Two local-spatial interpolators: regression kriging vs. geographically weighted regression

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Abstract

If spatial dependence and/or spatial heterogeneity are taken account of into the process of spatial interpolation, this prediction process can be named local-spatial prediction. Geographically weighted regression is a type of local-spatial prediction models since methodologically it incorporates spatial heterogeneity into a regression model. From the standpoint of spatial interpolation, regression kriging is presented as another local-spatial prediction model that incorporates local-spatial dependence, association between response and auxiliary variables, and the unbiased estimation with minimized variance into an interpolation process. The methodologies of regression kriging and geographically weighted regression are summarized to indicate how local-spatial correlation, spatial heterogeneity, and non-spatial correlation and are incorporated into interpolation process. This paper points out regression kriging applies the local variation of spatial dependence to regression parameter estimation and combines the estimated regression model with residual kriging considering spatial autocorrelation in residuals into a hybrid local-spatial interpolator. Using a raster data with two types of sampling approaches, this study examines and compares the performance of regression kriging and geographically weighted regression. The empirical examples indicate that both regression kriging and geographically weighted regression are powerful local-spatial prediction models, but regression kriging can be better in capturing spatial structure of the original data.

Keywords Regression kriging · Geographically weighted regression · Local-spatial prediction · Spatial dependence · Spatial non-stationarity

1. Introduction

A primary difference between geographic information science (GIScience) and other science disciplines is the description and modeling of spatial differences and similarities. In GIScience, an important research trend has been changed to the focus of differences instead of similarity across space (Fotheringham and Brunsdon, 1999). It is difficult to use global models to describe the differences across space because a hidden assumption of global models that variation is the same everywhere for a given study area, while spatial dependence generally varies across space. The first law of geography i.e., "Everything is related to everything else, but near things are more related than distant things (Tobler, 1970)" is a typical description of spatial dependence that forms the primarily foundation of geospatial modeling. It is convenient to use local models to model differences across space. For example, local indicator of spatial autocorrelation (LISA) is an efficient function modeling spatial dependence across space (Anselin, 1995). However, it is difficult to have all the measurements of interesting variables across a whole study area and predictions based on sample locations are usually the dominant way in practice. An efficient way is to use spatial prediction models to estimate the values at unsampled locations given both values at sampled locations and values of auxiliary variables across the whole study area for which remotely sensed images have been widely used as auxiliary variables. Incorporating the spatial characteristics of spatial autocorrelation or spatial heterogeneity into prediction, the spatial prediction models can be appropriate. Therefore, the spatial prediction models taking account of local-spatial characteristics (e.g., local dependence or spatial non-stationarity) can be called local-spatial prediction models (LSPM).

Spatial dependence and spatial heterogeneity determine the necessary of using LSPM to estimate values of a geographical property. Unwin and Unwin (1998) emphasized the spatially varying characteristics because of three important properties: (1) spatial dependence exists in most spatial data analysis, (2) many geographic analyses depend on the modifiable areal unit problem (MAUP), and (3) the assumption of spatial stationarity is difficult to build in the observed geographical processes over space. These properties are all determined by the nature of geographical objects while for the MAUP subjective judgments may play important roles in practice. From the standpoint of methodology, Fotheringham (1997) summarized three reasons why a global model may not be appropriate: (1) random sampling variations result in spatial variations in observed relationships; (2) Certain relationships intrinsically vary across space; and (3) a global model used to measure relationships is a gross misspecification of reality. For example, a geographical property like temperature, precipitation, pollution, and elevation varies from place to place and a LSPM can be better than a global model to estimate the values of this property at unsampled locations based on the values at locally sampled locations and known values of auxiliary variables (e.g., one typical auxiliary data are remote sensing data).

However, the development of prediction models taking account of local-spatial correlation and heterogeneity still has been got little attention in the fields of GISystems and GIScience. Geographically weighted regression (GWR) is a type of LSPM that incorporates spatial heterogeneity into a regression process. Regression kriging (RK) emphasizing spatial correlation and its local variation in interpolation process is another type of LSPM. Regression kriging takes account of local-spatial correlation into both regression parameter estimation and residual kriging.

