Using Genetic Algorithms to Estimate Local Shape Parameters of RBFs

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ABSTRACT

Estimation of *design rainfall* in unobservable places is important in hydrological engineering. The aim of this paper is to use genetic algorithms to find the optimal global and local shape parameters of *radial basis functions* (RBFs) to create an interpolation model to estimate scaling exponents of short term rainfalls across selected regions of Slovakia. Scaling exponents can be used later to estimate rainfalls intensity in places without observations. In this paper, we have used interpolation methods based on RBFs to model interpolation surfaces. We investigate the properties of shape parameters in RBFs, and we test some methods for finding an optimal shape parameter. The choice of the best basis function along with the optimal shape parameter has a significant impact on the accuracy of the interpolation models which best approximate the real model. We have found that Hardy's multiquadrics interpolant with the optimal local shape parameters can be used for estimation the rainfall intensities in areas without direct observation.

Keywords

Radial basis functions, genetic algorithms, thin plate spline, shape parameters, rainfall

1 INTRODUCTION

In hydrology, engineering designers often face the problem of unreliable estimation of design short term rainfall intensities in unobservable places, or insufficiently long time series of observations. Regionalization methods are often used to solve this problem. These methods use available spatial information, and they consequently achieve reliable estimates of design values without direct observation [Koh16].

This paper gives a new method to estimate scaling exponents using interpolation methods based on *radial basis functions* (RBFs) with optimal global/local shape parameters. Our new method has not yet been applied to such extent. Our aim is to create an appropriate model for spatial estimation of rainfall intensities in places without direct observation for selected months across selected regions in Slovakia.

From the mathematical point of view, we need to construct the interpolation surface as long as we have a few of data points arranged in an irregular mesh. We attempt to achieve high accuracy of used interpolation surface for data points, in which we have no observations.

From literature, RBFs are known as a very popular interpolation tool for solving our designed problem due to their simplicity and ability to accurately approximate underlying multidimensional scattered data. This methodology is competitive, and it gives a high numerical accuracy when we compare it with other interpolating methods. Some of the most recent applications of RBFs include, for example, cartography, neural networks, medical imaging, numerical solution of partial differential equations [Flw09], [Dyn87], [Dyn89], [Isk03], [Ska13]. Interpolation methods based on RBFs are also used in BSDF interpolation [WKB12], [Ward14]. Hierarchical genetic algorithms are proposed in [TR15] to tackle the problem of automatic curve fitting. In this paper, authors have used only the Gaussian RBF, they have not compared the global shape parameter with the local ones and as a test data they have used only analytically defined one dimensional functions. Rainfall approximation of the sparse rainfall data using RBFs is solved in [PC15], [PC16a] and [PC16b].

Many RBFs contain a free shape parameter c (see Table 1). The choice of the basis function and shape parameter has a significative impact on the accuracy of the method. In most papers authors choose this shape parameter by trial. Rippa [Rip99] has described a numerical algorithm to estimate the best value for shape parameter in radial basis interpolation using Leave One Out Cross Validation (LOOCV). Fasshauer and Zhang [FaZh07] used iterative approximative moving least squares approximation and RBFs pseudo-spectral method to estimate an appropriate shape parameter. Mongillo [Mon11] examined how to choose RBFs and shape parameters in a scattered data approximation.

Our paper introduces the idea of a global and local shape parameters estimation using genetic algorithms for scattered data. We discuss our method based on Leave Multiple Out Cross Validation (LMOCV) to estimate the best shape parameter(s).

The paper is organized as follows. Section 2 shortly describes the principle of the used interpolation methods based on RBFs. Section 3 presents our methodology and data. We discuss how an LMOCV strategy can be used in the context of finding the optimal shape parameter(s). Finally, section 4 presents our results. A comparison of the LOOCV and LMOCV method has been made. We have used root-mean-square error (RMSE) to compare selected interpolation methods based on RBFs.

2 INTERPOLATION METHODS BASED ON RBFS

The research of RBFs helps us understand how we can use these functions to solve practical problems. RBFs are preferred for image warping, geodesy, geography, digital terrain modeling, hydrology, etc. A good review of the theory of RBFs is given by Hardy [Har90], Powell [Pow91].

