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Multi-Source Geographically Weighted Regression for Regionalized Ground-Motion Models

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Abstract:	This work proposes a novel approach to the calibration of regionalized regression models, with particular reference to ground-motion models (GMMs), which are key for probabilistic seismic hazard analysis and earthquake engineering applications. A novel methodology, named multi-source geographically-weighted regression (MS-GWR), is developed, allowing one to \emph{(i)} estimate regionalized regression models depending on multiple sources of non-stationarity (such as site- and event-dependent non-stationarities in GMMs), and \emph{(ii)} make inference on the significance and stationarity of the regression coefficients. Unlike previous approaches to the problem, the proposed framework is fully non-parametric, the inference being based on a permutation scheme. MS-GWR is here used to calibrate a new regionalized ground-motion model for predicting peak ground acceleration in Italy, based on a large scale database of waveforms and metadata made available by the Italian Institute for Geophysics and Vulcanology (INGV).
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Dear Editor,

please consider for publication in *Spatial Statistics* the paper "Multi-Source Geographically Weighted Regression for Regionalized Ground-Motion Models" coauthored with Luca Caramenti, Sara Sgobba and Giovanni Lanzano.

In the paper, we address the problem of defining and calibrating *regionalized* linear models for ground motion prediction (a.k.a. ground motion models, GMMs) based on large-scale spatially distributed seismic records. Providing GMMs that are capable to precisely account for the regional factors influencing the propagation of ground motion is critical for probabilistic seismic hazard analysis and earthquake engineering applications.

We propose a novel method for the calibration of regionalized GMMs, named Multi-Source Geographically Weighted Regression (MS-GWR), which allows one to incorporate within the model multiple sources of non-stationarity (e.g., those arising from event- and site-effects in the propagation of ground motion). Unlike previous approaches to the problem, the proposed methodology is fully non-parametric, and prone to extensions to more complex types of intensity measures than scalar ones. In this vein, we also develop an inferential procedure based on a permutational approach to test for the significance and non-stationarity of the model coefficients.

We use the developed framework to calibrate a regionalized GMM for Italy, based on a large-scale database of waveforms and meta-data made available by the Italian Institute for Geophysics and Vulcanology (INGV).

We are confident that the readership of the *Spatial Statistics* will appreciate this work, which addresses from an original perspective a problem of primary importance in earth sciences.

My co-authors are aware that this manuscript is being submitted. The material contained in this manuscript has not been published in any journal, and it is not being considered for publication in any other journal. I will act as corresponding author.

Yours Respectfully,

A Menafoglio

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Multi-Source Geographically Weighted Regression for Regionalized Ground-Motion Models

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Abstract

This work proposes a novel approach to the calibration of regionalized regression models, with particular reference to ground-motion models (GMMs), which are key for probabilistic seismic hazard analysis and earthquake engineering applications. A novel methodology, named multi-source geographically-weighted regression (MS-GWR), is developed, allowing one to *(i)* estimate regionalized regression models depending on multiple sources of non-stationarity (such as site- and event-dependent non-stationarities in GMMs), and *(ii)* make inference on the significance and stationarity of the regression coefficients. Unlike previous approaches to the problem, the proposed framework is fully non-parametric, the inference being based on a permutation scheme. MS-GWR is here used to calibrate a new regionalized ground-motion model for predicting peak ground acceleration in Italy, based on a large scale database of waveforms and metadata made available by the Italian Institute for Geophysics and Vulcanology (INGV).

Keywords: Geographically-weighted regression, ground motion models, peak-ground acceleration, seismic risk analysis

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1. Introduction

Seismic risk analysis and earthquake engineering applications use empirical ground motion models (GMMs) to predict the intensity level of ground shaking caused by an earthquake event at a site. These models quantify the expected median level of a ground motion parameter, i.e. Intensity Measure (IM), along with the associated uncertainty, from a set of independent variables such as the earthquake magnitude and the event-to-site distance. GMMs are traditionally calibrated on global datasets, meaning that seismic records available in different parts of the world – which taken individually would not suffice for a robust calibration – are used together to perform the model calibration, which typically consists of a regression analysis. The obtained relationships are then applied globally, under the hypothesis that the conditional distribution of the ground motion parameter of interest given the magnitude, distance and site conditions, is identical at any site. This assumption however implies a high level of uncertainty associated with the estimated IMs, that reflects the large region-to-region variations observed on ground motion as a consequence of physical peculiarities at smaller scales, such as those related to different source and attenuation properties, as well as to site amplifications. Neglecting such region-specific variations leads not only to a larger variability but also to biased estimates of the IMs at more local scales for individual events and stations.

The current trend in the field of engineering seismology is thus moving towards region-specific GMMs. This is nowadays possible thanks to the increasing availability of seismic records in the majority of the most tectonically active countries. The resulting models provide different median predictions for different locations, instead of a single prediction that roughly averages all the ground motion effects at different scales. Recent studies have indeed focused on the development of new approaches for ground motion regionalization (Stafford [32], Kotha et al. [11], Sahakian et al. [30], Kuehn et al. [15], Sgobba et al. [31], Parker et al. [28], Kuehn and Abrahamson [14], Kotha et al. [12], Menafoglio et al. [27]). The main strategy in this field is providing regional adjustments of the median GMM prediction, assuming that there are repeatable source, path, and site effects, which can be estimated from residual decomposition (where the term “residual” stands for the logarithmic deviation of a data point from the predicted IM; [2], [3]).

Another approach grounds on the development of GMMs having a single functional form for all sites with coefficients that vary with the geographical location ([16], [13]). The pioneering work of [16] used a fully Bayesian approach built on the technique presented by Bussas et al. [5], to introduce a double spatial non-stationarity of the model coefficients, which were allowed to be constant, or dependent on site- or event-coordinates (without depending on both types of coordinates simultaneously). The methodology – which was applied to build a GMM in California – revealed to be promising in order to improve GMMs accuracy and reduce the associated uncertainty, with a significant impact on hazard and engineering-oriented applications. However, its modeling and computational complexity represents a limitation for its use in the seismological practice.

