean Squared Error; SE: stacked ensemble; SPDE: Stochastic Partial Differential Equations; Tropomi: Tropospheric monitoring instrument; UK: Universal Kriging (UK); OMI (Ozone Monitoring Instrument) VIIRS: Visible Infrared Imaging Radiometer Suite; XGB: XGBoost

⁴⁷ (Tropospheric monitoring instrument, NSO and ESA, 2019) onboard of Sentinel 5p satellite, mea-
⁴⁸ sures column density of a variety of gaseous air pollutants, in particular with an unprecedentedly
⁴⁹ high resolution for NO₂ (3.5 km x 5.5 km, across along track, since 06 August 2019).

⁵⁰ Statistical methods applied for spatial air pollution prediction can be broadly classified depending
⁵¹ on whether the spatial dependency is explicitly modelled. If not modelled, we refer to the methods
⁵² "non-spatial" and otherwise "spatial". Most of the spatial air pollution models were developed to
⁵³ predict at coarser resolutions, commonly 1 km or coarser (Young et al., 2016; Shaddick et al., 2018;
⁵⁴ Beloconi and Vounatsou, 2020). Non-spatial methods are more dominant in air pollution mapping,
⁵⁵ particularly in high-resolution (100 m resolution or higher) mapping. Among them, LUR (Land
⁵⁶ Use Regression) models which assumes linear relationships between NO₂ and geospatial predictors
⁵⁷ are the most studied (Briggs et al., 2000; Hoek et al., 2008). Most recently, statistical learning (in
⁵⁸ this study, "statistical learning" is used interchangeably with "machine learning") methods (Hastie
⁵⁹ et al., 2009), including regularised linear regression (e.g. Lasso and Ridge regression (James et al.,
⁶⁰ 2013)), kernel methods such as support vector machine (Suykens and Vandewalle, 1999), ensemble
⁶¹ tree-based methods such as random forest (RF, Breiman, 2001) and XGBoost (XGB, Chen and
⁶² Guestrin, 2016), have been applied for feature selection or capturing non-linear response-covariate
⁶³ relationships (Lu et al., 2020a; Chen et al., 2019a). In air pollution (not restricted to NO₂) mapping,
⁶⁴ several studies compared between statistical learning and conventional LUR methods (Chen et al.,
⁶⁵ 2019a; Kerckhoffs et al., 2019; Lu et al., 2020a; Ren et al., 2020; Rybarczyk and Zalakeviciute, 2018).

⁶⁶ Geostatistical models (e.g. Kriging) and Geographically Weighted Regression (GWR) are the
⁶⁷ most used spatial methods for air pollution prediction (Vicedo-Cabrera et al., 2013; Li et al., 2014;
⁶⁸ Wang et al., 2021; Zou et al., 2016) and these methods have been combined with dimension reduction
⁶⁹ Zhai et al. (2018) and RF (Zhan et al., 2018; Liu et al., 2020) to improve NO₂ prediction accuracy.
⁷⁰ A Bayesian geostatistical model is developed in Beloconi and Vounatsou (2020) to predict NO₂ by

71 integrating Tropomi satellite instrument measurements and chemical transport models. A GWR
72 model naturally models spatial varying coefficients by fitting multiple local regressions depending
73 on the homogeneity in response-covariate relationships when a number of observations are involved.
74 A typical geostatistical model can be viewed as consisting of two components: a mean function,
75 commonly a linear model, capturing the response-covariate relationships and a covariance function
76 modelling dependency of residuals from the mean (Bhatt et al., 2017). Conventional Kriging methods
77 suffer from the "big n problem", i.e. it may become computationally intractable with a large number
78 of observations. To deal with this problem, Lindgren et al. (2011) propose to use Stochastic Partial
79 Differential Equations (SPDE) to approximate the Gaussian Random Field (GRF) to a Gaussian
80 Markov Random Field (GMRF, Rue and Held (2005)). The main advantage of this is that the GMRF
81 has a sparse structure of the precision matrix, which is the inverse of the covariance matrix of a
82 GRF. Along with this, Rue et al. (2009) propose to use the Integrated Nested Laplace Approximation
83 (INLA) in a Bayesian framework to achieve the computational scalability of a geostatistical model
84 using approximations for all the estimations. This is especially advantageous when modelling NO₂
85 over a larger scale e.g., continental or global-scale modelling when a large amount of observations
86 are modelled, and in spatiotemporal modelling.

87 As spatial models are typically more complex compared to their non-spatial counterparts, several
88 studies compared spatial and non-spatial models to understand if the spatial effects could be simply
89 modelled by including certain covariates in LUR models. Young et al. (2016) studied the use of
90 universal Kriging (UK), OMI (Ozone Monitoring Instrument) satellite instrument (Earthdata) and
91 LUR models for NO₂ prediction at 2.5 km resolution. Young et al. (2016) indicated that either
92 using UK or adding OMI in the LUR model improves a LUR model but adding OMI in a UK
93 model only trivially improves the performance. Bertazzon et al. (2015) shows that the inclusion of
94 the meteorological variables accounts for spatial effects similarly to the use of spatial autoregressive

models(Anselin et al., 2001). However, even if the spatial dependency can be captured by involving certain covariates in a LUR model, we may still need geostatistical methods to understand the spatial structure present in the data. Linear models have been used for the mean function but the relationships between NO₂ and predictors have been shown to be better modelled with non-linear ML methods (Lu et al., 2020a). Most recent studies attempt to replace the linear mean function with ML models. Liu et al. (2020) applied a geostatistical model to the residuals from an RF model for the spatial prediction of PM_{2.5}. In disease mapping, Bhatt et al. (2017) proposes to stack ML models to replace the mean function in a geostatistical model.

Few studies have compared between geostatistical and ML methods, possibly because the ML methods are still relatively less studied in air pollution mapping and in the field of geostatistics. It might be more interesting to compare between geostatistical methods and ML methods than geostatistical methods and LUR, because ML methods may be more capable of (implicitly) capturing the spatial dependency by integrating covariates, when the number of observations is sufficient. Moreover, most comparison studies only compare the cross-validation accuracy of the prediction mean (e.g. using R-squared, mean absolute error, or root mean squared error), ignoring the prediction intervals. Also not discussed is the cause of the prediction errors, are they caused by missing covariants, violation of the model assumptions (e.g. data distribution, non-linearity), or inconsistent distributions between training and validation sets. Also, different cross-validation strategies, e.g., how do we split the train-test sets, may lead to different model validation results. Current studies typically solely rely on k-fold splitting (Kerckhoff et al., 2019; Larkin et al., 2017; Ren et al., 2020) or bootstrapping (Lu et al., 2020a) to randomly splitting between train-test sets, which may be one-sided and does not provide an indication of accuracy in spatial blocks (but only at the locations of ground stations).

In this study, we focus on ensemble tree-based methods (e.g. RF and boosting) in the ML

category and a hierarchical spatial model (Lindgren et al., 2015; Blangiardo and Cameletti, 2015; Moraga, 2019) called latent Gaussian model in the geostatistics category. Additionally, we invest in stacked models in integrating ML and geostatistical models and develop a LUR model using Lasso for comparison. Ensemble trees are nonparametric models, deriving prediction intervals is therefore less straightforward than a parametric model (e.g. a linear regression model) but has been studied and shown satisfactory results with simulated data. Prediction intervals have been most well studied for RF (Meinshausen, 2006; Wager et al., 2014; Stasinopoulos et al., 2007; Alakus et al., 2021) and more recently for boosting (Duan et al., 2020; Velthoen et al., 2021). Comparing probabilistic methods (i.e. prediction interval calculation) of RF and boosting is beyond the scope of this study and we focus on prediction intervals derived for RF to compare with geostatistical methods. Possibly, one of the most widely recognisable methods to derive RF prediction intervals is Quantile Random Forest (QRF) (Meinshausen, 2006). QRF has been shown to estimate middle quantiles well but may fall short at the extremes due to the limited number of observations in the tail regions (Velthoen et al., 2021). Velthoen et al. (2021) proposed to use extreme quantile regression to estimate for data outside the range of observations. Another well-recognised method is distributional regression forests (DF) (Schlosser et al., 2019), which embeds the GAMLSS (Generalised Additive Models for Location Scale and Shape) (Stasinopoulos et al., 2007) into RF.