Let us have a set $\mathscr{X}$ of N different input points $\mathscr{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N \mid \mathbf{x}_i \in \mathbb{R}^2\}$ with rainfall intensity values $\mathscr{F} = \{f_1, \ldots, f_N \mid f_i \in \mathbb{R}\}$. We search for such function $S : \mathbb{R}^2 \to \mathbb{R}$, for which the interpolation conditions are true:

$$S(\mathbf{x}_i) = f_i,\ i = 1, \ldots, N. \tag{1}$$

We can write the interpolation function $S(\mathbf{x})$ in the following form [Rip99]:

$$S(\mathbf{x}) = \sum_{i=1}^{N} \lambda_i \Phi(\|\mathbf{x} - \mathbf{x}_i\|) \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^2$, $\Phi(r)$ is a fixed real-valued RBF and $\|\cdot\|$ denotes the Euclidean norm.

The solution of the above interpolation conditions (1) is equivalent to the solution of a linear system of equations:

$$\mathbf{A} \cdot \boldsymbol{\lambda} = \mathbf{f},\ \mathbf{A} = \mathbf{A}_{i,j} = \Phi(\|\mathbf{x}_j - \mathbf{x}_i\|) \tag{3}$$

for the vector $\boldsymbol{\lambda} \in \mathbb{R}^2$ of unknown coefficients. This interpolation problem is solvable if and only if matrix $\mathbf{A}$ is nonsingular. The general conditions on $S(\mathbf{x})$ which guarantee nonsingularity of $\mathbf{A}$ are given in [Mic86], and they can be checked for many radial basis functions. In particular, these conditions are fulfilled for the choices of the function $\Phi(r)$ given in Table 1.

Radial basis function	$\Phi(r)$
Polyharmonic splines (PHS)	r^3
Thin plate splines (TPS)	$(1/2)r^2 \log r^2$
Gauss function (GAUSS)	$e^{-r^2/2c^2}$
Hardy's multiquadric (HMQ)	$\sqrt{c^2 + r^2}$
Inverse multiquadric (IMQ)	$1/\sqrt{c^2 + r^2}$
Inverse quadric (IQ)	$1/(c^2 + r^2)$

Table 1: Commonly used types of radial basis functions

The RBFs listed in Table 1 contain a shape parameter c that must be specified by the user. It is well known [Fra82], [Rip99], [Mon11] that the accuracy of the RBFs interpolants depends heavily on the choice of the parameter c. A smaller value of the shape parameter c corresponds to a surface with a higher curvature and a higher value of the shape parameter c corresponds to a flatter surface with a smaller curvature. The global shape parameter influences the whole surface, but local shape parameters influence the shape of the surface only in the neighborhood of each interpolated point.

2.1 Thin plate splines

One of the most commonly used interpolation methods based on RBFs is *thin plate splines* method. This method adds a polynomial term into equation (2) and does not contain any shape parameter.

We can write the TPS interpolating function $S(\mathbf{x})$ in the form [Fog96]:

$$S(\mathbf{x}) = S(x, y) = c_1 + c_2 x + c_3 y + \frac{1}{2} \sum_{i=1}^{N} \lambda_i r_i^2 \log(r_i^2), \tag{4}$$

where $[x, y] \in \mathbb{R}^2$, $r_i^2 = (x - x_i)^2 + (y - y_i)^2$ and $c_1,\ c_2,\ c_3,\ \lambda_i \in \mathbb{R}$ are unknown coefficients. The unknown values λ_i, $i = 1, \ldots, N$, have to satisfy the boundary conditions:

$$\sum_{i=1}^{N} \lambda_i = 0,\ \sum_{i=1}^{N} \lambda_i \mathbf{x}_i = \mathbf{0}. \tag{5}$$

Applying interpolation conditions (1) together with boundary conditions (5), we can compute the unknown values using a system of equations:

$$\mathbf{A} \cdot \mathbf{L} = \mathbf{F},$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & x_1 & x_2 & \cdots & x_n \\ 0 & 0 & 0 & y_1 & y_2 & \cdots & y_n \\ 1 & x_1 & y_1 & 0 & r_{21}^2 \log(r_{21}^2) & \cdots & r_{n1}^2 \log(r_{n1}^2) \\ 1 & x_2 & y_2 & r_{12}^2 \log(r_{12}^2) & 0 & \cdots & r_{n2}^2 \log(r_{n2}^2) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & y_n & r_{1n}^2 \log(r_{1n}^2) & r_{2n}^2 \log(r_{2n}^2) & \cdots & 0 \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \lambda_1/2 \\ \lambda_2/2 \\ \vdots \\ \lambda_N/2 \end{pmatrix}, \; \mathbf{F} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix}$$

and $r_{ij}^2 = r_{ji}^2 = (x_j - x_i)^2 + (y_j - y_i)^2$.