In our work, we follow the same regionalization strategy adopted by Landwehr et al. [16] to introduce a spatial non-stationary GMM for Italy, but we embed the inference on this model in a different methodological framework based on the theory of geographically weighted regression (GWR, [4]). GWR allows one to model all the regression coefficients of a linear model as varying over space, and estimate them by localizing the model through spatial kernels. Although a generalization of this methodology – named mixed geographically weighted regression (MGWR, Fotheringham et al. [8]) – allows one to keep some coefficients constant over space, none of the available GWR methods enables one to include *multiple* spatial non-stationarities within the model, i.e., non-stationarities deriving from the presence of multiple spatial indexes in the random process (hereafter called *multi-source* non-stationarity). In fact, even though GWR represents the natural framework to develop spatially variable GMMs, this methodological gap still represents an important limitation to its use, as GMMs need to incorporate both site- and event-coordinates within the model. As a key innovative contribution of this work, we thus further extend the GWR methodology, leading to multi-source GWR (MS-GWR), that allows one to jointly include *(i)* a set of stationary coefficients, and *(ii)* a double spatial non-stationarity within the model. We here propose a computational methodology to estimate the model parameters, as well as to quantify the associated uncertainty. We also develop an inferential framework for hypothesis testing on the model coefficients, based on a permutation approach. These developments enable us to propose a novel approach to build region-specific GMMs, which is here used to calibrate a GMM for the peak-ground acceleration over the entire Italian territory. This model shall be here built upon a large-scale dataset, collecting the seismic measures related with 4784 events recorded in Italy along 40 years.

The remaining part of this work is organized as follows. In Section 2 we recall the seismological background of this work, with particular reference to the state-of-the-art GMM in Italy (ITA18, Lanzano et al. [19]), and the GMM proposed by Landwehr et al. [16]; we here also describe the calibration dataset being considered in our study. Section 3 describes the MS-GWR, and the inferential framework we propose for hypothesis testing on the model coefficients. An extensive simulation study assessing the performance of MS-GWR is illustrated in the Supplementary Material, and briefly summarized in Section 4. Section 5 describes the calibration of the GMM based on MS-GWR for Italy, and its validation. Section 6 eventually concludes the work. Codes and support material for the use of MS-GWR in ground-motion modeling are available on GitHub at `https://github.com/lucaramenti/ms-gwr`.

2. Background and data

The proposed methodology aims to extend to a spatial non-stationary framework the ITA18 model [19], which is the most updated version of the reference GMM for shallow crustal earthquakes in Italy. ITA18 provides the median value and associated uncertainty of a set of intensity measures (IMs), modeled as log-normal random variables. It was calibrated via a maximum likelihood approach, based on a linear model for the logarithmic transformation of the IMs. For ease of exposition, in this work we shall focus on a single IM, which is the peak ground acceleration (PGA) — Figure 1, although an analogous approach can be used on the other IMs considered by Lanzano et al. [19]. PGA is defined as the maximum absolute amplitude of an accelerogram recorded at a site during an earthquake [7]. It is the most commonly used ground motion parameter by engineers, as well as the main parameter considered by design codes to define seismic hazard at a site.

For the scope of the present work, it is relevant to recall the functional form of ITA18 for the PGA. In Lanzano et al. [19], the PGA is modeled as:

$$
\begin{aligned}
\log_{10} PGA = a &+ b_1(M_w - M_h)\mathbb{1}_{(M_w \leq M_h)} + b_2(M_w - M_h)\mathbb{1}_{(M_w > M_h)} \\
&+ [c_1(M_w - M_{ref}) + c_2)] \log_{10} \sqrt{R_{JB}^2 + h^2} + c_3\sqrt{R_{JB}^2 + h^2} \\
&+ k \left[\log_{10}(\tfrac{V_{S30}}{800})\mathbb{1}_{(V_{S30} \leq 1500)} + \log_{10}(\tfrac{1500}{800})\mathbb{1}_{(V_{S30} > 1500)}\right] \\
&+ f_1 SoF_1 + f_2 SoF_2 + \epsilon,
\end{aligned}
\tag{1}
$$

where the explanatory parameters M_w, R_{JB}, V_{S30} and SoF are respectively the event moment magnitude, the Joyner-Boore distance (i.e. a metric that defines the distance from a site to the surface projection of the fault rupture, Joyner and Boore [10]), the shear wave velocity in the uppermost 30 meters (i.e. a proxy of the site response) and the style of faulting (i.e. a parameter describing the relative movement of the two sides of the fault plane), varying between normal, reverse and strike-slip. M_h, M_{ref} and h are fixed parameters, which have been estimated by a non-linear regression [19] and are here assumed to be known. Symbols a, b_1, b_2, c_1, c_2, c_3, f_1, f_2 and k denote the regression coefficients, which are the parameters of the model together with the variance σ^2 of the error ϵ. Note that Lanzano et al. [19] further decomposed the variance of the error term ϵ in components due to event- and site-effects, in a mixed-effect framework. This latter decomposition is not considered further here, as the variability attributable to event- and site-effects shall be here captured through the non-stationarity of the model, as in Landwehr et al. [16].

We here aim to regionalize model (1), to allow for spatially varying coefficients in the GMM, similarly as done by Landwehr et al. [16] in the formulation of a non-ergodic GMM for California. These authors proposed to model the PGA through the following model – rewritten in log-10 units, for the ease of comparison with model (1)

$$\begin{aligned}\log_{10} PGA = \beta_{-1}(u_e, v_e) + \beta_0(u_s, v_s) + \beta_1 M + \beta_2 M^2 \\ + [\beta_3(u_e, v_e) + \beta_4 M] \ln \sqrt{R_{JB}^2 + h^2} + \beta_5(u_e, v_e) R_{JB} \\ + \beta_6(u_s, v_s) \ln V_{S30} + \beta_7 F_R + \beta_8 F_{NM} + \epsilon,\end{aligned} \tag{2}$$

where (u_e, v_e), (u_s, v_s) denote the event and site coordinates respectively. Landwehr et al. [16] calibrated the model for California in a Bayesian setting, by considering a Gaussian process prior over the spatially varying coefficients. In the following, we shall consider a GWR framework instead, as this represents a simpler but fully non-parametric alternative to the approach of Landwehr et al. [16]. An approach based on GWR is also extendable to the setting of functional data analysis (FDA, Ramsay and Silverman [29]), as we further discuss in Section 6, which could be used to model the entire response spectrum, as proposed by Menafoglio et al. [27].

For consistency reasons, the dataset being considered in this study is substantially the same as the one used for calibration of ITA18, with the only modification consisting in the removal of some worldwide earthquakes, which were introduced in order to better constrain the regression at higher magnitudes. In particular, events occurred in Turkey, Japan, New Zealand, California (USA), Iceland, Iran and Greece are here removed as not relevant to the Italian data, while all the Italian earthquakes are kept in the dataset, along with events located in Slovenia, France and Croatia, which are neighboring countries. The resulting dataset is composed by 4784 observations of 137 events from 925 stations, recorded between 1976 and 2016, with magnitudes ranging from 3.5 to 6.9. The adopted acceleration waveforms and metadata are taken from the Engineering Strong Motion database, ESM [22] and the ITalian ACcelerometric Archive, ITACA [6].