Fouedjio and Klump (2019) compared prediction accuracy and uncertainty quantification between KED (Kriging with external drift) and QRF by simulating data with various levels of spatial dependency. It concluded that an optimal model choice depends on the level of spatial dependency and response-covariate relationships. However, it does not account for the fact that in practice, as an ensemble tree-based method can make use of a large number of (possibly correlated) predictors without being constrained to certain (e.g. linear) relationships, the spatial dependency may be explained by the covariates despite not being explicitly modelled.

¹⁴³ The objective of our study is to compare geostatistics and non-spatial ensemble tree-based models
¹⁴⁴ for NO₂ mapping, in terms of their prediction accuracy, uncertainty quantification, and model inter-
¹⁴⁵ pretation and to understand effect of modelling spatial structures. More specifically, the following
¹⁴⁶ sub-objectives are reached:

- ¹⁴⁷ 1. Optimising a set of spatial hierarchical and ML models for NO₂ prediction in Germany and
¹⁴⁸ the Netherlands.
- ¹⁴⁹ 2. Developing a non-spatial and a geostatistical stacked ensemble model, i.e., a stack of various
¹⁵⁰ ML learners.
- ¹⁵¹ 3. Model comparison regarding the predicted mean, prediction interval, and model interpretation.

¹⁵² The spatial Hierarchical model incorporates the spatial random effect along with other covariates
¹⁵³ and the estimation is performed using the R package **INLA** (Rue et al., 2009; Martins et al., 2013).
¹⁵⁴ XGB, RF and Lasso are chosen for the comparison with the geostatistical model and they also
¹⁵⁵ form the base learners in the two (geostatistical and non-spatial) stacked learning models. The ML
¹⁵⁶ methods are chosen for their dissimilarity. Specifically, Lasso is a linear regression model without
¹⁵⁷ accounting for spatial dependency. RF and XGB are non-linear models with regression trees as base-
¹⁵⁸ learners and are not affected by dependent covariates. XGB is a highly scalable boosting method
¹⁵⁹ that builds tree models subsequently over the residuals of previous trees and has multiple routines
¹⁶⁰ to penalise model over-fitting (Chen et al., 2019b), which has been reported in various studies to
¹⁶¹ obtain the highest prediction accuracy Lu et al. (2020a).

¹⁶² 2 Data

¹⁶³ NO₂ concentration measurements of 2017 from national ground stations of Germany and the Nether-
¹⁶⁴ lands are used. The original hourly data is downloaded from the EEA (European Environment

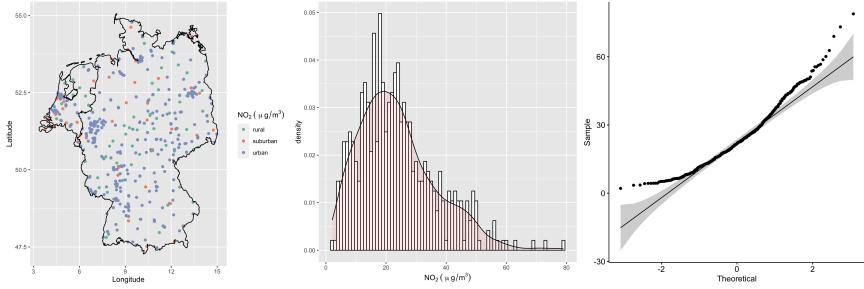


Figure 1: Spatial distribution of NO₂ stations, histogram and Q-Q plot of the NO₂ measurements.

Agency, Nelson, 1999; EEA, 2021). Negative values are considered as missing. The data is aggregated to annual concentrations by taking the mean and omitting missing values. The spatial distribution of NO₂ stations and the station types, histogram and Q-Q plot for normality are shown in fig. 1. We conducted a Shapiro test for normality, with the result implying the distribution of data being significant different from normal distribution ($p\text{-value} = 8.605e-12$, "normal distribution" and "Gaussian distribution" are used interchangeably in this study). A Gamma distribution test was conducted using the method proposed in Villaseñor and González-Estrada (2015) and implemented in Gonzalez-Estrada and Villasenor-Alva (2020). The test result ($p\text{-value} = 0.32$) indicates that the data distribution is not significantly different from Gamma distribution.

The geospatial predictor grids (table 1) are calculated or re-sampled at 100 m resolution. They are either spatial attributes aggregated in a circular ring centred at each sensor or prediction location, called buffered predictors, or values of the spatial attribute at the observation or prediction location, called gridded variables. The buffered predictors include total road length, total industry areas, VIIRS (Visible Infrared Imaging Radiometer Suite) Nighttime Day/Night Band radiances values (nightlight, NOAA, 2021) and population. Variables that are originally grids include wind speed and temperature (Dee et al., 2011), elevation (NASA), annual mean Tropomi level 3 product of NO₂ column density (Copernicus, 2021) from 2019 (due to the increased resolution compared to 2018).

182 The buffered predictors of road and industry are calculated from OpenStreetMap (OpenStreetMap
183 contributors, 2019). For detailed descriptions of the processing of the geospatial predictors please
184 refer to Lu et al. (2020a).

185 **3 Methods**

186 The methods considered in this study are classified as spatial and non-spatial and are given the
187 names below in this study.

188 **Spatial models:**

- 189 1. INLA: A spatial hierarchical model fit using INLA with a Gaussian likelihood.
- 190 2. INLA-G: A spatial hierarchical model fit using INLA with a Gamma likelihood.
- 191 3. SE-INLA: using the spatial hierarchical model to stacked learning with Lasso, RF and XGB
192 models as base learners;

193 **Non-spatial models:**

- 194 1. LA: A Lasso regression model;
- 195 2. RF: A RF model;
- 196 3. XGB: An XGB model assuming a Gaussian objective function;
- 197 4. XGB-G: An XGB model assuming a Gamma objective function;
- 198 5. QRFLA: using Lasso to aggregate QRF trees (Hastie et al., 2009);
- 199 6. SE: stacked learning with Lasso, RF and XGB models as base learners;
- 200 7. QRF: quantile regression forest (Meinshausen, 2006);
- 201 8. DF: distributional regression forest (Schlosser et al., 2019).

Table 1: Geospatial predictors considered in this study. ”_mon” indicates months (mon = 1, 2....,12). ”_buf” indicates buffer radius in meters. The road length and industrial areas are calculated with buffer radii of 100 m, 300 m, 500 m, 800 m, 1000 m, 3000 m and 5000 m. The night lights digital numbers are calculated with buffer radii of 450 m, 900 m, 3150 m and 4950 m. The original resolution is provided for gridded variables and data types for vector variables.

Predictor	Variable name	Unit	Resolution/data type
Monthly wind speed at 10 m altitude.	Wind_speed_10m_mon	km/hr	10 km
Monthly temperature at 2 m altitude.	temperature_2m_mon	Celsius	10 km
TROPOMI 2018 mean vertical column density.	trop_mean_filt; Tropomi	mol/cm^2	0.01 arc degrees
Population in 5 km grid	population_5000	count	5 km
Population in 3 km grid	population_3000	count	3 km
Population in 1 km grid	population_1000	count	1 km
Nightlight	nightlight_bufnl	$Wcm^{-2}sr^{-1}$	500 m
Total length of highway	road_1_buf	m	polygon, lineString
Total length of primary roads	road_2_buf	m	polygon, lineString
Total length of local roads	road_M345_buf	m	polygon, lineString
Area of industry	I_1_buf	m^2	polygon, lineString

202 **3.1 Non-spatial methods**

203 Lasso is a linear regression algorithm with the L1 regularisation to shrink variable coefficients to
204 zero, which enables "feature selection". In the cost function, the absolute value of coefficient is added
205 to the original least squares as a penalty term. RF and XGB in this study use trees as base learners
206 and ensemble them to reduce variability of single trees (Friedman, 2001). RF firstly randomly draws
207 a subset of features, and then choose features from this subset to build the tree. RF (Breiman, 2001)
208 grows trees independently and then take the mean of the predictions of each tree.