2.2 Hardy's multiquadrics with local shape parameters

This method is very similar to the previous method, but it uses different RBFs, does not have a polynomial term and uses local shape parameters. For our interpolation problem, we obtain the following interpolation function:

$$S(\mathbf{x}) = S(x,y) = \sum_{i=1}^{N} \lambda_i \sqrt{c_i^2 + r_i^2}. \tag{6}$$

The local shape parameters c_i significantly change the shape of the resulting interpolation surface. In general, a smaller value of the parameter c_i creates so-called "sharp extremes" at point $\mathbf{x}_i$ in the graph of the function, while its greater value "smoothes" the function. Using local shape parameters instead of one global parameter allows not only to change the shape of the interpolation surface at each interpolation point but also can increase accuracy of the created interpolation model. Introducing local shape parameters has one drawback - matrix that is created by RBFs (see equation (3)) is not symmetric anymore, which leads to the problem of finding optimal local shape parameters c_i using standard optimization methods.

3 METHODOLOGY

Different RBFs and their different shape parameters give different interpolation surfaces for the same data set. Finding the best RBF and the best estimation of the shape parameter(s) that produces the most accurate results is one of the topics of our paper. In this section we investigate *cross validation methods* for optimizing the shape parameter(s) with respect to the error in interpolation methods based on RBFs.

We decide to exclude at most K data points in one step (interpolation function calculation) from a data set with sample size N (number of interpolation points), where K corresponds to approximately 10% of the sample size N.

3.1 Cross validation methods

Cross validation methods are used for evaluating the accuracy of the created model (e.g. interpolation function) by splitting the input data set into validation and training data. The model is created from the training data so that it fits the validation data with some small error.

In practical use, there are several rounds of cross validations using different partitions of the data set. The resulting statistical measure giving the accuracy of the model is given as the average of the errors calculated in the individual rounds.

Let M (number of rounds) be the number of the sets of points indices of the excluded points. For LOOCV method, we have $M = N$ and for LMOCV method, we have M given in advance such that $M > N$.

Leave one out cross validation (LOOCV)

LOOCV method uses 1 element as validation data and $N-1$ remaining elements as training data, from which we get N singleton sets $I_p = \{p\},\ p = 1,\ldots,N$ of indices of excluded points for model determination.

Leave multiple out cross validation (LMOCV)

LMOCV method uses a random number of elements for the validation data, while their number is limited by in advance given value K.

Let set $I_p = \left\{{}^p i_1, \ldots, {}^p i_{n_p}\right\}$ denote the p-th set of indices of the excluded data points for $p = 1,\ldots,M$, where ${}^p i_{n_k}$ is a random integer, $1 \leq {}^p i_{n_k} \leq N$, while cardinality $\left|I_p\right|$ (number of elements) of the set of indices varies from 1 to K.

3.2 Shape parameter estimation

Let $S^{(p)}(\mathbf{x})$ be the p-th interpolant of the reduced data set obtained by removing n_p points $\mathbf{x}_{{}^p i_1}, \ldots, \mathbf{x}_{{}^p i_{n_p}}$ and the corresponding data values $f_{{}^p i_1}, \ldots, f_{{}^p i_{n_p}}$ from the original data set. Our algorithm estimates the shape parameter c by minimizing the error vectors ${}^{p}\boldsymbol{\varepsilon} = ({}^{p}e_1, \ldots, {}^{p}e_{n_p})^{\mathsf{T}}$, where

$$ {}^{p}e_j = S^{(p)}(\mathbf{x}_j) - f_j, \; j \in I_p, \; p = 1, \ldots, M. \qquad (7) $$

The error vectors are calculated by using standard LOOCV or our proposed LMOCV method. We take RMSE as a measure of the quality how well the interpolation function calculated from reduced data set fits the interpolation function created from all data points.