Figure 2 shows the spatial distribution of the stations that recorded the

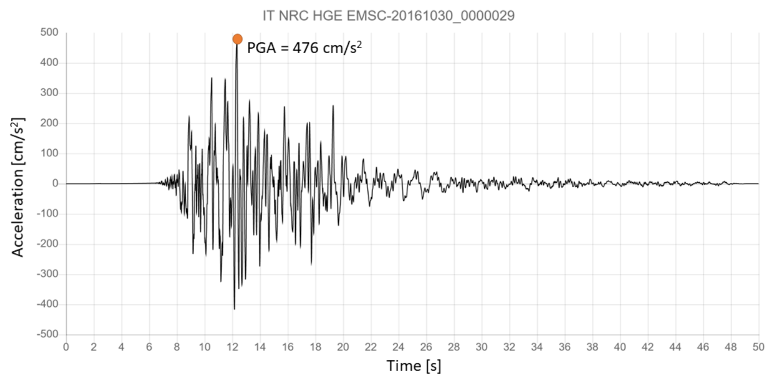


Figure 1: Indication of PGA on the acceleration waveform as recorded by the NRC station during the October 30, 2016 earthquake 06:40:18 UTC event (data are taken from ITACA database).

events included in the dataset; here, each event is connected, with lines of the same colour, to all the stations which recorded it.

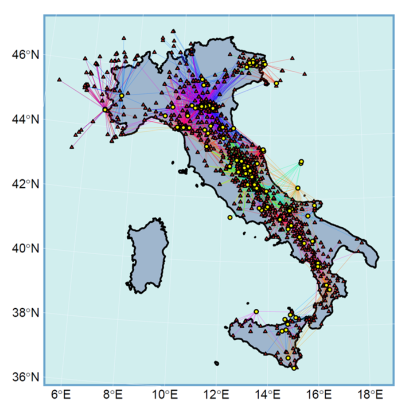


Figure 2: Map of the sampled ray-paths (colored lines) from the events (circles) to the stations (triangles).

3. Multi-source geographically weighted regression

3.1. Geographically weighted regression

Geographically weighted regression [4] is a family of statistical methods aimed to estimate a regionalized linear model, characterized by spatially varying (a.k.a. non-stationary) coefficients. In this context, the general form of the regression model is

$$y_i = \sum_j \beta_j(u_i, v_i)x_{ij} + \epsilon_i, i = 1, ..., n, \tag{3}$$

where y_i is the response variable at the i-th site with coordinates (u_i, v_i), x_{ij} is the j-th regressor associated with the i-th unit, $\{\beta_j(u_i, v_i)\}_j$ are the regression coefficients, and $\{\epsilon_i\}_i$ are the i.i.d. random errors. Methods of GWR to estimate model (3) usually consist of localizing the estimation procedure, by calibrating the model in a *neighborhood* of the target site (u_0, v_0). This is typically selected through a spatial kernel K, which is a positive non-increasing function such that *(i)* $K(0) = 0$, and *(ii)* $\lim_{d->\infty} K(d) = 0$. In practice, the spatial kernel allows one to attribute a weight $K(d_{i0})$ to the available data based on their distance d_{i0} from the target site, thus naturally down-weighting data being distant from the target. A widely-used example for K is the Gaussian kernel, which shall also be employed in the following

$$K(d) = \exp\left\{-\frac{d^2}{2h^2}\right\},$$

where h denotes the kernel *bandwidth.*

When a spatial kernel is used, GWR reduces to a weighted least square regression, the weights being determined by the spatial kernel itself. That is, for a target location (u_0, v_0), the vector of coefficients $\boldsymbol{\beta}(u_0, v_0)$, is estimated as

$$\hat{\boldsymbol{\beta}}(u_0, v_0) = (X^T W_0 X)^{-1} X^T W_0 Y, \quad i = 1, ..., n, \tag{4}$$

with X the design matrix, Y the vector of observations of the response variable, and W_0 the diagonal matrix of kernel weights $W_{0,ii} = K(d_{i0})$.

To allow for the introduction of spatially stationary regression coefficients in model (3), GWR was lately extended to Mixed GWR (MGWR, Fotheringham et al. [8]). Here, the general form of the model is

$$y_i = \sum_{j \in C} \beta_j x_{ij} + \sum_{j \in NS} \beta_j(u_i, v_i) x_{ij} + \epsilon_i, i = 1, ..., n, \tag{5}$$

where C denotes the set of spatially stationary terms, and NS the set of spatially non-stationary ones. An estimate of model (5) can be effectively obtained by using a two-steps algorithm, as advocated by Mei [24]. Here, first the constant term is estimated via OLS on an auxiliary regression problem, and then the non-stationary term is fitted by GWR on the residuals from the stationary term. The algorithm is recalled in details in the Supplementary Material, Section A. In the following Section, this methodology is generalized to the case of multi-source non-stationarity, to enable the estimate of a model of the kind (2).

3.2. Multi-source GWR: model and estimation algorithm

We now extend GWR to allow for the presence of two sources of spatial non-stationarity, which are here representative of event- and site- effects in the GMM. The general model we aim to estimate takes the form

$$y_i = \sum_{j \in C} \beta_{j_C} x_{ij} + \sum_{j \in E} \beta_{j_E}(u_{e_i}, v_{e_i}) x_{ij} + \sum_{j \in S} \beta_{j_S}(u_{s_i}, v_{s_i}) x_{ij} + \epsilon_i, \quad i = 1, ..., n, \tag{6}$$

where (u_{e_i}, v_{e_i}), (u_{s_i}, v_{s_i}) are the event- and site-coordinates, respectively, of the i-th observation, C is the set of spatially stationary coefficients, E, S are the sets of spatially non-stationary coefficients, depending on event- or site- coordinates respectively, and ϵ_i zero-mean i.i.d. errors with variance σ^2.

In order to formulate the calibration algorithm, we first introduce two auxiliary estimation equations. Denote by $\tilde{y}_i$ and $\tilde{y}_i^{(s)}$ the following partial residuals

$$\tilde{y}_i = y_i - \sum_{j \in C} \beta_{j_C} x_{ij}; \quad \tilde{y}_i^{(s)} = \tilde{y}_i - \sum_{j \in S} \beta_{j_S}(u_{s_i}, v_{s_i}) x_{ij}. \tag{7}$$

The auxiliary estimation equation then reads

$$\tilde{y}_i = \sum_{j\in E} \beta_{j_E}(u_{e_i}, v_{e_i}) x_{ij} + \sum_{j\in S} \beta_{j_S}(u_{s_i}, v_{s_i}) x_{ij} + \epsilon_i \tag{8}$$

$$\tilde{y}_i^{(s)} = \sum_{j\in E} \beta_{j_E}(u_{e_i}, v_{e_i}) x_{ij} + \epsilon_i. \tag{9}$$

For ease of notation, $\beta_{j_E}(u_{e_i}, v_{e_i})$ and $\beta_{j_S}(u_{s_i}, v_{s_i})$ will be denoted hereafter by $\beta_{j_E,i}$ and $\beta_{j_S,i}$ respectively and, moreover, $\beta_{E,i} = (\beta_{1E,i}, ..., \beta_{pE,i})^T$, and $\beta_{S,i} = (\beta_{1S,i}, ..., \beta_{rS,i})^T$.