209 QRF is a non-parametric prediction interval estimation method which keeps all the observations
210 in the terminal node for estimating the conditional probability function. Specifically, it samples
211 from all the response values in each terminal node and use the ratio between the number of samples
212 that is taken from each terminal node and the number of total observations in the terminal node as
213 weights to aggregate the samples. The weights of all the trees are summed. The summed weights
214 computed for each observation are then used to construct the empirical conditional cumulative
215 distribution function (Meinshausen, 2006). QRFLA uses Lasso as a post-processing of QRF (Hastie
216 et al., 2017, page 617). This method firstly preserves all the trees instead of aggregating them
217 (e.g. taking the mean of all the predictions) and then apply Lasso regression to all the trees for
218 aggregation. This leads to a shrinkage of the tree space and theoretically reduces model variance.
219 DF (Schlosser et al., 2019) firstly divide data into regions as homogeneous as possible with respect
220 to a parametric distribution, thus capturing changes in location, scale and shapes. For each tree,
221 maximum likelihood is used to fit distributions and recursively select and split covariates according
222 to the instability of the gradient of the likelihood at each observation along each co-variate. Then,
223 the distributional trees are ensembled for DF.

224 XGB is a variation of gradient boosting, which grows trees subsequently by fitting to model
225 residuals of the previous step. XGB is scalable to multiple threads. It enables multiple penalisation

226 paths to control model complexity to prevent model over-fitting, including regularisation (e.g. L1
227 regularisation) on tree width and terminal node values, as well as drop-out (dropping trees), sampling
228 observations (take a subset of observations in each run), and early stopping (stop iterating when after
229 a few rounds the loss does not decrease or the node does not meet the splitting rule). The default
230 objective function for regression assumes normal distribution of target variables (and the prediction
231 is the mean of the distribution). This assumption is used in all the air pollution mapping studies.
232 Here, we additionally fit a model with the objective function assuming the target variable follows a
233 Gamma distribution (XGB-G) as the distribution of NO₂ measurements is closer to Gamma than
234 normal distribution.

235 Different from the ensembling in RF or XGB,SE (Stacking Ensemble) refers to a class of al-
236 gorithms that trains a second-level “meta-learner” to optimise the combination of a collection of
237 prediction algorithms (base-learners). The base-learners are preferably diverse to capture different
238 relationships or patterns. In this study, Lasso, RF, and XGB are the base-learners. Cross-validated
239 predicted values (commonly known as level-one data) are used to train the meta-learner.

240 **3.2 Hyperparameter setting for XGB and RF**

241 To optimise the hyperparameters of XGB (known as ”model tuning”), we used grid search to optimise
242 hyperparameters in 5-fold cross-validation basing on the minimum RMSE (Root Mean Squared
243 Error) and additionally manual adjustment of the hyperparameters to look at the prediction patterns.
244 The grid search is used instead of more computationally efficient methods (e.g. Bayesian or random
245 search) as the optimal hyperparameter range is largely known from our previous experiences (Lu
246 et al., 2020a, 2021). The search grid for the number of iterations (nrounds) was from 200 to 3000,
247 with a step of 200; maximum tree depth (max-depth) from 3 to 6 with a step of 1, learning rate
248 (eta) from 0.001 to 0.1 with a step of 0.05, the penalty term Gamma (Chen et al., 2019b) from 1

249 to 5 with a step of 1, the subsample is set to 0.7, L1 norm penalisation (lambda) is set to 2 and L2
 250 norm penalisation (alpha) is set to 0. RF is not sensitive to hyperparameter tuning. We used the
 251 default setting of number of variables that are randomly drawn for each tree (Breiman, 2001), which
 252 is the integer part of the total number of variables divided by three. The number of trees is set to
 253 2000 for a safe choice as the high number of trees will not negatively affect model performance.

254 3.3 Geostatistical models

255 Suppose we assume that NO_2 values y_i measured at locations \mathbf{s}_i , $i = 1, \dots, n$, follows a Gaussian
 256 distribution with mean μ_i and variance σ^2 , where the mean μ_i is expressed as a sum of covariates
 257 and a spatially structured random effect following a zero-mean Gaussian process with a spatial
 258 covariance function (Moraga, 2019).

$$y_i \sim N(\mu_i, \sigma^2), \quad i = 1, 2, \dots, n \quad (1)$$

$$\mu_i = \mathbf{d}_i \boldsymbol{\beta} + \mathbf{x}(\mathbf{s}_i) \quad (2)$$

259 Here, $\mathbf{d}_i = (d_{i1}, \dots, d_{ip})$ is the vector of covariates at location \mathbf{s}_i , $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)'$ is the
 260 coefficient vector, and $\mathbf{x}(\mathbf{s}_i)$ denotes a spatial Gaussian random field. That is, $\{\mathbf{x}(\mathbf{s}_1), \dots, \mathbf{x}(\mathbf{s}_n)\} \sim$
 261 $\mathcal{N}_n(\mathbf{0}, \boldsymbol{\Sigma})$, where N_n is a Normal multivariate distribution for the spatial process specified by its
 262 mean $\mathbb{E}(\mathbf{x}(\mathbf{s}))$, and covariance function $C(\mathbf{s}_1, \mathbf{s}_2) = \text{Cov}(\mathbf{x}(\mathbf{s}_1), \mathbf{x}(\mathbf{s}_2))$. The Gaussian random field
 263 can be stationary and isotropic, where the covariance function depends only on the distance and not
 264 direction between points, that is $C(\mathbf{s}_1, \mathbf{s}_2) = \text{Cov}(\|\mathbf{s}_1 - \mathbf{s}_2\|)$ and its dependence is commonly modeled
 265 using a Matérn function (Stein (2012); Yuan (2011); Diggle et al. (2013)). Since incorporating the
 266 spatial dependence directly with a large number of observations using a Gaussian random field is
 267 computationally expensive, Rue and Held (2005) proposed the approximation of a Gaussian random
 268 field by a Gaussian Markov random field for a more efficient computational process of estimation.

269 The main property of the Gaussian Markov random field is that it uses a conditional dependency
270 structure through the precision matrix \mathbf{Q} .

271 In this study, we compare two spatial hierarchical models with geospatial predictors as covariates,
272 one uses a Gaussian likelihood and the other a Gamma likelihood. The Gamma model has the same
273 hierarchical structure as the Gaussian model: the response variable in (1) can be represented by
274 $y_i \sim \text{Gamma}(\alpha, \beta)$ where α is the shape parameter and β the rate parameter. The INLA-SE model
275 uses a Gaussian likelihood.

276 **3.4 INLA and SPDE**

277 To fit the geostatistical models, we use the R package **INLA** which facilitates the application of the
278 INLA and the SPDE approaches. Following the expression proposed in (1), the structure for the
279 hierarchical model is:

$$\mathbf{y} | \mathbf{x}, \theta_1 \sim N(\mathbf{D}\boldsymbol{\beta} + \mathbf{A}\mathbf{x}, \theta_1) \quad (3)$$

$$\mathbf{x} | \theta_2 \sim \text{GRF}(\mathbf{0}, \mathbf{Q}(\theta_2)^{-1}) \quad (4)$$

$$\boldsymbol{\theta} = \{\theta_1, \theta_2\} \quad (5)$$

280 where $\boldsymbol{\theta}$ is the vector of hyperparameters with $\theta_1 = \sigma^2$, $\theta_2 = \{\log(\tau), \log(\kappa)\}$, \mathbf{x} is the spatial
281 latent field, \mathbf{A} is the projector matrix and \mathbf{y} is the vector of the response variable $f(\cdot | \mathbf{x}, \boldsymbol{\theta})$,
282 commonly from the exponential family of distributions. \mathbf{D} is a covariate matrix and $\boldsymbol{\beta}$ a coefficient
283 matrix.

284 The R package **INLA** can be used to perform direct numerical calculation of the posterior distri-
285 bution for a Bayesian hierarchical model (Rue et al. (2009), Martino and Rue (2009)). If we use \mathbf{x}
286 as a latent Gaussian field (a Gaussian Markov random field), $\boldsymbol{\theta}$ a vector of (hyper)parameters and

²⁸⁷ \mathbf{y} a vector of observations, assuming independent observations given the vector of the spatial latent
²⁸⁸ field (\mathbf{x}) and the hyperparameters ($\boldsymbol{\theta}$), the likelihood can be expressed as:

$$p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}) = \prod_{i \in \mathcal{I}} p(y_i \mid \eta_i, \boldsymbol{\theta}), \quad (6)$$

²⁸⁹ where η_i is the linear predictor and \mathcal{I} contains the indices of the observed values \mathbf{y} .