RMSE for LOOCV method is defined by:

$$ \mathrm{RMSE}(c) = \sqrt{\frac{\sum_{j=1}^{N} \left[S^{(p)}(\mathbf{x}_j) - f_j\right]^2}{N}}, \qquad (8) $$

RMSE for LMOCV method is defined by:

$$ \mathrm{RMSE}(c) = \sqrt{\frac{\sum_{p=1}^{M} \left(\sum_{j \in I_p} \left[S^{(p)}(\mathbf{x}_j) - f_j\right]^2\right)}{\sum_{p=1}^{M} |I_p|}}. \qquad (9) $$

Global shape parameter estimation

The optimal value of the global shape parameter c is defined as the value of c that minimizes RMSE(c). Any standard numerical estimation method can be used for finding the optimal shape parameter.

Local shape parameters estimation

Both previously defined RMSE measures can be used for local shape parameters estimation, with the only difference that vector $\mathbf{c} = (c_1, \ldots, c_N)$ of the local shape parameters c_i (see Section 2.2) is used instead of one global parameter c.

We use a genetic algorithm because standard optimization methods like quasi-Newton methods are not robust enough when searching the optimal vector of local shape parameters.

4 DATA AND EMPIRICAL RESULTS

In order to demonstrate the functionality of our LMOCV method for computing the interpolation function, we have used 5 sample datasets that consist of scaling exponents of maximum rainfall intensities with duration between 5 and 1440 minutes (short–term rainfall) for the warm season, from April to September in 34 rain gauge stations measured in Slovakia. The rain gauge stations are summarized in Table 2 and the area of the three regions is displayed in Figure 1.

During April, it was possible to measure rainfall only for $N = 29$ rainfall stations, while in other months we have recorded the scale exponent for $N = 34$ rainfall stations.

Region	Rain gauge stations
1	Myjava, Senica, Kuchyňa - Nový Dvor, Jaslovské Bohunice, Oravská Lesná, Čadca, Piešťany, Prievidza
2	Bratislava - Koliba, Bratislava - letisko, Nitra - Veľké Janíkovce, Telgárt, Sliač, Boľkovce, Dolné Plachtince, Bzovík, Kamenica nad Cirochou, Somotor, Rožňava, Lom nad Rimavicou, Štós - kúpele, Moldava nad Bodvou, Hurbanovo, Košice, Liptovská Osada
3	Javorina, Červený Kláštor, Poprad, Švedlár, Tatranská Lomnica, Medzilaborce, Liptovský Hrádok, Štrbské Pleso, Jakubovany

Table 2: Selected Slovakia regions with the rain gauge stations distribution

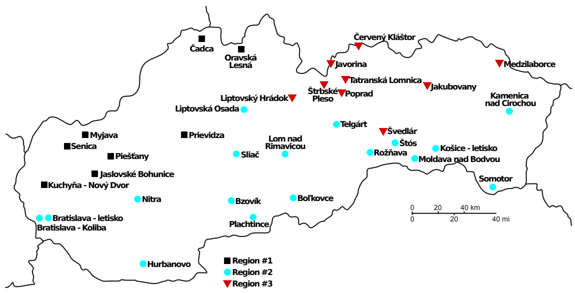

Figure 1: Map of the three selected regions and rain gauge stations

For our LMOCV method, we set $K = 4$, the maximum number of excluded data points in one step of interpolation function $S^{(p)}(\mathbf{x})$ calculation. We have created $M = 120$ sets I_p of excluded indices of rainfall stations.

We have discovered that searching the local shape parameters using classical optimization methods like quasi-Newton methods is inappropriate because these methods have found a local minimum instead of the global minimum. Therefore, we have decided to use genetic algorithms to find the global minimum. We have used the GA (see [Scr11], [Scr16]) and the GENOUD (see [Meb11]) genetic algorithm which are available as packages for **R** (**R** is a programming language and software environment for statistical computing). These packages combine the genetic algorithms approach with the standard optimization approach using BFGS optimization method and others.

We present the results of numerical experiments involving interpolation of the given datasets by polyharmonic splines, thin plate splines, Gaussian function, Hardy's multiquadric, inverse multiquadric and inverse quadric interpolants. We have compared the LOOCV and LMOCV method for excluding data points. Some selected results of the obtained interpolation surfaces for various datasets and various interpolation methods are shown in Figures 4–8.

Estimating the global shape parameter c for Hardy's multiquadrics is not suitable in general because of a very high curvature (peaks) at input points $\mathbf{x}_i$ on the created interpolation surfaces (see Figure 4). This undesirable shape is caused by the fact that the estimated shape parameter c is zero because of numerical instability of calculations in the optimization process. Consequently, we decide to find local shape parameters $\mathbf{c} = (c_1, \ldots, c_N)$ using genetic algorithms and with the LMOCV method, see Figure 5b.