To clear the understanding of regression kriging and emphasize how the two local-spatial interpolators RK and GWR incorporate spatial correlation, spatial heterogeneity, and non-spatial association into a local-spatial interpolation process, this study states that the methodological characteristics of regression kriging and geographically weighted regression in section 2. Using a raster data as an example and two types of sample schemes, this study examines and compares the performance of the two local-spatial prediction models in section 3. This study closes with concise discussion and conclusion that suggest both regression kriging and geographically weighted regression are powerful in local-spatial prediction and in the process of interpolation regression kriging can be better to capture spatial structure of the original data.

2. Methodology

A local-spatial prediction model can be defined as the process to interpolate a real valued function of $z(s)$ given the set of values $z(s_1), z(s_2), ..., z(s_n)$ at the neighboring locations $\{s_1, s_2, \ldots, s_n\}$. It is necessary to allow for uncertainty in our descriptions of the predicted results for the insufficient knowledge of a given geographic property. From the standpoint of local-spatial prediction, a concise methodological summarization of the RK and GWR is presented below.

2.1 *Regression kriging*

Odeh et al. (1994, 1995) was originally suggested using the term of regression kriging to employ correlation between response variable and auxiliary variables and spatial autocorrelation within the response variable, while kriging with external drift (KED) is often used when external drift is described through some auxiliary variables (Chiles and Delfiner, 1999; Wackernagel, 1998). Goovaerts (1999) used the term of kriging after detrending to define this kriging process. One advantage of RK is that it does not suffer from instability in practice (Goovaerts, 1997) and RK can be easily integrated with statistical computation like general additive modeling or regression tree (McBratney et al., 2000). The RK is used in this study since it indicates that regression is combined with kriging.

In a local-spatial prediction process, let the values to be predicted for the given locations indicate as $z(s_1)$, $z(s_2)$, $z(s_3)$, …, $z(s_n)$, where, for example, $s_i = (x_{latitude}, y_{longitude})$ is a location with the coordinates of $x_{latitude}$ and $y_{longitude}$, and location i = 1, 2, 3,…, n. The value to be predicted at a new and unsampled location (s_0) can be predicted using RK by adding the spatial trend and random components (i.e., residuals) (Odeh et al., 1994) using the equation below.

$$\hat{z}(s_0) = \hat{m}(s_0) + \hat{e}(s_0) \tag{1}$$

where the residuals $\hat{e}$ are interpolated using ordinary kriging, and the trend is modeled using a linear regression as follows:

$$\hat{z}(s_0) = \sum_{k=0}^{p} \hat{\beta}_k \cdot q_k(s_0) + \sum_{i}^{n} w_i(s_0) \cdot e(s_i) \tag{2}$$

where $\hat{\beta}_k$ are the kth estimated drift model coefficient, q_k is the kth external auxiliary variable or predictor at location s_0 (while, $q_0(s_0) = 1$), p is the number of auxiliary variables, $w_i(s_0)$ are the weights determined by the covariance function and $e(s_i)$ are the regression residuals.

Rewrite the RK model in a matrix notation using the following equations:

$$z = q^T \cdot \beta + \varepsilon \tag{3}$$

$$\hat{z}(s_0) = q_0^T \cdot \hat{\beta} + \lambda_0^T \cdot e \tag{4}$$

where ε is the regression residuals, q_0 is the vector of p auxiliary variables at s_0, $\hat{\beta}$ is the vector of p +1 estimated drift model coefficients, λ_0 is the vector of n kriging weights and e is the vector of n residuals. Taking into account the spatial correlation of residuals the model coefficients are solved by a generalized least squares estimation below (Cressie, 1993).