²⁹⁰

²⁹¹ The main aim is to approximate the posterior density for the posterior of the spatial latent field
²⁹² and the hyperparameters. The marginal densities can be obtained:

$$p(x_i \mid \mathbf{y}) = \int p(x_i \mid \boldsymbol{\theta}, \mathbf{y}) p(\boldsymbol{\theta} \mid \mathbf{y}) d\boldsymbol{\theta}, \quad (7)$$

²⁹³ and

$$p(\boldsymbol{\theta}_j \mid \mathbf{y}) = \int p(\boldsymbol{\theta} \mid \mathbf{y}) d\boldsymbol{\theta}_{-j}. \quad (8)$$

²⁹⁴ respectively (Lindgren et al. (2015); Krainski et al. (2018)).

²⁹⁵

²⁹⁶ To model data indexed in space, Lindgren et al. (2011) proposed a new methodology based mainly
²⁹⁷ on the approximation of the Gaussian random field with the Matérn function using the Stochastic
²⁹⁸ Partial Differential Equations (SPDE) as follows:

$$(\kappa^2 - \Delta)^{\alpha/2}(\tau(\mathbf{s})x(\mathbf{s})) = \mathbf{W}(\mathbf{s}), \quad (9)$$

²⁹⁹ where κ is a scale parameter, $x(\mathbf{s})$ is a spatial random field, Δ is the Laplacian, α is the parameter
³⁰⁰ that controls the smoothness of the realizations, τ controls the variance and $\mathbf{W}(\mathbf{s})$ is a Gaussian
³⁰¹ spatial white noise process (Lindgren et al. (2015)). For the above we can use a Gaussian Markov
³⁰² random field that approximates to a Gaussian random field using a triangulation of the region of

303 study without specifying an explicit covariance structure through the SPDE method. This approx-
304 imation leads to a decrease in computational burden from $\mathcal{O}(n^3)$ to $\mathcal{O}(n^{3/2})$.

305 3.5 Geospatial predictor selection for the INLA model

306 As involving too many covariates (e.g. more than 12) in the INLA model brings problems in model
307 inferencing and multicollinearity, we used Lasso to reduce the number of variables. The Lasso was
308 used instead of ensemble tree-based methods for feature selection because it is also a linear model
309 (same as the INLA and INLA-G models in our study). Variables are selected with the L1 norm
310 penalty that returns a model with errors that are within one standard error of the minimum mean
311 cross-validated error. Lasso is applied to 80% data randomly sampled from all the observations
312 and this process is repeated 20 times. Variables that are selected more than 90% of the times (i.e.
313 18) will be considered as covariates in INLA. The times that the Lasso selected certain variables is
314 shown in table 2. The INLA modelling process applies the same bootstrapped samples for training
315 and validation. In addition, AIC (step-wise) model selection is applied to the entire dataset to
316 suggest a model as a further reference. The variables selected by AIC are almost the same as
317 Lasso selected variables, besides it does not choose road_class_3_3000, which is highly correlated
318 with road_class_1_5000. Based on this, the road_class_3_3000 is not used as a covariate in INLA.

319 3.6 INLA model parameterisation

320 The triangulated mesh constructed in the SPDE approach is shown in supplementary material
321 (supfig. 1), with size of the inner and outer extensions around the data locations (*offsets*) 1/8 of
322 the maximum distance among all the observations for both the inner and outer extensions. The
323 maximum allowed triangle edge lengths in the region and in the extension (*max.edge*) are set
324 to respectively 1/30 and 1/5 times maximum distance among all the observations. The Matern

Table 2: Frequency (number of times) of variables selected by Lasso in 20 times bootstrapping and variables that are selected more than 90% times (i.e. 18) are listed below. These variables are considered in INLA besides road_class_3_3000.

	Variables	Frequency
1	nightlight_450	20
2	population_1000	20
3	population_3000	20
4	road_class_1_5000	20
5	road_class_2_100	20
6	road_class_3_300	20
7	trop_mean_filt	20
8	road_class_3_3000	19
9	road_class_1_100	18

325 SPDE model is constructed with $\alpha = 2$. The SE-INLA model has the same specification (i.e.
326 mesh structure, likelihood, objective function, priors, optimisation process) as the INLA model
327 parameterisation described above.

328 4 Model evaluation

329 4.1 Cross validation

330 We use RMSE, MAE (Mean Absolute Error), IQR (Interquartile Range) and R^2 (R-squared) to
331 compare model performance. RMSE is calculated as the square root of the differences between
332 predictions and observations; MAE is calculated as the absolute differences between predictions
333 and observations; IQR is the differences between the third and first quartiles of the prediction. R^2
334 indicates the explained variance and is calculated as $R^2 = 1 - \text{var}(\text{error})/\text{var}(y)$, where $\text{var}(\cdot)$
335 indicates variance, error indicates model residuals and y indicates observed response values. When
336 different data is used in CV (e.g. separating between close and far-away from roads), we additionally
337 calculated the RRMSE (relative RMSE), RMAE (relative MAE), RIQR (relative IQR) to account
338 for the differences in the magnitudes of response values. The RRMSE and RMAE are calculated by
339 dividing the RMSE and MAE, respectively, by the mean of observations. The RIQR was calculated
340 by dividing the IQR by the median of observations. The three CV methods we designed and used
341 to assess our model performance are:

- 342 1. Bootstrapped CV. 20-times randomly bootstrapped splitting of training and test sets (Lu et al.,
343 2020a).
- 344 2. Spatial-blocked CV. Dividing data into spatial blocks, each time use one block for test and
345 other blocks for training.

346 3. Customised CV. Splitting train-test based on values of certain covariates. In this study, three
347 sub-areas are defined, 1) close to traffic and with high population ("tr-hp"), 2) close to traffic
348 and with middle low population ("tr-lmp"), 3) far away from traffic ("far"). High population is
349 defined as the variable population of 1000 m buffer that is in the last quartile. Low population
350 is defined as the variable population of 1000 m buffer is below the median. Close to road is
351 defined as (please refer to table 1 for the definition of covariates):

```
352       road_class_2_100 > 0 |  
353       road_class_1_100 > 0 |  
354       road_class_3_100 > quantile(road_class_3_100, .75))
```

355 Far away from road is defined as:

```
356       road_class_2_100 == 0 &  
357       road_class_1_100 == 0 &  
358       road_class_3_100 < quantile(road\class\_3\_100, .5)
```

359 where "&" indicates "and" and "|" indicates "or". The second variable of the function
360 "quantile(.)" indicates the percentage quantile of the variables.

361 This yields 85, 65, and 177 samples in each category. This ensures a balanced number of samples
362 between close to traffic and far-away from traffic. Each time, 30 samples (7% of the entire dataset)
363 are drawn from the corresponding category for CV. For example, each time, 30 samples are drawn
364 from the 85 samples as the test set to obtain the prediction accuracy CV for the situation "tr-hp"
365 and the rest is used for training.

366 **4.2 Prediction intervals**

367 CRPS (Continuous Ranked Probability Score) and coverage probabilities are used as quality indica-
368 tors of prediction intervals. CRPS is an uncertainty measure that assesses the similarities between

369 two distributions. We use it to indicate how the predicted distribution matches the observed dis-
370 tribution. The CRPS implemented as an R package **ScoringRules** (Jordan et al., 2017) is used.
371 CRPS is calculated for the INLA and QRF models. For the INLA model, the prediction intervals
372 are calculated by simulating from the response $Y \sim N(\theta, \sigma^2)$ where θ and σ^2 are the fitted mean and
373 variance. The mean of CRPS for all the points within each test block is calculated in spatial-blocked
374 CV. Coverage probabilities are calculated as the ratio between the number of predictions within
375 the upper and lower quantile and the total number of predictions (in the test set). The prediction
376 intervals are mainly compared between INLA, INLA-G, QRF and DF. The prediction interval for
377 QRFLA is compared with QRF to investigate the effects of Lasso tree-aggregation strategy on the
378 prediction intervals.

379 4.3 Model interpretation

380 We inspect fixed and spatial random effects modelled by INLA and compare the spatial random field
381 with modelled prediction intervals and model residuals to understand the contribution of spatial
382 random effects. Different from linear regression methods, which themselves are the best models for
383 interpretation, interpreting ensembling tree-based methods requires external models (Lundberg and
384 Lee, 2017). We use SHAP (SHapley Additive exPlanations, Lundberg et al., 2018; Lundberg and
385 Lee, 2017), a unified method based on additive feature attribution, to estimate variable influence in
386 RF and XGB models.