Note that, one may estimate model (9) for the partial residuals $\tilde{y}_i^{(s)}$ via GWR, as the right term in (9) only depends on a single set of coordinates (u_{e_i}, v_{e_i}). This yields

$$\hat{\beta}_{E,i} = (X_E^T W_{E,i} X_E)^{-1} X_E^T W_{E,i} \tilde{Y}^{(s)} = A_{E,i} \tilde{Y}^{(s)}, \quad i = 1, ..., n, \tag{10}$$

and the following estimate of the partial residuals

$$\hat{\tilde{Y}}^{(s)} = \begin{pmatrix} X_{E,1}\hat{\beta}_{E,1} \\ \vdots \\ X_{E,n}\hat{\beta}_{E,n} \end{pmatrix} = \begin{pmatrix} X_{E,1}(X_E^T W_{E,1} X_E)^{-1} X_E^T W_{E,1} \\ \vdots \\ X_{E,n}(X_E^T W_{E,n} X_E)^{-1} X_E^T W_{E,n} \end{pmatrix} \tilde{Y}^{(s)} = H_E \tilde{Y}^{(s)} \tag{11}$$

where $\tilde{Y}^{(s)} = (\tilde{y}_1^{(s)}, ..., \tilde{y}_n^{(s)})^T$ is the vector of partial residuals, $X_{E,i}$ stands for the i-th row of the design matrix X_E – containing the event-dependent covariates – and $W_{E,i}$ is the weighting matrix associated with the i-th sample unit, and built through the spatial kernel (see Subsection 3.1).

Plugging-in the estimated coefficients in eq. (8), leads to

$$\tilde{Y} - H_E \tilde{Y}^{(s)} = \begin{pmatrix} X_{S,1}\beta_{S,1} \\ \vdots \\ X_{S,n}\beta_{S,n} \end{pmatrix} + \epsilon, \tag{12}$$

with $\epsilon = (\epsilon_1, ..., \epsilon_n)^T$. Replacing the definition of $\tilde{Y}^{(s)}$ (given in eq. (7)) in (12) and rearranging the terms yields

$$(I - H_E)\tilde{Y} = (I - H_E) \begin{pmatrix} X_{S,1}\beta_{S,1} \\ \vdots \\ X_{S,n}\beta_{S,n} \end{pmatrix} + \epsilon. \tag{13}$$

Note that eq. (13) can be interpreted as a regionalized model for a modified response vector ($(I - H_E)\tilde{Y}$) based on a modified regressors ($(I - H_E)X_{S,i}$, $i = 1, ..., n$). Hence, GWR can be applied again, finding the following estimates:

$$\begin{aligned}\hat{\beta}_{S,i} &= \left[X_S^T(I - H_E)^T W_{S,i}(I - H_E)X_S\right]^{-1} X_S^T(I - H_E)^T W_{S,i}(I - H_E)\tilde{Y} \\ &= A_{S,i}\tilde{Y}, \quad i = 1, ..., n\end{aligned} \tag{14}$$

from which we get

$$\begin{pmatrix} X_{S,1}\hat{\beta}_{S,1} \\ \vdots \\ X_{S,n}\hat{\beta}_{S,n} \end{pmatrix} = \begin{pmatrix} X_{S,1}A_{S,1} \\ \vdots \\ X_{S,n}A_{S,n} \end{pmatrix} \tilde{Y} = H_S\tilde{Y}. \tag{15}$$

Replacing all the estimated coefficients in the first auxiliary equation (8), and recalling again the definition of the partial residuals (7), we obtain

$$Y - H_E\tilde{Y}^{(S)} - H_S\tilde{Y} = X_C\beta_C + \epsilon \tag{16}$$

and substituting eq. (9) in this expression we get

$$Y - H_E(\tilde{Y} - H_S\tilde{Y}) - H_S\tilde{Y} = X_C\beta_C + \epsilon. \tag{17}$$

Replacing Equation (8) in Equation (17) we find

$$Y - H_E\left[Y - X_C\beta_C - H_S(Y - X_C\beta_C)\right] - H_S(Y - X_C\beta_C) = X_C\beta_C + \epsilon \tag{18}$$

which leads to

$$(I - H_E + H_EH_S - H_S)Y = (I - H_E + H_EH_S - H_S)X_C\beta_C + \epsilon. \tag{19}$$

Setting $B = (I - H_E + H_EH_S - H_S)$, we can apply OLS to Equation (19), obtaining

$$\hat{\beta}_C = (X_C^TB^TBX_C)^{-1}X_C^TB^TBY. \tag{20}$$

It is possible to write an explicit formulation of the resulting hat matrix,

Initialization: Define H_E, H_S as in eq. (11) and (15), and set $B = I - H_E + H_E H_S - H_S$.

Estimation steps:

- Estimate β_C as $\hat{\beta}_C = (X_C^T B^T B X_C)^{-1} X_C^T B^T B Y$;
- Evaluate the estimated partial residuals $\hat{\tilde{Y}} = Y - X_C \hat{\beta}_C$;
- Estimate $\beta_{S,i}$ as $\hat{\beta}_{S,i} = A_{S,i} \hat{\tilde{Y}}, \quad i = 1, ..., n$;
- Evaluate the estimated partial residuals $\hat{\tilde{Y}}^{(S)} = \hat{\tilde{Y}} - H_S \hat{\tilde{Y}} = (I - H_S)\hat{\tilde{Y}}$;
- Estimate $\beta_{E,i}$ as $\hat{\beta}_{E,i} = A_{E,i} \hat{\tilde{Y}}^{(S)}, \quad i = 1, ..., n$.

Figure 3: Estimation algorithm of Multi-source GWR

using all the previous estimates:

$$\begin{aligned} \hat{Y} &= X_C \hat{\beta}_C + \begin{pmatrix} X_{E,1}\hat{\beta}_{E,1} \\ \vdots \\ X_{E,n}\hat{\beta}_{E,n} \end{pmatrix} + \begin{pmatrix} X_{S,1}\hat{\beta}_{S,1} \\ \vdots \\ X_{S,n}\hat{\beta}_{S,n} \end{pmatrix} \\ &= X_C \hat{\beta}_C + H_E \tilde{Y}^{(s)} + H_S \tilde{Y} \\ &= HY \end{aligned} \tag{21}$$

where

$$H = I - B + B X_C (X_C^T B^T B X_C)^{-1} X_C^T B^T B. \tag{22}$$

Summing up, all the coefficients can be estimated in cascade, through the algorithm reported in Figure 3.