$$\hat{\beta} = (q^T \cdot C^{-1} \cdot q)^{-1} \cdot q^T \cdot C^{-1} \cdot z \tag{5}$$

where q is the matrix of auxiliary variables at all the observed locations, z is the vector of sampled response observations, and C is the n × n covariance matrix of residuals below.

$$C = \begin{bmatrix} C(s_1, s_2) \cdots C(s_1, s_n) \\ \vdots \quad \ddots \quad \vdots \\ C(s_n, s_2) \cdots C(s_n, s_n) \end{bmatrix} \tag{6}$$

The covariance matrix between sampled pairs $C(s_i, s_j)$ can be estimated using a semivariogram model, which incorporates spatial correlation and its local variations of residuals into the parameter estimations of regression models. At the same process, in order to minimize the spatial autocorrelation in residua and potentially increase the prediction accuracy, the predicted results from the estimated model are added to residual kriging considering local-spatial autocorrelation of residuals. In other words, two spatial processes spatial estimation of regression parameters and local kriging of residuals are incorporated into regression kriging.

In summarization, if we would like to illustrate the regression kriging process using simple numerical examples, we need to conduct a simple or multiple-linear regression, select an optimal semivariogram model to explore the residuals, compute the regression coefficients, process the weight matrix, and at last conduct the regression kriging model and obtain the predictions at all unsampled points. Regession kriging is a hybrid interpolator that incorporates spatial correlation and its local variation into the combination of either a simple or multiple-linear regression model with residual kriging. In the process of RK, kriging with uncertainty introduces the regression residuals (i.e., the model uncertainty) into the kriging system, which is then applied directly to predict the response variable. The predictions are combined from two parts: one is the estimation obtained from regression considering spatial correlation, and the second part is the residual estimated from the ordinary kriging. Therefore, a general format of RK can be rewrite in a matrix notation below as Christensen (1990).

$$\hat{z}(s_0) = q_0^T \cdot \hat{\beta} + \lambda_0^T \cdot (z - q \cdot \hat{\beta}) \quad (7)$$

2.2 *Geographically weighted regression*

Geographically weighted regression was first explored by Fotheringham (1997), Brunsdon et al. (1998), Fotheringham and Brunsdon (1999), and Fotheringham (2000). Fotheringham et al. (2002) discussed in detail of geographically weighted regression.

For the value z (s_0) at a given location s_0, it can be estimated using it's neighbors with the set of values $z = z(z(s_1), z(s_2), ..., z(s_n))$. Considering k predictors of q, The GWR model can be written as Eq. 8.

$$\hat{z}(s_0) = \sum_{k=0}^{p} \hat{\beta}_k \cdot q_k(s_0) + \varepsilon \quad (8)$$

where ε is the residuals, and other notes as above. The objective of GWR is to obtain non-parametric estimates for each predictor q_i and at the location s_0. This can be processed using neighboring data of the location s_0. The basic process using GWR for spatial prediction can be summarized below: (1) determine the samples, (2) determine the unsampled location s_0, (3) design and compute a weight matrix (W) based on this location (i.e., Eq. 9), (4) compute the model coefficients using weighted least-squares regression using Eq. 10, and (5) estimate the values of an interesting property at the given locations using the fitted GWR model.

$$W_{s_0} = \begin{pmatrix} w_{01} & 0 & . & . & . & 0 \\ 0 & w_{02} & . & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & 0 & . & . & . & w_{0n} \end{pmatrix} \quad (9)$$

$$\hat{\beta}_{s_0} = (Q^T \cdot W_{s_0} \cdot Q)^{-1} \cdot Q^T \cdot W_{s_0} \cdot z \tag{10}$$

A number of weighting functions can be used. Gaussian function is given as an example as follows, and the weight at the location s_0 is calculated as:

$$w_{s_0} = \exp(-0.5(d/\tau)^2) \tag{11}$$

where d is the Euclidean distance between the location s_0 and its neighbors, τ is the bandwidth of the kernel. Detailed discussion of bandwidth and weight matrix can be found in the software of GWR (Fotheringham et al, 2002). Once the w for each unsampled location has been calculated, the coefficient matrix can be computed by repeated application of Eq. 10. Therefore, without specifying a function of the spatial variation a set of estimates of spatially varying parameters can be obtained at the unsampled locations. In the process of interpolation, each regression coefficient is predicted to characterize each predictor at a given location, and the GWR "lets the data speak for themselves" (Brunsdon et al., 1998).