In case of the inverse multiquadrics (see Figure 6) and other RBFs from Table 1, we do not face a problem with finding the optimal value of the global shape parameter. Except Hardy's multiquadrics, there is no problem with numerical instability for other RBFs. However, their accuracy is worse than that of Hardy's multiquadrics.

An example of interpolation surface created by the TPS method which does not need to estimate shape parameters is shown in Figure 7.

Table 3 and Figure 2 present RMSE calculated according to formula (8) and formula (9) for the optimal (best) global shape parameter c for interpolation methods based on RBFs from Table 1. We can see that the best accuracy is obtained for Hardy's multiquadric interpolant, the thin plate spline is second in order. The worst results have been achieved for the Gaussian RBF. As we can see, the LMOCV method gives smaller RMSE in comparison to the LOOCV method.

Figure 3 shows dependence between the RMSE and the global shape parameter c for dataset *June–July* while using Hardy's multiquadrics interpolation function. The LOOCV method gives the optimal value of the shape parameter c equal to 0.0854, and the LMOCV method gives the optimal value of the shape parameter c equal to 0.0621.

In estimating the global shape parameter for the dataset *April*, we would not be able to find its appropriate value due to numerical instability (see Figure 4). Even when we have used Q-R decomposition and SVD method for matrix equation calculation, we have experienced the same problem. In the optimization procedure, we have tried many statistical measures for the error vectors computation (MSE, MAE, MAPE, MASE and SMAPE) but we have not obtained acceptable results. We have decided to find optimal local shape parameters instead of the global parameter using the LOOCV and our proposed LMOCV method.

The LOOCV method for local shape parameter estimation gives low RMSE values (see Table 4), but the obtained function often oscilates (see Figure 5a) and has extreme values at the surface border. Using the LMOCV method, the RMSE is slightly higher, but the surface appears to be normal (see Figure 5b). Based on the above experiments, we propose that the value of the parameter c can be estimated by minimizing RMSE(c) using the LMOCV method.

5 CONCLUSION

We have found that the optimization procedure for estimating the global shape parameter of Hardy's multiquadrics interpolation function gives approximately zero value for many data sets. This zero value is unacceptable because it creates an inappropriate surface shape. Therefore, we have decided to use and estimate the local shape parameters. Classical optimization methods for the local shape parameters estimation is inapropriate because these methods rapidly converge to a local optimum. We have consequently decided to use two genetic algorithms - GA and GENOUD. Both algorithms combine genetic algorithms with the standard optimization method BFGS. We have also found that optimization process in the GENOUD package converges faster than in the GA package. Because standard LOOCV (Leave One Out Cross Validation) method for the model creation did not give good results for local shape parameters estimation, we have proposed the LMOCV (Leave Multiple Out Cross Validation) method.

Figure 5 and Table 4 show that the use of the optimal local shape parameters creates a smooth surface and gives lower RMSE values than the use of one global shape parameter. We conclude Hardy's multiquadrics interpolant with local shape parameters calculated using our proposed LMOCV method can be subsequently used in estimating the rainfall intensities in Slovakia, especially in areas without direct observation.

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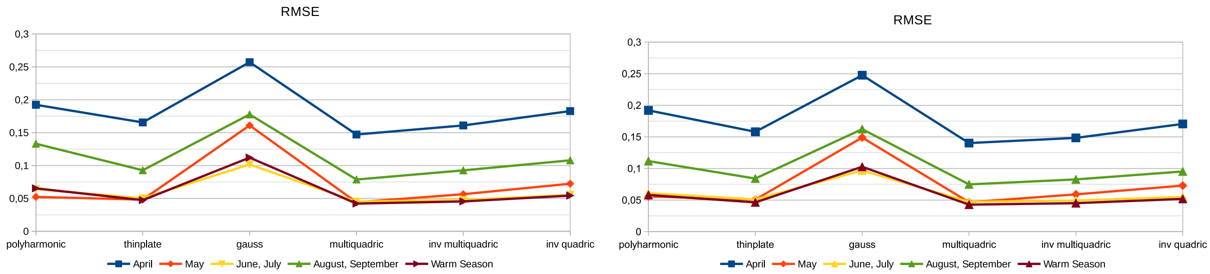
	PHS	TPS	GAUSS	HMQ	IMQ	IQ
Apr	0.192	0.166	0.257	0.147	0.161	0.183
May	0.052	0.048	0.161	0.044	0.056	0.072
Jun-Jul	0.064	0.050	0.102	0.045	0.048	0.055
Aug-Sep	0.133	0.093	0.178	0.079	0.093	0.108
Jun-Sep	0.065	0.047	0.112	0.042	0.045	0.054