Note that the order of estimation has been selected arbitrarily. In fact, using an analogous approach as that here discussed we may obtain six different estimation methods (one for each possible permutation of the estimation order). The following subsections shall assume that the estimation order is set as in Fig. 3, although they could be restated analogously with any other permuted order. In Section 4, we shall illustrate a simulation study aiming to investigate the effect of the estimation order on the quality of the resulting estimates. The study is described in greater details in the Supplementary Material, Section S.B.

3.3. Parameter estimation accuracy and prediction uncertainty

In order to quantify the error made in estimating the coefficients, set

$$A_C = (X_C^T B^T B X_C)^{-1} X_C^T B^T B,$$

and let e_k be a column vector whose k^{th} element is one, and the other elements are null. Then, denoting by $\hat{\beta}_{k,i}$ the estimate of the coefficient vector $\hat{\beta}_C$, $\hat{\beta}_{E,i}$, or $\hat{\beta}_{S,i}$ for $k = 1, 2, 3$ respectively, one has

$$\hat{\beta}_{k,i} = e_k^T \begin{pmatrix} \hat{\beta}_C \\ \hat{\beta}_{E,i} \\ \hat{\beta}_{S,i} \end{pmatrix} = e_k^T \begin{pmatrix} A_C Y \\ A_{E,i} \tilde{Y}^{(S)} \\ A_{S,i} \tilde{Y} \end{pmatrix} = e_k^T Q_i Y, \quad i = 1, ..., n \tag{23}$$

where

$$Q_i = \begin{pmatrix} A_C \\ A_{E,i}(I - H_S)(I - X_C A_C) \\ A_{S,i}(I - X_C A_C) \end{pmatrix}, \quad i = 1, ..., n. \tag{24}$$

Denoting by $\hat{\beta}_{\cdot,i}$ all the regression coefficients at location i, and noting that $\hat{\beta}_{\cdot,i} = Q_i Y$, one may compute the standard error of the estimator of the coefficients at location i as

$$Var(\hat{\beta}_{\cdot,i}) = \sigma^2 Q_i Q_i^T. \tag{25}$$

Using the unbiased estimate of σ^2 given by $\hat{\sigma}^2 = \frac{RSS}{\delta_1}$, where $\delta_1 = tr\{(I - H)^T (I - H)\}$ are the effective degrees of freedom of the estimator [21], we finally get

$$\widehat{Var}(\hat{\beta}_{\cdot,i}) = \frac{RSS}{\delta_1} Q_i Q_i^T, \quad i = 1, ..., n. \tag{26}$$

The variance (26) can also be used to provide an estimate of the prediction uncertainty at a target site (u_{S0}, v_{S0}) and for a target event at (u_{E0}, v_{E0}), as

$$\widehat{Var}(\hat{y}_0) = \widehat{Var}(x_0^T \hat{\beta}_{\cdot,0}) = S_0 \hat{\sigma}^2, \tag{27}$$

where $S_0 = x_0^T Q_0 Q_0^T x_0$, and Q_0 is defined analogously as in (24), but with the weight matrices $W_{S,0}$, $W_{E,0}$ (see eq. (14), (10)) computed through spatial kernel centred in (u_{S0}, v_{S0}) and (u_{E0}, v_{E0}) respectively. This result is fully analogous to the prediction uncertainty obtained for GWR by [8].

Notice that in seismological applications uncertainty is commonly split into two components, namely *aleatory* variability and *epistemic* uncertainty. Aleatory variability is intended as the natural randomness in a process, while epistemic uncertainty is defined as the uncertainty in the model of the process, caused by limited data and knowledge [1]. One way to reduce aleatory variability is to identify those components of ground motion variability that are not completely random and to transfer them to the quantification of the epistemic uncertainty, for instance introducing spatially varying coefficients. For instance, consider a simple linear model

$$y = \beta_0 + \beta_1 x + \epsilon_1 \tag{28}$$

and its (single-source) non-stationary counterpart

$$y = \beta_0 + \beta_1(u, v)x + \epsilon_2 \tag{29}$$

where $Var(\epsilon_1) = \sigma_1^2$ and $Var(\epsilon_2) = \sigma_2^2$. The aleatory variability of the models (28) and (29) is represented by σ_1 and σ_2 respectively, while the epistemic uncertainty includes also the variability associated with the estimation of the model coefficients, resp. $\{\beta_0, \beta_1\}$, and $\{\beta_0, \beta_1(u, v)\}$. Introducing spatial non-stationarity in model (28) –yielding model (29)– may allow us to remove repeatable effects from σ_1, leading to $\sigma_2 < \sigma_1$, but also to an increased uncertainty related to parameter estimation. The advantage of transferring repeatable effects to epistemic uncertainty is that, unlike aleatory variability, it can be reduced introducing new data or knowledge. In fact, aleatory variability of a stationary linear model is constant over space and can be estimated using the variance of the error, while epistemic uncertainty for MS-GWR varies over space and can be partially quantified by estimating the statistical variability in the median predictions using eq. (27). This point shall be further explored in Section 5, and will be part of the comparative study between the proposed non-stationary GMM and the model of Lanzano et al. [19].

3.4. Permutational inference for MS-GWR

In order to carry out inferential tests on regression parameters without relying on the normality assumption over residuals, we here develop a set of permutation tests, following the Freedman and Lane permutation scheme [9]. Its distinctive trait is that the permutations are carried out, under the null hypothesis, over the model residuals. Notice that this is an approximate test, since it is based on empirical residuals.

The general idea is that, if the null hypothesis being tested holds, the derived datasets should be equivalent to the original one: a small reported significance level indicates an unusual dataset under the null assumption.