Using GWR, the parameters are estimated using Eq. 11. For a given unsampled location s_0, the estimated value is calculated using Eq.12, where $q_{s_0}^T$ are the s_0 row of the Q, and $\hat{\beta}_{s_0}$ are the estimated parameter vector at the location s_0.

$$\hat{z}(s_0) = q_{s_0}^T \cdot \hat{\beta}_{s_0} = q_{s_0}(Q^T W_{s_0} Q)^{-1} Q^T W_{s_0} z \tag{12}$$

2.3 *Evaluation methods*

The GWR could provide better fits in terms of the residual because of the flexible estimations of the GWR coefficients at a given location. Regression kriging is another powerful model for local predictions because it takes into account the local dependence of the response variable into both regression parameter estimation and residual kriging. It is necessary to compare the performance of the two local spatial prediction models.

Visual comparisons are necessary to indicate the quality of local predictions of interpolations although the visual analysis is subjective. Statistical methods are performed to objectively quantify the differences between the original image and the predicted images using RK or GWR. (1) Basic statistics including mean, median, range, minimum, maximum, standard deviation (SD), kurtosis, skewness, and histogram are used to describe the basic distribution of the predicted imagery data and the original image data and compare their differences. (2) Root mean square error (RMSE) is used to compare the differences between the original and the predicted imagery across the whole study area; while mean absolute error (MAE) is used to compare the differences at per-pixel level. (3) Pearson correlation coefficient is applied to check the similarity of the distributions between the original and predicted images. (4) Using a raster data Ikonos images, the original images and the interpolated images are processed using two morphological functions of dilate and erode in order to compare performance of RK and GWR. Assessment of spatial structure is then conducted using Pearson correlation index.

Morphological processing typically is used to understand the structure of an image and identify boundaries or objects within an image. Morphological techniques here are used to indicate the potential spatial structure of spectral values within an image. To evaluate spatial effects of these local predictions, morphological processes with 3x3, 5x5, and 7x7 neighborhoods and the two morphological functions are applied to the predicted images and the original band 2. Dilate is used as a maximum operator to select the greatest values in the neighborhood, while erode is used as a minimum operator to select the smallest values in the neighborhood. Then, Person correlation coefficient is used to measure the agreement between the processed predictions and the original data.

3. Empirical Assessment

An Ikonos image with spatial resolution of 4 meter (i.e., band 2 is used as the response variable, and band 3 is used as an auxiliary variable) is used as an example. The GWR models are applied first according to Fotheringham et al (2002). Regression kriging is applied to model the images based on Gstat software package (Pebesma and Wesseling, 1998). The prediction models of RK and GWR are applied to interpolate pixel values of band 2 using band 3 as the predictor. Because all the locations in imagery have recorded values, it is relatively easy to conduct sampling techniques and use the sample data to build local-spatial prediction models. It also is relatively convenient to assess the performance of regression kriging and geographically weighted regression using the predicted values of the unsampled locations in the imagery.

3.1 *The data*

The coastal area located in Camp Lejeune (34.57° N latitude, 77.28° W longitude, Fig. 1), southeastern North Carolina, is used as the study area. Camp Lejeune is a coastal plain that changes in elevation from sea level to 19.2 m (63 feet) (Rootsweb, 2007). Different landscapes including hardwoods, mixed softwoods, vegetated wetlands, and roads cover this region (Fig.1).

Two popular sample techniques are applied to assess the local predictions using RK and GWR. 528 regularly distributed points are sampled and a simple random sampling is conducted to generate 264 points (Fig. 1).