(a) LOOCV method

	PHS	TPS	GAUSS	HMQ	IMQ	IQ
Apr	0.192	0.158	0.248	0.140	0.148	0.171
May	0.056	0.051	0.149	0.047	0.059	0.073
Jun-Jul	0.061	0.051	0.097	0.047	0.049	0.055
Aug-Sep	0.112	0.084	0.162	0.075	0.083	0.095
Jun-Sep	0.058	0.046	0.103	0.043	0.045	0.052

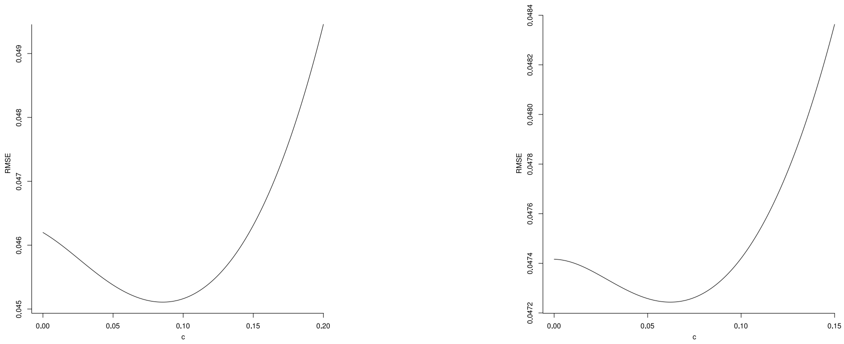
(b) LMOCV method

Table 3: RMSE comparison for various datasets and various RBFs with the global shape parameter



(a) LOOCV method (b) LMOCV method

Figure 2: RMSE comparison of two methods for points exclusion for various RBFs with the global shape parameter



(a) LOOCV method, $c = 0.0854$ (b) LMOCV method, $c = 0.0621$

Figure 3: RMSE vs. the value of the global shape parameter c of HMQ interpolation function for dataset *June–July*

	HMQ
Apr	7.546E-05
May	3.139E-09
Jun-Jul	2.229E-02
Aug-Sep	4.797E-05
Jun-Sep	9.438E-06

(a) LOOCV method

	HMQ
Apr	8.291E-02
May	2.625E-02
Jun-Jul	2.717E-02
Aug-Sep	5.015E-02
Jun-Sep	2.454E-02

(b) LMOCV method

Table 4: RMSE for HMQ interpolation function with the local shape parameters

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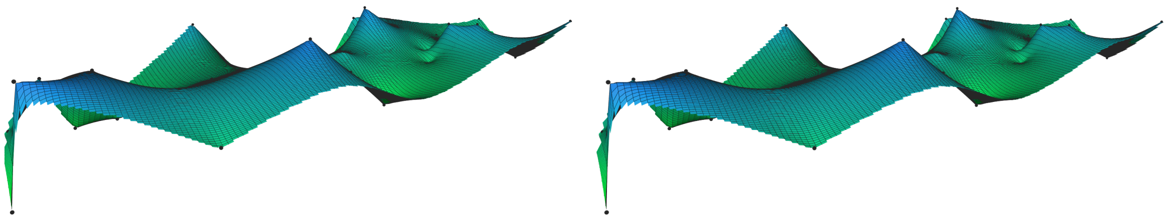
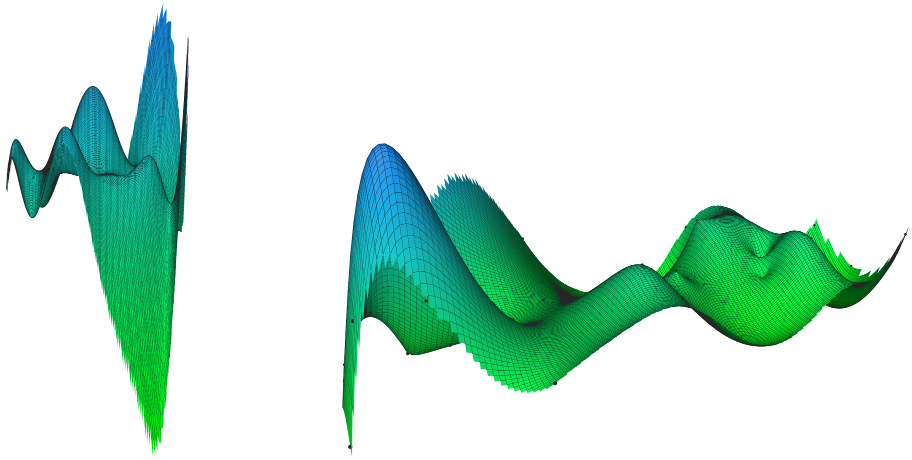