Consider the test

$$\begin{aligned} &H_0 : \text{a given coefficient, other than the intercept, is constant} \\ &H_1 : \text{all coefficients, except for the intercept, vary over space} \end{aligned} \tag{30}$$

As test statistic consider

$$T = \frac{RSS_{H_0} - RSS_{H_1}}{RSS_{H_1}} = \frac{Y^T[R_{H_0} - R_{H_1}]Y}{Y^T R_{H_1} Y}, \tag{31}$$

where $R_{H_i} = (I - H_{H_i})^T(I - H_{H_i})$, $i = 0, 1$. The statistic (31) has already been used in GWR and MGWR literature for testing analogous assumptions on simpler models ([26], [21], [25]), and compare, on a relative scale, the residuals of the models under H_0 and under H_1. To perform the test, we propose a permutation procedure which consists of the following steps

1. Find the optimal bandwidths, under H_0, for the spatial kernels involved in the computation of $W_{E,i}, W_{S,i}$ – appearing in (10) and (14);
2. Calibrate the models under H_0 and H_1 with the bandwidths found at Step 1.; compute the statistic T and the residuals under H_0, $\hat{\epsilon}_{H_0} = (I - H_{H_0})Y$;
3. Permute the residuals $\hat{\epsilon}_{H_0}$, obtaining $\hat{\epsilon}^{*b}$;
4. Build $Y^{*b} = H_{H_0}Y + \hat{\epsilon}^{*b}$;

5. Recalibrate both models under H_0 and H_1 using Y^{*b}, always with the same bandwidths, and compute T_i^{*b};
6. Repeat Steps 3. to 5. for B times;
7. Estimate the distribution of T^* from the replicates $\{T^{*b}\}_{b=1,\dots,B}$ and compare it with T, computing the *p-value* of the test as

$$p = \frac{1}{b}\sum_{b=1}^{B} \mathbb{1}_{(T^{*b}>T)},$$

the symbol $\mathbb{1}$ denoting the indicator function.

Finding the optimal bandwidths at Step 1. is not strictly necessary, the crucial part is calibrating the model under H_0 and H_1 with the same bandwidths, since this is the only way to obtain comparable values, thus a meaningful *p-value*. Moreover, we remark that one needs not to recompute the hat matrices for the recalibration at Step 5., as T_i^{*b} can be computed as

$$T^{*b} = \frac{(Y^{*b})^T[R_{H_0} - R_{H_1}]Y_i^{*b}}{(Y^{*b})^T R_{H_1} Y^{*b}}. \tag{32}$$

Note that considering T as test statistic yields a computational procedure which is much more efficient than that obtained by considering any test statistic based on the coefficients themselves, as in the latter case the hat matrices would need to be recomputed at any iteration.

Although formulated so far for testing on a single coefficient, the proposed test is very general, and can be used for testing the joint stationarity of multiple coefficients, or the single-source stationarity. This can be achieved by properly setting H_0 and H_1, and by consistently interpreting eq. (31). Moreover, to evaluate whether some explanatory variables in the stationary part of the model are significant or not, one may set a null model such that the coefficients corresponding to these explanatory variables are all zero.

Summing up, a possible approach, inspired by the bootstrap procedure proposed by [26], is the following.

1. Test one at a time, exploiting also *a priori* knowledge if possible, the non-stationarity of the coefficients;

2. Test simultaneously the coefficients identified as not-significant at Step 1., considering them as spatially stationary under H_0;
3. Test singularly whether a stationary coefficient is significant or not, setting it to zero under H_0 and comparing two spatially varying models;
4. Test simultaneously the coefficients identified as not-significant at Step 3., considering them as null under H_0.

In the following Section 4 we summarize the results of the extensive simulation study we carried out to assess the performances of the proposed inferential procedure, in terms of level and power of the tests. A detailed account of the simulation study is provided in the Supplementary Material, Section S.B.

4. MS-GWR: summary of the supporting simulation studies

In this section, we briefly describe the performances of MS-GWR when this was applied to simulated data; the extensive simulation study is described in greater details in the Supplementary Material, Section B.

4.1. Assessment of the estimation procedure

We assessed the performances of MS-GWR, with particular regard to the estimation and prediction accuracy when changing *(i)* the order of estimation in the algorithm of Section 3 and *(ii)* the bandwidth of the spatial kernels involved in the GWR estimates. Simulated data and coefficients were generated in a four-dimensional coordinate space and training and test sets were randomly and repeatedly drawn, in a Monte Carlo setting. Note that in all simulation studies we included the intercept in one component only, which means that it was considered either spatially stationary or depending only on one type of coordinate (site or event), to avoid identifiability issues.

The performance of the estimation procedure was assessed based on

(i) the accuracy in the estimate of the coefficients;

(ii) the prediction accuracy on the test set.

As far as notation is concerned, all the different permutations have been named after the estimation order, which has to be read from right to left: C stands for spatially stationary, S for site-dependent and E for event-dependent. The main results of our simulation study concerning the order of estimation are the following:

- SEC and ESC (i.e., estimating the stationary part first) proved to work significantly better than all the other estimation orders, especially for low and medium bandwidth values;
- the best results were always obtained when considering the intercept as stationary, even when this was a misspecification of the model for the intercept; in this latter case, the consideration of a stationary intercept led anyway to improved results in terms of quality in the estimation of the remaining coefficients.

Considering the prediction accuracy rather then the coefficients estimates, simulations show that there is no significant difference between the standardized error when permuting the order of estimation, regardless of the chosen bandwidth. This result suggests that the order of estimation has no relevant impact on the quality of point estimates of the response variable, but only on the coefficients.

4.2. Permutational inference

To assess the performance of the inferential procedure proposed in Section 3, we designed the simulation study by taking inspiration from the simulation setting used by [26] to assess the performances of the bootstrap test for the stationary coefficients of MGWR. Simulated data were generated so that collinearity can be introduced in a controlled way; here, two different models for model errors ϵ_i were tested, namely normal and uniform distributions. The main results of these simulation studies are:

- the method yields rejection rates under the null hypothesis reasonably close to the significance level, under all the tested scenarios;

- the method proved to be robust to collinearity and different error distributions as far as detecting stationarity coefficients is concerned (H_0 true);

- the power increased with increasing sample size;

- the method proved to be robust to different error distributions as far as detecting non-stationarity is concerned (H_0 false); a slight loss in power was observed when introducing collinearity, without substantially compromising the goodness of the final results.

5. Case study

5.1. Model calibration

In this section we calibrate via MS-GWR a non-ergodic GMM to describe the PGA, extending eq. (1) [19] to a spatially varying formulation inspired by the model (2) of Landwehr et al. [16]. However, unlike Landwehr et al. [16], we here consider a stationary intercept, consistent with the results of the simulation study summarized in Section 4, and reported in the Supplementary Material, Section S.B. The model for the PGA we aim to estimate is

$$\begin{aligned}\log_{10}PGA &= a + b_1(M_w - M_h)\mathbb{1}_{(M_w \leq M_h)} + b_2(M_w - M_h)\mathbb{1}_{(M_w > M_h)} \\ &+ [c_1(M_w - M_{ref}) + c_2(u_e, v_e)] \log_{10}\sqrt{R_{JB}^2 + h^2} + c_3(u_e, v_e)\sqrt{R_{JB}^2 + h^2} \\ &+ k(u_s, v_s)\left[\log_{10}(\tfrac{V_{S30}}{800})\mathbb{1}_{(V_{S30} \leq 1500)} + \log_{10}(\tfrac{1500}{800})\mathbb{1}_{(V_{S30} > 1500)}\right] \\ &+ f_1 SoF_1 + f_2 SoF_2 + \epsilon.\end{aligned} \tag{33}$$

Notice that M_h, M_{ref} and h are fixed parameters; M_w, R_{JB} and V_{S30} represent the covariates and a, b_1, b_2, c_1, c_2, c_3, f_1, f_2 and k the regression coefficients.