3.2 *Results*

Based on the simple random sample of 264 pixels and the regularly sampled 528 pixels, GWR and RK are applied to predict the values of band 2 at the unsampled locations. The predicted pixels using GWR are depicted in Fig. 2, and RK predictions are portrayed in Fig.3. It seems that there is little visual difference between the original band 2 and the predicted bands obtained using GWR and RK. Contrast is a little strong in the predicted band 2 using GWR and the 528 sampled pixels (Fig.2). The band 2 obtained using RK and the 528 sampled pixels also results in a little strong contrast (Fig.3).

The GWR and RK have almost similar values of the basic statistics of mean, median, range, minimum, maximum, SD, kurtosis, and skewness as the original band 2 (Table 1). The predictions using both the sampled 264 and 528 pixels also have the similar values in these statistics. The prediction using RK and 528 sampled pixels has closer values of kurtosis and skewness to the original band 2 while relatively large differences in mean, minimum, and maximum between this prediction and the original band 2. The comparisons of histogram are consistent with the basic statistics, and there is not big difference of distribution between these predictions and the original band 2 (Fig. 4).

The diagnostic check of the GWR and RK using mean absolute error, relative mean absolute error, root mean square error, and Pearson correlation coefficient is consistent with the above descriptive comparisons. These diagnostics indicate there is not any significant difference between the prediction of GWR and that of RK (Table 2). There is not any significant difference between the prediction using the simple random sample of 264 pixels and the regularly sampled 528 pixels. There are very strong positive associations between all the predictions and the original band 2 (i.e., correlation coefficients are from 0.979 to 0.994). The higher the correlation coefficients, the better is the consistency between the predictions and the original data (e.g., the higher the correlation coefficients, the better the spectral similarity between the predicted imagery and the original imagery). Furthermore, the absolute errors are very small (i.e., from 4.97 to 8.62) and the values of the relative mean absolute error are only between 1.8 % and 3.2%.

Both the basic statistics and the diagnostics indicate that satisfied predictions are achieved using both the GWR and RK models. Also, the simple random sample (i.e., the 264 pixels) results in almost the same predictions as the much dense sample (i.e., the regularly distributed 528 pixels).

We may wonder whether the GWR and RK models perform similar in characterizing the spatial structure in their predictions. Are there some differences in spatial structures between the predicted values and the original values? Morphological analysis of the predicted pixel values and the original band 2 can help answer the two questions. We use two morphological functions of dilate and erode to process the predicted and the original band 2, and then for the processed bands Pearson correlation coefficients are calculated. The higher the correlation coefficient, the better is the spatial consistence between the predictions and the original band data. Given a window size, the dilate function is used to select the maximum values while the erode function is used to select the minimum values within the given neighborhood. In order to have a relative comprehensive analysis on spatial structure, window sizes of 3x3, 5x5, and 7x7 are applied for the morphologically processed bands. The correlation coefficients are then calculated and summarized in Table 3.

The very high correlation coefficients show that the RK model can be better than GWR model in characterizing spatial structure in the original data (Table 3). The relatively lower values of correlation coefficients between the GWR prediction and the original band 2 indicate that GWR performs relatively poor in maintaining local maximum values (i.e., after dilate functions are processed, the GWR predicted bands and the original band 2 are relatively lower correlated). The simple random sample (i.e., 264 pixels) and the much dense 528 pixels (i.e., the regularly distributed sample) result in similar values in correlation coefficients, and these similar correlation coefficients indicate that the much dense sample of 528 pixels cannot have apparent advantages to maintain the spatial structure in prediction.

4. Discussions and Conclusions

Regression kriging and geographical weighted regression model the quantitative association between the dependent variable and the predictor variables, therefore, the performance of local-spatial prediction also depends on the correlation represented among response and predictor variables. The higher the correlation between response and predictor variables, the better is the spatial prediction. The selection of auxiliary variables that are highly correlated with the variable of interest is important for local-spatial prediction of environmental or social-economic variables for which the measurement is time consuming and expensive. Remotely sensed images are typically the first choice of auxiliary variables that are relatively cheap of acquiring up-to-date information over a large area.