387 5 Results

388 5.1 Accuracy assessment and uncertainty quantification

389 Non-spatial CV

390 Both ensemble tree-based methods with a Gaussian objective function and INLA with a Gaussian
391 likelihood function obtain higher prediction accuracy than Lasso (table 3), indicating the necessity of
392 using a more flexible model and modelling spatial random fields. Among individual methods, in terms
393 of R^2 and RMSE, INLA with Gaussian likelihood obtained the highest prediction accuracy, followed
394 by XGB-G and QRFLA. QRFLA greatly improves from original RF. Despite the distribution of
395 response being closer to Gamma distribution compared to Gaussian distribution, using Gamma
396 regression in XGB and specifying Gamma likelihood in INLA both decrease the prediction accuracy
397 considerably. Compared to INLA, XGB obtained lower RMSE and R^2 despite it obtained lower
398 MAE and IQR, indicating that the XGB model predicts less well at more extreme ranges. The
399 QRF and DF results are not shown in table 3 as the results are very similar to RF. Their prediction
400 intervals are compared.

401 SE-INLA improves prediction accuracy compared to SE and INLA, obtained the best results in
402 terms of root mean squared error (6.83, 24.5% of the mean of observations) and R^2 (0.71). This in-
403 dicates the spatial structures could further improve prediction accuracy despite flexible relationships
404 captured from ML models.

405 **Spatial-blocked CV**

406 Spatial-blocked CV provides information about prediction accuracy in spatial blocks. The R^2
407 map (fig. 2) shows that the XGB, RF and INLA predict relatively well in most parts of Germany
408 besides blocks at the boundaries. The R^2 for the block western the Netherlands is also relatively low
409 with all the three methods and especially for XGB (R^2 : 0.2). RF obtains the best result for the block
410 of western the Netherlands (R^2 : 0.5). The INLA model outperforms RF and XGB in the blocks
411 at south-east and north. The R^2 between blocks are the most heterogeneous with XGB, which is
412 consistent to the result of bootstrapped CV that the XGB falls short at predicting extremes.

413 The spatial-blocked CRPS fig. 3 is computed for QRF and INLA (the DF is not shown as it will

Table 3: Prediction accuracy matrix for different models using 20 times bootstrapped cross-validation. Non-spatial models: LA: Lasso; RF: random forest, XGB: XGBoost using the default Gaussian loss; XGB-G: XGBoost using a Gamma loss; QRFLA: quantile random forest with Lasso for shrinkage aggregation of regression trees; SE: stacked ensembling. Spatial models: INLA: a latent Gaussian model implemented using INLA assuming a Gaussian likelihood. INLA-G: a latent Gaussian model implemented using INLA assuming a Gamma likelihood. SE-INLA, geostatistical stacked ensembling.

	LA	RF	XGB	XGB-G	QRFLA	SE	INLA	INLA-G	SE-INLA
RMSE	7.54	7.45	7.14	8.91	7.23	7.18	7.06	9.21	6.83
IQR	8.47	7.39	6.54	9.21	7.27	7.30	7.1	7.4	6.8
MAE	5.69	5.51	5.05	6.27	5.28	5.31	5.3	6.2	5.0
R ²	0.65	0.65	0.68	0.51	0.67	0.69	0.69	0.45	0.71

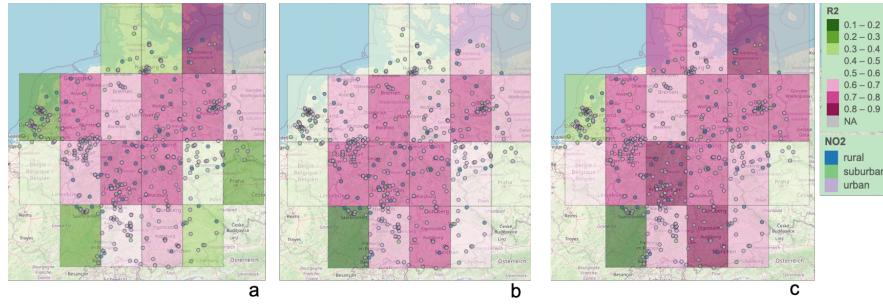


Figure 2: The R-squared of each block, using the rest of the blocks for training. The models are a) XGB, b) QRF, c) INLA.



Figure 3: The CRPS (Continuous Ranked Probability Score) of each block, using the rest of the blocks for training. a) RF, b) INLA.

414 be shown that the QRF and DF performed similarly in prediction interval prediction (section 5.2)).
 415 The INLA predicted prediction distribution deviates considerably from observed distribution for the
 416 block of western the Netherlands, as reflected by the high value of mean CRPS. This is consistent
 417 to the relatively low R^2 observed for the same block. However, some blocks with relatively high R^2
 418 (in the north and south) have high CRPS. This indicates that the prediction mean is well-predicted
 419 but not the prediction interval (too narrow).

420 **Customised CV**

421 There is a distinctive difference between model performance in areas close to traffic (i.e. *tr-hp*
422 and *tr-lmp*) and far away from traffic (i.e. *far*). The INLA model outperformed other non-spatial
423 methods in both *tr-hp* and *tr-lmp*, especially for the latter while the XGB model outperformed the
424 INLA model (and all the other models) in *far*. This indicates the importance of modelling spatial
425 dependency in areas close to traffic and possibly non-linear relationships far-away from roads. All the
426 ensemble tree-based methods obtained much worse results compared to linear regression methods in
427 *tr-lmp*. A linear regression model typically outperforms ensemble tree-based methods when there are
428 relatively few observations for a flexible relationship to be justified. As the number of observations
429 that are close to traffic and far away from traffic is balanced, the results indicate that the population
430 density alters relationships between NO₂ and road density (i.e. the relationships between NO₂ and
431 road density is different with different population density) in areas close to traffic.

432 5.2 Prediction interval

433 The 90% prediction intervals for INLA, INLA-G, DF, QRF and QRFLA are shown in figs. 4 to 6.
434 The RF-based methods, namely DF, QRF and QRFLA reach the coverage probability higher than
435 0.9, but the DF predicts a more realistic prediction quantile, notably, it covers four observations that
436 are not covered by the same prediction quantiles predicted by the QRF. The INLA 90% prediction
437 interval is too narrow. The coverage probability is 0.41 for INLA and 0.36 for INLA-G. The predicted
438 90th quantile of the INLA-G turned to better capture extreme high values but the model also turned
439 to miss more at lower values. The QRFLA predicted a slightly narrower prediction interval compared
440 to QRF. This indicates that Lasso reduced the variance of a QRF model by aggregating trees.

Table 4: Results with customised CV. tr-hp: close to traffic and high population, tr-lmp: close to traffic and middle and low population, far: far away from traffic. RRMSE (relative RMSE), RMAE (relative MAE), RIQR (relative IQR).

	RMSE	RRMSE	IQR	RIQR	MAE	RMAE	R^2
LA_tr-hp	12.4	0.3	17.3	0.4	10.2	0.3	0.11
RF_tr-hp	11.9	0.3	17.8	0.5	9.8	0.3	0.18
XGB_tr-hp	11.6	0.3	15.3	0.4	9.3	0.2	0.21
INLA_tr-hp	11.3	0.3	16.6	0.4	9.5	0.3	0.26
LA_tr-lmp	7.5	0.3	10.4	0.5	6.1	0.3	0.21
RF_tr-lmp	8.2	0.4	10.9	0.5	6.4	0.3	0.05
XGB_tr-lmp	8.2	0.4	10.5	0.5	6.4	0.3	0.04
INLA_tr-lmp	6.7	0.3	8.7	0.4	5.3	0.2	0.36
LA_far	5.0	0.4	4.9	0.4	4.2	0.3	0.47
RF_far	4.9	0.3	4.0	0.3	3.6	0.3	0.47
XGB_far	3.4	0.2	3.6	0.3	2.5	0.2	0.74
INLA_far	4.0	0.3	4.3	0.3	3.2	0.2	0.65