Bandwidth selection. The calibration is carried out for grid with step equal to 10 km, covering the whole Italian territory, except for Sardinia, which is non-seismic; as a result, the considered grid is made of 2760 grid cells.

We carry out the whole calibration using SEC and then we select the best between ESC and SEC, by comparing their generalized cross-validation criterion values (GCV, [24]) found with the same bandwidths. More in details, we first select the optimal bandwidths for model (33) using the SEC order, finding $bw_E = 25$ km and $bw_S = 75$ km, and then carry out all the following tests using the same bandwidths. The reason for this choice is that selecting the optimal bandwidths bw_E and bw_S is the computationally heaviest step in the whole calibration, which is thus applied once, on the model we are most likely to use based on the prior knowledge on the GMM.

Model selection. Having fixed the bandwidths, we verify whether introducing spatial non-stationarity leads to improved results with respect to a stationary approach. A joint test for the stationarity of the coefficients shows a strong evidence of non-stationarity (*p-value*=0.000).

By analogy with [17] we expect that c_2 and c_3 –controlling geometric divergence and anelastic attenuation, respectively– shall depend on event-location. Moreover, we expect that k –which characterizes the soil under the station– shall depend on site-coordinates. A joint test on the non-stationarity of c_2, c_3 and k (H_0: all the coefficients are stationary; H_1: all the coefficients except c_2, c_3, k are stationary) shows evidence (level 10%) of their non-stationarity (*p-value*=0.078). These coefficients are hereafter considered as non-stationary, consistent with [17].

For the sake of completeness, Table 1 reports the results of hypothesis testing on the stationarity of the coefficients, when these tests are carried out one at a time. Note that one would reject (at the same level 10%) the null hypothesis for f_2. However, a non-stationary f_2 would hinder the physical interpretation to the model; in the following, f_2 is thus considered as constant.

Looking at how influential stationary covariates are, we refer to the results reported in Table 2. Here, one can see that b_2 and f_2 seem not to be significant at level 10%, consistently with the results obtained in the calibration of ITA18. Despite their limited impact on model predictions, these covariates were kept in ITA18, and shall be included in our model as well, to ease the comparison. This choice is also supported by the joint test on these coefficients, according

Null hypothesis	*p-value* PGA
$H_0 : b_{1,i} = b_1$	0.988
$H_0 : b_{2,i} = b_2$	0.116
$H_0 : c_{1,i} = c_1$	0.156
$H_0 : c_{2,i} = c_2$	**0.047**
$H_0 : c_{3,i} = c_3$	**0.012**
$H_0 : f_{1,i} = f_1$	0.972
$H_0 : f_{2,i} = f_2$	**0.033**
$H_0 : k_i = k$	**0.087**

Table 1: Permutation tests for stationary coefficients (1000 permutations). P-values lower than 10% are highlighted in bold.

Null hypothesis	*p-value* PGA
$H_0 : a = 0$	**0.000**
$H_0 : b_1 = 0$	**0.000**
$H_0 : b_2 = 0$	0.151
$H_0 : c_1 = 0$	**0.000**
$H_0 : f_1 = 0$	**0.031**
$H_0 : f_2 = 0$	0.117

Table 2: Permutation tests for null coefficients (1000 permutations). P-values lower than 10% are highlighted in bold.

to which they are jointly significant at level 10% (*p-value*=0.048).

Finally, the comparison of GCV values obtained for ESC or SEC –on the final model, estimated using the same bandwidths– leads to the selection of SEC over ESC (GCV=450.8 for SEC, GCV=498.6 for ESC).

5.2. Interpretations

In Table 3 the estimated *stationary* coefficients are reported together with their standard deviation, and compared with the ones obtained in ITA18. No evident discrepancy between the two models is observed in this stationary part.

Figure 4a to 4c displays the spatial representation of the non-stationary coefficients, each referred to the corresponding domain of variation (i.e., event-coordinates (u_e, v_e) for c_2, c_3 and site-coordinates (u_s, v_s) for k). The site-dependent estimate varies much more smoothly than the event-dependent ones. This is likely to be due to the different density of events with respect to stations and to the differing bandwidths that have been previously selected.

As far as c_2 and c_3 are concerned, one can see that they behave in a complementary way, higher values of geometrical spreading being associated with

	a	b_1	b_2	c_1	f_1	f_2
MS-GWR	3.5502	0.2354	-0.0513	0.2654	0.0510	0.0394
	(0.0454)	(0.0326)	(0.0372)	(0.0188)	(0.0205)	(0.0240)
ITA18	3.4210	0.1940	-0.0220	0.2871	0.0860	0.0105
	(0.0459)	(0.0332)	(0.0411)	(0.0104)	(0.0359)	(0.0344)

Table 3: Point estimate of the stationary coefficients; standard deviations are reported between brackets.

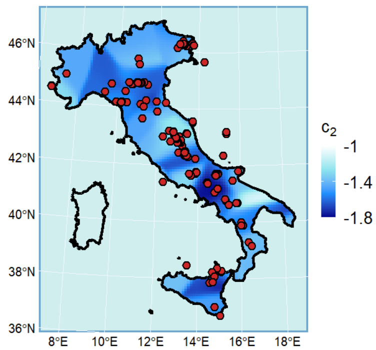
lower values of anelastic attenuation and vice versa.

Notice that, in the calibration of ITA18, c_3 was set to 0 when positive, since it would lead to an enhancement of the spectral amplitudes, which is not physically meaningful in general. Nevertheless, in the calibration using MS-GWR, positive values of c_3 have been kept, since this phenomenon can be observed in the Po Plain, where we may have reflection effects, for both long and short periods, due to Moho discontinuity, which marks the transition in composition between the Earth's rocky outer crust and the more plastic mantle [18].