Both geographically weighted regression and regression kriging are powerful local-spatial prediction models. The descriptive comparisons between the original data and the predicted data and the diagnostic check of GWR and RK indicate both the LSPM of GWR and RK perform very well in spatial interpolation. Based on the sampled locations and the spatial non-stationarity, GWR provides flexible estimations of parameters and then uses these spatially varying regression parameters to interpolate values at unsampled locations but does not directly consider spatial dependence in the process of model development. The regression kriging model predicts values at unsampled locations by building a spatial regression model (i.e., incorporating spatial autocorrelation and its local variation into parameter estimation) combined with residual kriging (i.e., taking account of local-spatial autocorrelation in residuals). Additionally, regression kriging does not suffer from spatial non-stationarity in practice (Goovaerts, 1997).

The mophorlogical analysis and Pearson correlation coefficients show that regression kriging has a little superiority to geographically weighted regression in predicting spatial structure. Geographically weighted regression emphasizes the spatial non-stationarity but methodologically takes no-account of spatial correlation when model is developed. A distance-decreased function (e.g., Gaussin function is tested as an optimal one in this study) typically is used to calculate the weight matrix used in geographically weighted regression. In the process of prediction using regression kriging, the weight matrix for residual kriging and the spatial semivariogram for regression parameter estimation are determined by a relatively optimal semivariogram function that quantitatively models the spatial dependence and structure.

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Table 1. Descriptive comparisons of GWR and RK for local-spatial prediction

	Mean	Median	Range	Minimum	Maximum	*SD*	*K*	*S*
Band2	272	250	372	191	563	60	3.33	1.84
GWR-264	274	249	376	187	563	59	3.05	1.78
GWR-528	274	249	378	185	563	60	3.11	1.80
RK-264	274	248	376	187	573	60	3.02	1.79
RK-528	271	248	364	164	528	57	3.22	1.81

SD, standard deviation; *K*, kurtosis; *S*, skewness;

GWR-264 (or 528), geographically weighted regression using 264 (or 528) sampled pixels; RK-264 (or 528), regression kriging using 264 (or 528) sampled pixels.

Table 2. Diagnostic check of GWR and RK

	MAE	RMSE	*r*
GWR-264	5.81	2.236	0.992
GWR-528	4.97	2.000	0.994
RK-264	7.70	2.000	0.983
RK-528	8.62	3.162	0.979

MAE, mean absolute error; RMAE, relative MAE; RMSE, root mean square error; *r*, Pearson correlation coefficient between the predicted and original band 2. Other notes as Table 1.

Table 3. Correlation between the original band and the predicted bands after morphological processes

		GWR-264	RK-264	GWR-528	RK-528
3x3 window	Dilate	0.8717	0.9765	0.7318	0.9752
	Erode	0.9588	0.9707	0.9766	0.9633
5x5 window	Dilate	0.8783	0.9775	0.7471	0.9756
	Erode	0.9488	0.9653	0.9846	0.9462
7x7 window	Dilate	0.8829	0.9785	0.7580	0.9758
	Erode	0.9373	0.9575	0.7775	0.9287

Notes as Table 1.