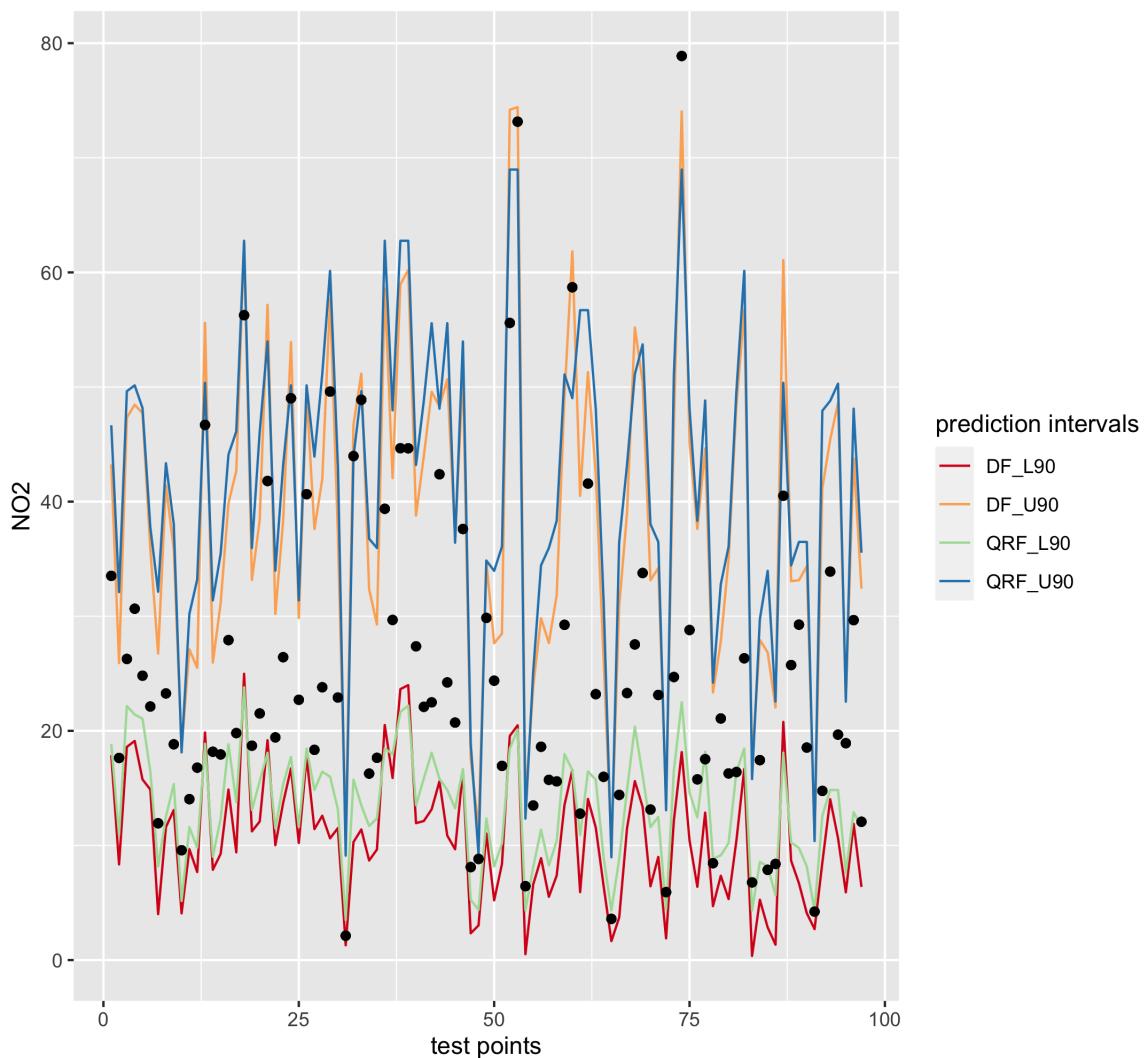


Figure 4: The 90% prediction interval predicted by DF and QRF. The black dots indicate observations in the test dataset.

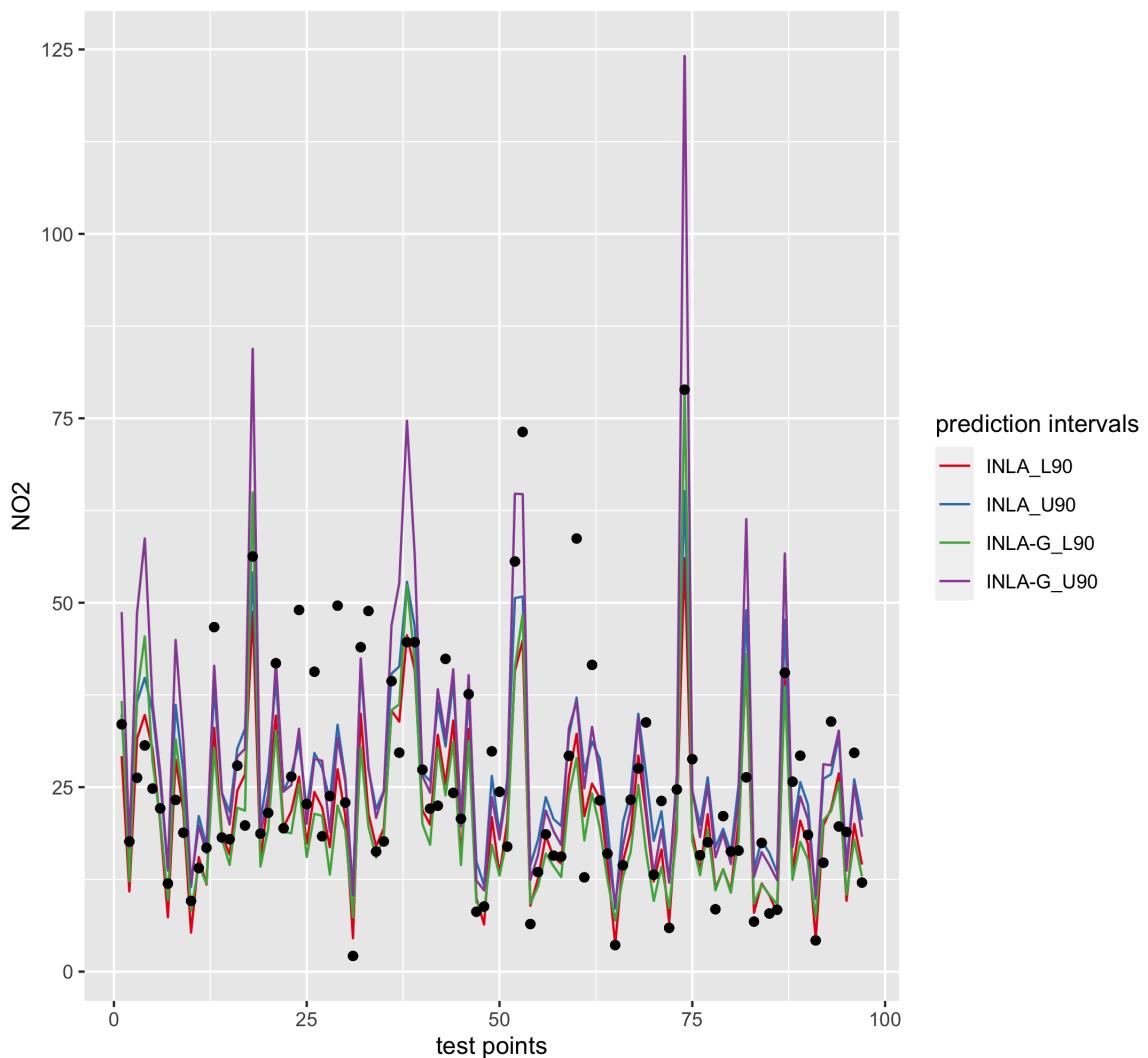


Figure 5: The 90% prediction interval predicted by INLA and INLA-G. The black dots indicate observations in the test dataset.