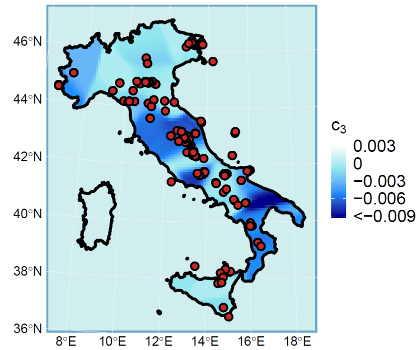
5.3. Residuals and uncertainty

Focusing on the residuals, they do not show relevant patterns (see the Supplementary Material, Section S.C), thus indicating that the model succeeds in capturing the effects of the input variables. We now compare the uncertainty of our model and associated predictions with those of ITA18. Recall that RSS/δ_1, with δ_1 the effective degrees of freedom, is an unbiased estimate of the variance of the error σ^2 (see Section 3). On this basis, we obtain an estimated standard deviation of $\hat{\sigma} = 0.3001$ against a standard deviation for ITA18 of $\hat{\sigma}_{ITA18} = 0.3362$. Introducing spatial non-stationarity thus leads to a moderate reduction of the aleatory variability.

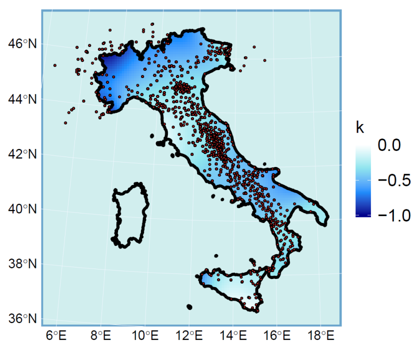
While the aleatory variability of the model is constant over space, epistemic uncertainty for MS-GWR is spatially varying. The joint effect of both variabilities can be assessed by evaluating the statistical variability in the median



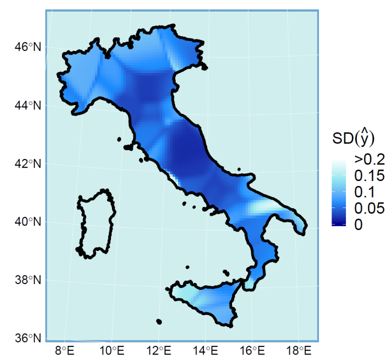
(a) Coefficient $c_2(u_e, v_e)$ (ITA18: $c_2 = -1.4056$)



(b) Coefficient $c_3(u_e, v_e)$ (ITA18: $c_3 = -0.0029$)



(c) Coefficient $k(u_s, v_s)$(ITA18: $k = -0.3946$)



(d) Standard deviation of $\hat{y}$ (in $\log_{10}$ units) for a given input

Figure 4: Maps of non-stationary coefficients, estimated via MS-GWR ((a) to (c)), and prediction uncertainty fo a fixed input.

predictions. To evaluate its spatial variation, we set the input variables to M_w=5, V_{S30}=300$\frac{m}{s}$, SoF=NF and R_{JB}=10km and predict the response for PGA. For the sake of simplicity and following Landwehr et al. [17], the same event-station coordinates are considered (i.e., $(u_e, v_e) = (u_s, v_s)$). Graphical inspection of Figure 4d suggests that the lowest values of predictive uncertainty are located in areas with a very high density of data, both of stations and events. On the other hand, its highest values are observed in areas characterized by a lack of data, e.g., in the region of the Alps, Apulia and Sicily. These values are generally higher than the epistemic uncertainty related to ITA18, coherently with the transferral of repeatable effect from aleatory variability to epistemic uncertainty.

5.4. Model validation

In order to validate the model, we carry out a 10-fold cross-validation, splitting the dataset completely at random in 10 folds $F_1, ..., F_{10}$ and comparing the mean squared error, defined as

$$MSE_{10-fold} = \frac{1}{10} \sum_{j=1}^{10} \frac{\sum_{i \in F_j} (y_i - \hat{y}_{-j})^2}{N_j}, \tag{34}$$

where $\hat{y}_{-j}$ is the predicted value using the model calibrated using all folds except for F_j. Results show that MS-GWR leads to improved results ($MSE_{10-fold} = 0.09252$) with respect to ITA18 ($MSE_{10-fold} = 0.11996$), supporting the introduction of spatially varying coefficients. Further validation results of the resulting GMM on independent events (i.e., events outside the calibration dataset) can be seen in the Supplementary Material, Section S.D.

6. Discussion and conclusion

In this work, we proposed a novel approach to calibrate regionalized regression models accounting for multiple spatial non-stationarities, with a particular focus on non-stationary ground motion models depending on site- and event-effects. The proposed approach is of general validity, and could be potentially applied in varied environmental and industrial settings, ranging from climatology to the oil and gas industry. In the field of seismology, the approach represents an alternative to the Bayesian methodology described by Landwehr et al. [16], presenting the significant advantage of being simpler and fully non-parametric. From the application viewpoint, the proposed approach allowed us to regionalize the state-of-the-art model for PGA in Italy [20], making explicit the non-stationary relation between the response variable (PGA) and the predictors. The extensive validation study (illustrated in Section 5, and in the Supplementary Material, Section S.D) allows us to conclude that the proposed model exhibits (a) a good capability to capture the main physical aspects related to the source, site and path terms; (b) a model uncertainty which is generally higher for the Italian regions where data are sparse (Western Sicily, Southern Apulia) and lower where data are densely sampled (Central Italy); (c) a lower aleatory variability, as a consequence of the regionalization process through spatially varying predictions, which necessarily reflects on a larger epistemic uncertainty; and (d) a decrease in the overall prediction error (both in cross-validation and on independent events) with respect to the state-of-the-art stationary model (ITA18, Lanzano et al. [20]). The results here presented thus appear very promising, and classify the methodology as a good candidate for the regionalization of global ground motion models when enough sampling coverage is available. This opens important perspectives for the computation of site-specific Probabilistic Seismic Hazard Analysis (PSHA), as well as for the development of shaking scenarios in loss prediction and emergency planning purposes.

Grounding on the theory of geographically weighted regression (GWR), the approach here proposed is also prone to be extended to more complex settings as functional data analysis (FDA, Ramsay and Silverman [29]) and object oriented data analysis (OODA, Marron and Alonso [23]). Such extension could potentially allow one to consider functional intensity measures, such as the spectral acceleration $SA(T)$ as a function of the period of oscillation T (of which PGA is a point evaluation at $T = 0$). A pioneering study in this direction was recently proposed by Menafoglio et al. [27], who presented a functional simulation setting for these types of data, based on the residuals of the GMM ITA18. The development of functional GMMs is seen by the authors as a powerful perspective of research, which could lead to breakthrough advances in engineering seismology, and could naturally stem from the research proposed in this work.

Supplement S: further details and additional material

The Supplementary Material is divided in four sections:

- section S.A contains a brief review of MGWR;
- section S.B shows the complete simulation study on MS-GWR;
- section S.C contains the plot of the residuals concerning PGA;
- section S.D contains validation results on independent events.

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