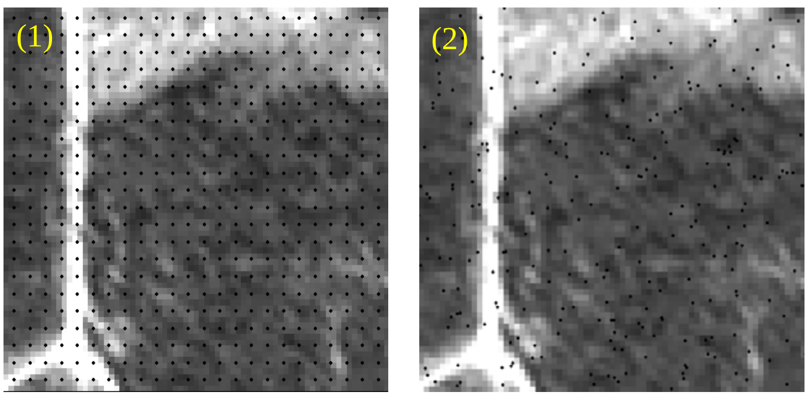

Fig. 1 Study area is located in North Carolina, US, center coordinates of 34.57° N / 77.28° W. 528 regularly distributed pixels (1) and 264 pixels obtained using a simple random sampling (2) are portrayed using Iknons band 2. Solid dark points are for sampled pixels.

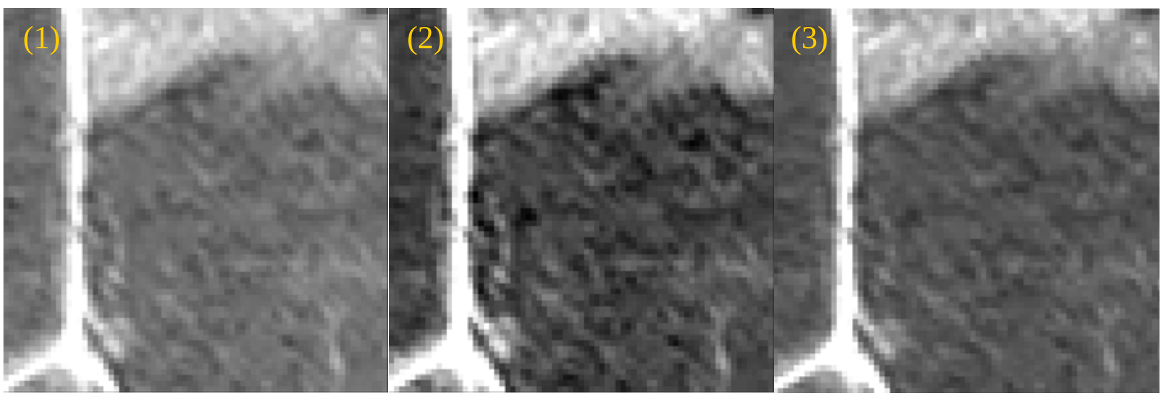

Fig. 2 Visual comparison of spatial prediction using geographically weighted regression (GWR). (1), predicted band 2 using GWR and 264 sample pixels; (2) predicted band 2 using GWR and 528 sample pixels; (3) the Ikonos band 2.

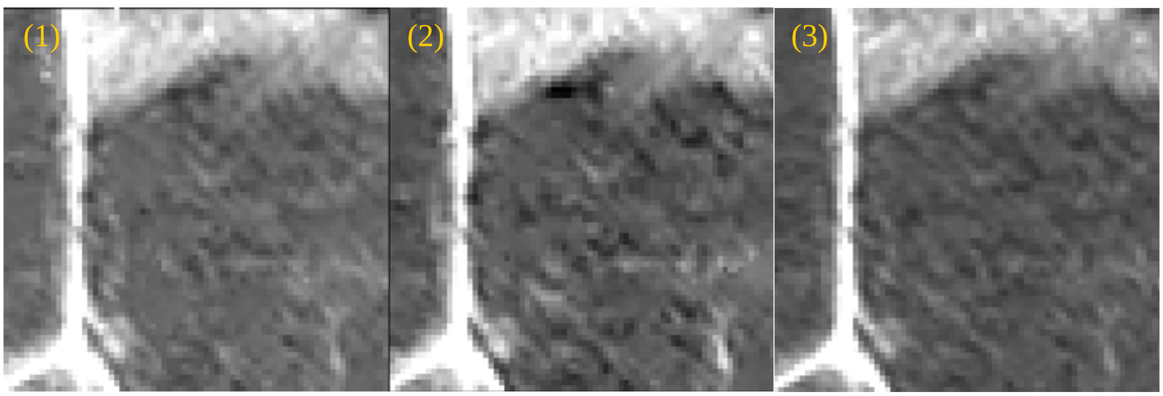

Fig. 3 Visual comparison of spatial predictions using regression kriging (RK). (1), predicted band 2 using RK and 264 sample pixels; (2) predicted band 2 using RK and 528 sample pixels; (3) the Ikonos band 2.