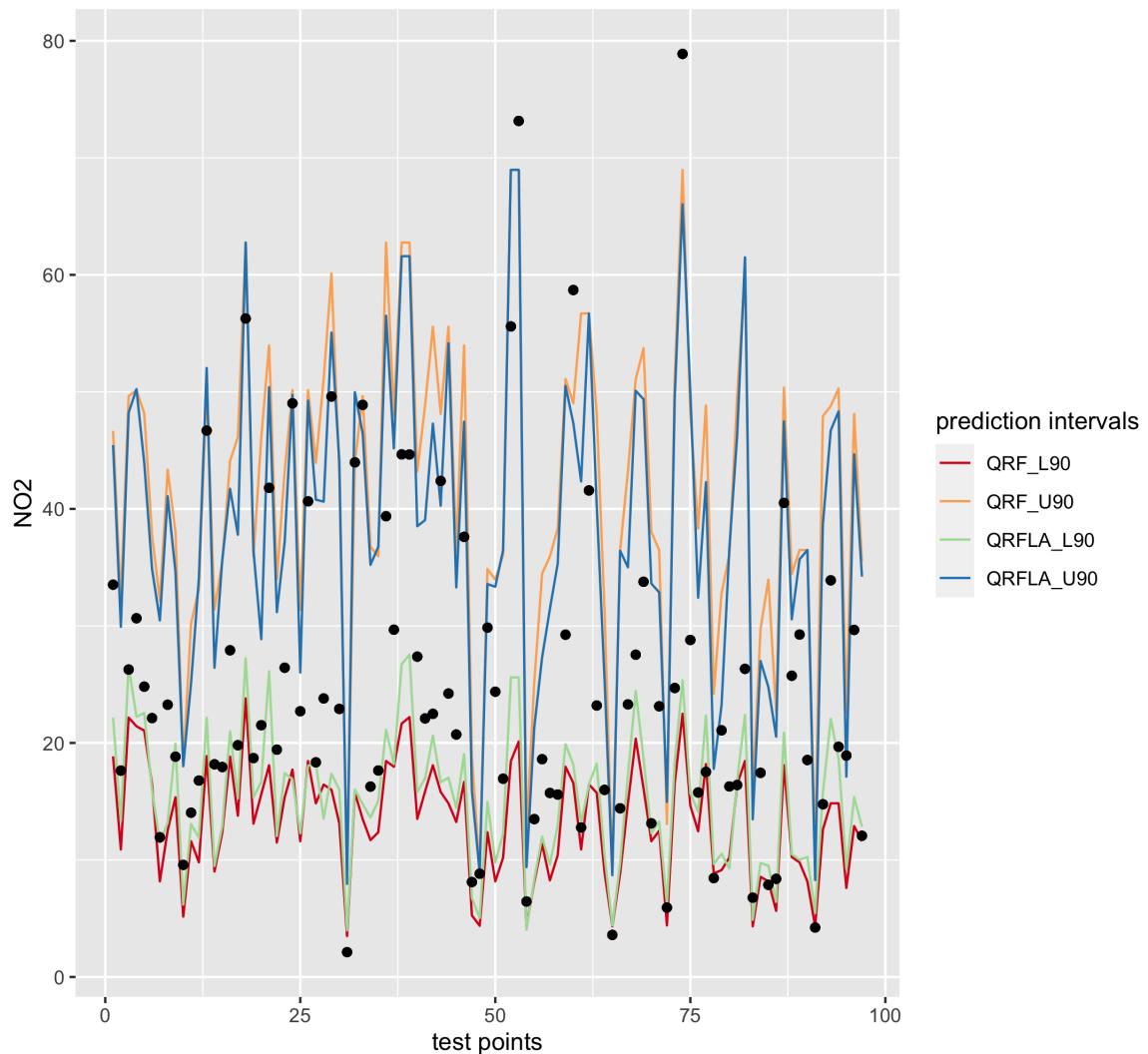


Figure 6: The 90% prediction interval predicted by QRF and QRFLA. The black dots indicate observations in the test dataset.

441 5.3 Model Interpretation

442 SHAP values are calculated for RF and XGB methods using all the data. The variables are ranked by
443 their variable importance, which is calculated as the sum of SHAP magnitudes over all the samples. It
444 can be observed from fig. 7 that the variable rankings and the pattern of variable impacts on model
445 output are similar. Both methods ranked road_class_2_100 at the top. The variable importance
446 calculated by the SHAP indicates a pattern that matches well with our expectation in the emission
447 sources (e.g. high pollution close to primary roads). To illustrate, we observe a positive trend of
448 SHAP values along with road_class_2_100 values, this matches with the explanation that areas with
449 higher primary road density generally experience higher NO₂ concentrations.

450 To analyse the effect of each covariate in the INLA model, we firstly normalised all the covariates
451 (by subtracting the mean and dividing the centred columns by their standard deviations) and used
452 all the data to fit the INLA model. road_class_2_100 has the highest effect (mean = 4.37), follows by
453 the population_3000 (3.08), these are consistent to the XGB variable importance (fig. 7b). Then,
454 the road_class_3_300 (3.00) has a notably higher effect (besides the top 2) than other covariates,
455 which has coefficients from 0.72 to 1.88. This differs from the XGB and RF variable importance
456 which ranked the population_1000 higher above, while in the INLA model the population_1000 has
457 the lowest effect (0.72). This may be because of the high correlation between population_1000 and
458 population_3000, as SHAP is a permutation test, it ignores the dependency between covariates.
459 In general, both geostatistical and ML methods estimated covariate effects match their physical
460 explanations. The statistics (mean, standard deviation, mode) and predicted quantiles of each
461 coefficient are shown in the supplementary material figure 3.

462 The differences between the predicted NO₂ and the mean of the spatial random field fig. 8
463 indicates the effects of covariates. The highest values of the mean of the spatial random field are
464 shown close to the Stuttgart region. Relatively high values can be observed in northern, southern

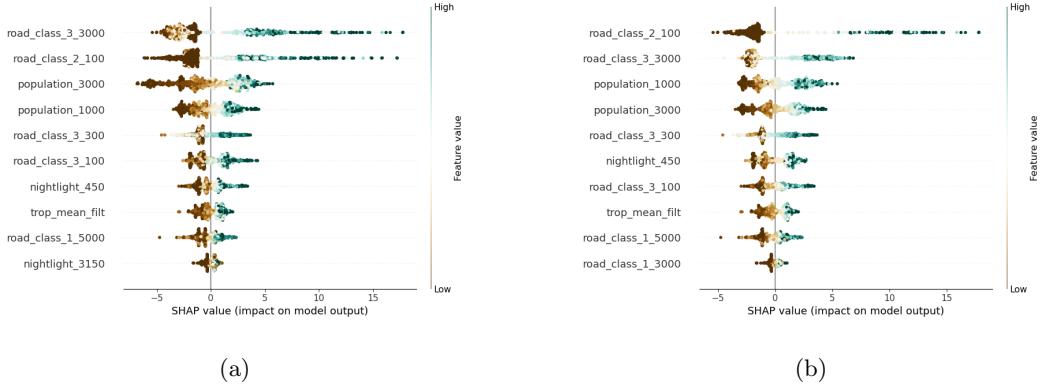


Figure 7: Variable impact calculated by SHAP (SHapley Additive exPlanations), a) the RF model, b) The XGB model. The horizontal location shows whether the effect of that value is associated with a higher or lower prediction. The covariate ranking is based on the sum of SHAP magnitudes over all the samples.

and western Germany. Compared to fig. 9, the areas close to the Stuttgart (Germany) region where the mean values of the spatial random field are high corresponds to the high magnitudes of NO₂ concentrations. Also, the differences between the observations and predictions are relatively large in magnitudes in this region. To facilitate visualisation, we also calculated the differences between INLA model predictions and the observations (supplementary material, figure 2).

6 Discussion

In this study, we compared geostatistical methods with ML methods for spatial NO₂ prediction in Germany and the Netherlands. The comparison consists of the predicted mean, prediction intervals, and model interpretation. Spatial and non-spatial CV strategies are used to reveal prediction accuracy in different aspects. We also implemented the Lasso post-processed RF and geostatistical stacked learning for NO₂ mapping (which to our knowledge have not been applied in air pollution

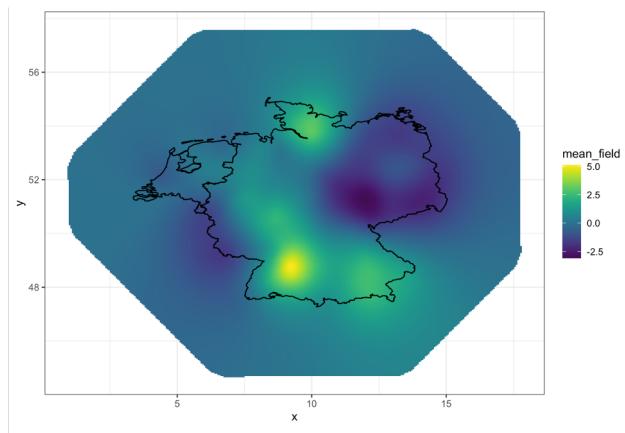


Figure 8: Mean of the spatial random field fitted by the INLA model.