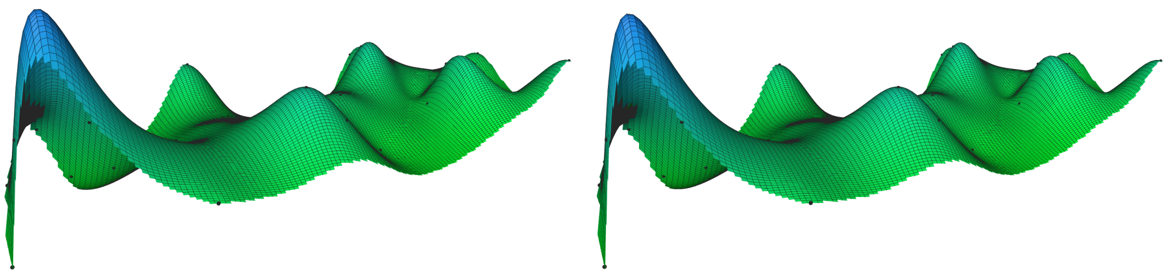
(a) LOOCV method, $c = 1.0\text{e}{-10}$ (b) LMOCV method, $c = 1.0\text{e}{-10}$

Figure 4: Dataset *April*: HMQ interpolation function with the optimal global shape parameter



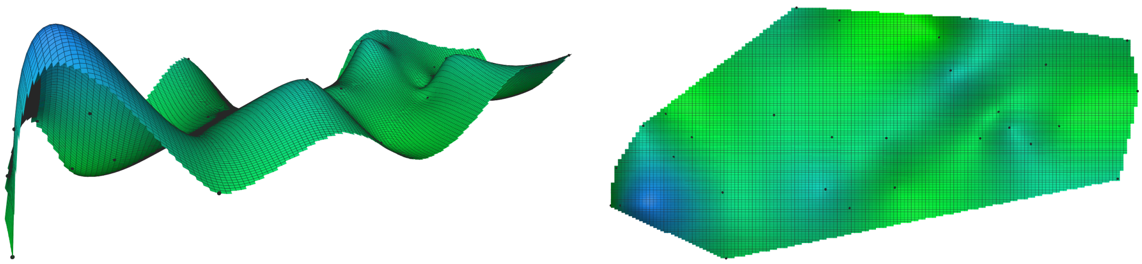
(a) LOOCV method (b) LMOCV method

Figure 5: Dataset *April*: HMQ interpolation function with the optimal local shape parameters



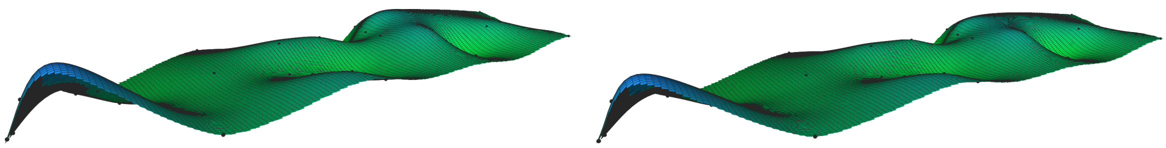
(a) LOOCV method, $c = 0.148$ (b) LMOCV method, $c = 0.143$

Figure 6: Dataset *April*: IMQ interpolation function with the optimal global shape parameter



(a) LOOCV method (b) Convex hull

Figure 7: Dataset *April*: TPS interpolation function with its top view



(a) LOOCV method, $c = 0.0854$ (b) LMOCV method, $c = 0.0621$

Figure 8: Dataset *June–July*: HMQ interpolation function with the optimal global shape parameter