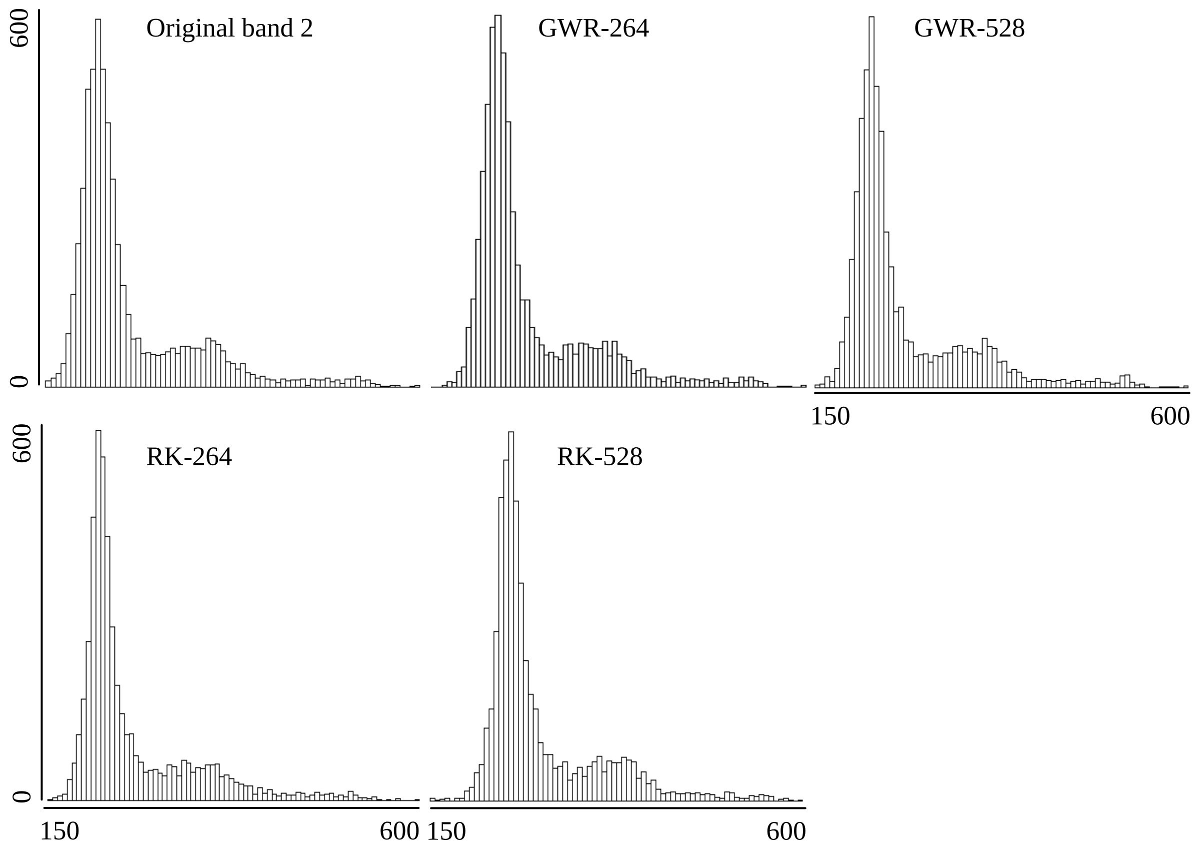

Fig. **4** Histogram of the original band 2 and its prediction using geographically weighted regression (GWR) and regression kriging (RK). GWR-264 (or 528), prediction using GWR and 264 (or 528) sampled pixels; RK-264 (or 528), prediction using RK and 264 (or 528) sampled pixels.