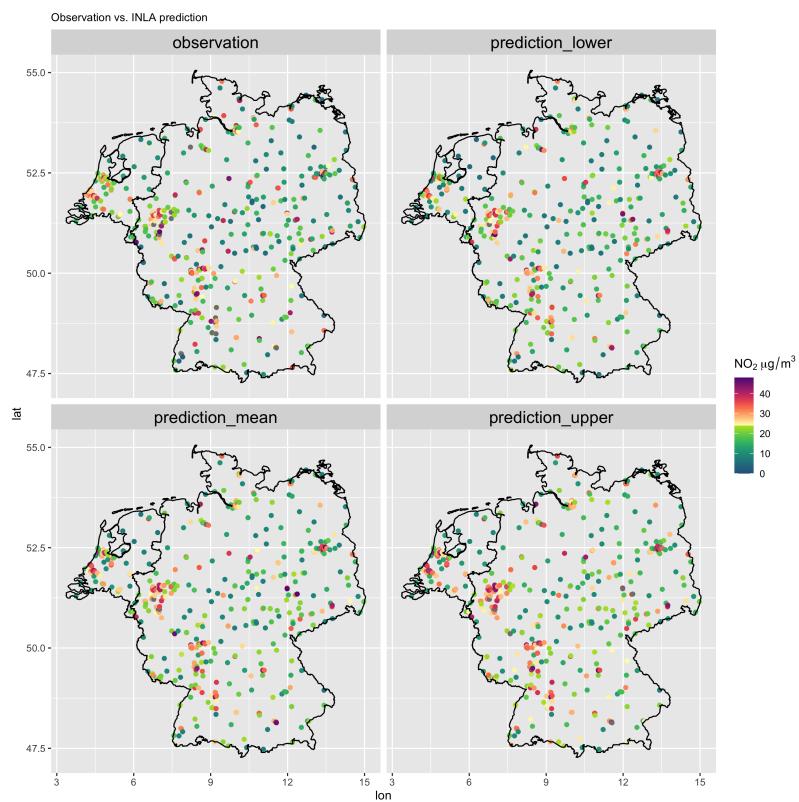


Figure 9: INLA predicted NO₂ at the ground stations with mean (prediction_mean), high (prediction_high, 0.975) and low (prediction_low, 0.925) quantiles and the observed NO₂ (observation).

⁴⁷⁶ mapping before) and these two methods considerably improve from the original RF and stacked
⁴⁷⁷ learning methods, respectively.

⁴⁷⁸ Several venues were attempted to further improve the geostatistical model fitted with INLA.
⁴⁷⁹ Firstly, as we observed in general worse results at the geographical boundaries (figs. 2 and 3), we
⁴⁸⁰ inspected if different meshes with edge-effects fully accounted (e.g. the mesh is sufficiently large for
⁴⁸¹ observations at the edge) could improve the prediction accuracy. It turned out that the same perfor-
⁴⁸² mance is obtained. Secondly, we suspected that the deviation from assumed distribution (Gaussian)
⁴⁸³ is the cause of narrow prediction intervals of the INLA model. However, assuming a Gamma distri-
⁴⁸⁴ bution likelihood did not improve the model performance (in terms of the accuracy matrix, CRPS
⁴⁸⁵ and coverage probability). We also experienced the square transformation of the observations and
⁴⁸⁶ the use of the log-normal likelihood but that also decreases the model performance. Thirdly, we
⁴⁸⁷ additionally added two factor variables, namely "country code" (country code, "DE" for Germany
⁴⁸⁸ and "NL" for the Netherlands) and "urban types" (rural, urban, city centre according to (Dijkstra
⁴⁸⁹ and Poelman, 2014)). However, that also does not increase the model performance. In future works,
⁴⁹⁰ using a different spatial model (e.g. by specifying different hyperparameters), using the country and
⁴⁹¹ urban types as mixed-effects, and modelling spatial varying coefficients may improve the modelling
⁴⁹² results. Major improvement may also be achieved by integrating mobile sensing measurements and
⁴⁹³ other geospatial predictors (e.g. traffic count, urban morphological matrix) (Moraga et al., 2017).

⁴⁹⁴ We implemented an INLA model without modelling the spatial random effect (called non-spatial
⁴⁹⁵ INLA) to deepen our understanding of the effect of modelling the spatial process in our INLA model.
⁴⁹⁶ The non-spatial INLA model obtained lower DIC (Information Criterion) 3286.66 vs. 3251.97 (with
⁴⁹⁷ spatial effects) and WAIC (Watanabe-Akaike information criterion) 3291.75 vs. 3253.93 (with spa-
⁴⁹⁸ tial effects). These suggest the advantage of modelling the spatial effects. We normalised covari-
⁴⁹⁹ ates before inputting into the spatial and non-spatial INLA models and compared the differences

500 between the fixed-effects obtained by the original and non-spatial INLA model (supplementary ma-
501 terial figure 3-4) and found the most notable change is on the increased effect on the covariate
502 population_1000 for the non-spatial INLA model. This can be explained by that part of the effects
503 of population_1000 is modelled in the spatial random field. The second most notable change is on
504 the decreased effect of nightlight_450 for the non-spatial INLA model. After the spatial process is
505 modelled, the nightlight_450 has a higher contribution to the model. Together with the decreased
506 effects of road_class_2_100 and road_class_3_300 for the non-spatial INLA model, these may indicate
507 that the spatial model could better account for traffic-related variables (i.e. road and nightlight in
508 smaller buffers).

509 Model performance differs between the three road and population situations. The "far" situation
510 obtained the best modelling accuracy while the "tr-hp" the worst. This is likely due to the fact that
511 the urban NO₂ process is more complex due to urban forms and traffic conditions. This may also
512 indicate that more detailed traffic counts and meteorological data are needed for modelling the NO₂
513 emission sources.

514 Different from non-parametric models such as ensemble trees, a parametric geostatistical model
515 fitted with INLA as the one developed in our study requires feature selection and the assumption
516 of the distribution of the response. Several studies used the whole dataset for variable selection and
517 then use selected variables for CV (Lu et al., 2020b; Larkin et al., 2017). This may however lead to
518 an information leak as the validation data is also used in CV. To avoid this problem, one can include
519 the variable selection process in each CV (i.e. use the same training data for variable selection and
520 test). However, variable selection in each run added in additional error and uncertainty, therefore,
521 a determined set of covariates may be preferred. We obtain a fixed set of selected variables while
522 reducing information leakage to a negligible level by choosing only the variables that are selected
523 90% -100% times of all the bootstraps of Lasso.

524 Using the geostatistical method to stack learners obtained higher prediction accuracy in terms
525 of the mean prediction compared to the non-spatial stacking. This suggests the complex response-
526 covariate relationships modelled by the ML learners do not fully capture the spatial process. The
527 geostatistical stacked models obtained the highest prediction accuracy and with high-performance
528 computation, it is possible to apply them to a large-scale and at a high resolution. The limitation of
529 such stacked methods is that they cannot be used to analyse the effects of covariates and therefore
530 NO₂ emission sources. But these models could be a reference to the level of accuracy a statistical
531 predictive model could reach with the data available and the characteristics of the base learners
532 (here: if the base learners are global or local models).

533 7 Conclusion

534 We proposed a model comparison process to comprehensively compare between models considering
535 not only the predicted mean but also prediction intervals and model interpretation. We also showed
536 that the information provided by commonly single-used non-spatial CV may miss reflecting model
537 behaviours. With the model comparison process, we compared the use of geostatistical and ML
538 methods for the spatial prediction of NO₂ in Germany and the Netherlands and found noticeable
539 differences in their limitations and strength. The geostatistical models are preferred especially for
540 urban area prediction and provide the spatial process of observations and indicate the insufficient
541 modelling of spatial random-effects of fixed-effects. But the uncertainty assessment of geostatistical
542 methods, which is commonly known as strength, fails to provide a prediction interval that meets
543 the expectation. The QRF and DF obtained satisfying prediction intervals, with the DF slightly
544 more capable of predicting the extremes. Using Lasso to aggregate trees in random forest increase
545 model performance and reduce model variance. Using the geostatistical method to stack learners
546 obtained the highest accuracy in terms of the mean prediction. Despite the NO₂ observations follow

⁵⁴⁷ closer to a Gamma distribution than a Gaussian, the use of a Gamma likelihood in the geostatistical
⁵⁴⁸ model and Gamma objective in the XGBoost obtained much worse results than using a Gaussian
⁵⁴⁹ likelihood or objective. By comparing with the non-spatial stacking, geostatistical stacking suggests
⁵⁵⁰ the necessity of modelling the spatial process.

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