Optimisation of Interpolation Parameters Using a Cross-validation

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1. Introduction

The high-quality and reliable data are a basic precondition for a successful implementation of any environmental project. Spatial complexity of terrain features in different landscapes (e.g. floodplains, mountains) imposes a challenge to automated digital terrain mapping. A new high-resolution data sources, such as SRTM and LIDAR are used, but their processing is not straightforward and requires more empirical experience and in-depth understanding. Divers approaches have to be adopted to meet specific demands of users. E.g., requirements for a digital elevation model in hydrological and sediment-flow applications are different from those in resource mapping.

There are many interpolation methods that can be used in digital terrain modelling. The interpolation is generally controlled by a set of parameters that enable to modify behaviour of the mathematical function so that a resulting surface meets the criteria of the user. Often, proper setting of these parameters is difficult and not clear to users.

The interpolation methods implemented in geographic information systems (GIS) have often control parameters set up as default constants or their functionality is poorly explained and influence on results is unclear. Instead of a clearly controlled procedure, the spatial interpolation becomes a black box for the user. In such case it is difficult to provide the end user with information on the uncertainty associated with the estimates generated during the interpolation. Therefore robust interpolation methods are needed that offer comprehensible parametrisation.

There are various approaches how to find optimal interpolation parameters. In practice, a trial-and-error method is often used, but much effort is needed, and less-experienced users can get quite poor results. There are also user-independent computational approaches. The best known is a cross-validation (CV), widely used in the interpolation applications (e.g Hancock and Hutchinson, 2003). The main advantage of the method is a clearly defined and user-independent algorithm that can be easily implemented in the software. The method is less reliable for surfaces with insufficient number of representative input points.

The Regularised Spline with Tension (RST) interpolation has been implemented as *s.surf.rst* and *v.surf.rst* commands and is widely used by the GRASS GIS users community (Neteler and Mitasova, 2002). Very recently, the RST method in GRASS GIS has been enhanced by a CV procedure. This option enables automation of the interpolation in a sense of choosing optimised interpolation parameters, but the applicability to different datasets is still not fully investigated. Also, the computational demands are rather high, and therefore it is currently applicable only to small datasets (up to 10^3-10^4 input points). Large datasets must be divided to smaller, representative subsets.

The goal of this paper is to test reliability and applicability of CV in an automatic optimisation of interpolation control parameters on an example of the regularized spline with tension and elevation data. The input elevation points are derived by random sampling with various densities from grid-based digital elevation models (DEM) with two different spatial resolutions (25m and 100m). The CV is applied on each sampled set of points to identify the optimum RST parameters. These parameters are subsequently applied in the interpolation of new surfaces, and their deviations to the original DEMs are analysed.

2. Interpolation by Regularised Spline with Tension

The RST method has been described by Mitasova and Mitas (1993) and Mitasova et al (1995). We briefly recall the basic principles of the method and focus on issues related to parameters that control the interpolation result.

The RST function $S(\mathbf{x})$ is a radial basis spline based on the condition of minimizing the deviation from the measured points and, at the same time, its smoothness seminorm $I(S)$ (e.g., Wahba 1990):

$$\sum_{j=1}^{N} \left| p^{[j]} - S\left(\mathbf{x}^{[j]}\right) \right|^2 w_j + w_0 I(S) = minimum \qquad (1)$$

where $p^{[j]}$ are the values measured at discrete points $\mathbf{x}^{[j]} = \left(x_1^{[j]}, x_2^{[j]}\right)$, $j = 1,\ldots,N$ within a region of a 2-dimensional space, w_j, w_0 are positive weighting factors and $I(S)$ is the measure of smoothness (smooth seminorm or roughness penalty). For $w_j / w_0 = 0$ the function $S(\mathbf{x})$ passes exactly through the data. The general solution of the minimization problem given by equation (1) can be expressed as a sum of two components (Talmi and Gilat 1977):

$$S(\mathbf{x}) = T(\mathbf{x}) + \sum_{j=1}^{N} l_j R\left(\mathbf{x}, \mathbf{x}^{[j]}\right) \qquad (2)$$

where $T(\mathbf{x})$ is a 'trend' function and $R(\mathbf{x}, \mathbf{x}^{[j]})$ is a *radial basis function* with an explicit form depending on the choice of the $I(S)$. The smoothness seminorm $I(S)$ for the RST method has been designed to synthesize in a single function properties of several previously known splines, such as Thin Plate Spline (Duchon, 1976), Thin Plate Spline with Tension (Franke, 1985; Mitas and Mitasova, 1988), Regularized Thin Plate Spline (Mitas and Mitasova, 1988). These desired properties include an explicit form, multi-variate formulation, smooth derivatives of higher orders, variational freedom through tension, and anisotropy. In 2-D formulation, the RST function generally defined by (2) has the following explicit form (Mitasova et al, 1995):

$$S(\mathbf{x}) = a_1 + \sum_{j=1}^{N} l_j \{-[E_1(r) + \ln r + C_E]\}, \qquad (3)$$

where $r = (j\, r/2)^2$, $r^2 = \sum_{i=1}^{d} \left(x_i - x_i^{[j]}\right)^2$ is the squared distance, C_E =0.577215 is the Euler constant, $E_1(.)$ is the exponential integral function (Abramowitz and Stegun, 1964), and j is a generalized tension parameter which provides the control over the influence of derivatives of certain order on the resulting function. The tension parameter controls the behaviour of the resulting surface from a thin membrane to a stiff steel plate.

3. The RST Control Parameters

One of the advantages of the RST interpolation is its flexibility within the single radial basis function, as opposed to often subjective selection of a suitable variogram in kriging. To properly consider the variability of a modelled phenomenon, the function can be tuned by a set of the following parameters:

- tension j ,
- smoothing w,
- anisotropy: rotation and scale (q, s),
- minimum and maximum distances between points.

The tension j , smoothing *w*, anisotropy (q, s) are internal RST parameters and they control the character of the resulting surface (Mitas and Mitasova, 1999). The parameters can be selected empirically, based on the knowledge of the modelled phenomenon, or automatically, by minimisation of the predictive error estimated by a CV procedure (Mitasova et al, 1995). In this study, we have tested only the tension and smoothing, as these are main parameters that control the interpolation result.

The tension parameter j plays a key role in areas with a steep change of modelled phenomenon where overshoots and undershoots of the interpolated surface occur. The RST method is scale dependent and the tension works as a rescaling parameter (high tension "increases the distances between the points" and reduces the range of impact of each point, low tension "decreases the distance" and the points influence each other over longer range). Surface with tension set too high behaves like a membrane (rubber sheet stretched over the data points) with peak or pit ("crater") in each given point and everywhere else the surface goes rapidly to trend. Surface with tension set too low behaves like a stiff steel plate and overshoots can appear in areas with rapid change of gradient (GRASS, 2000).

Using the smoothing parameter *w*, the RST behaves like an approximation function, i.e. the resulting surface does not pass through the given points, but approximates the input values. This parameter is useful in modelling of noisy data, where higher smoothing can filter out the noise, or alternatively, when a phenomenon is to be modelled at a lower level of detail.

The anisotropy parameters (q, s) can be used in the interpolation of anisotropic data. The orientation of the perpendicular axes characterising the anisotropy is defined by the rotation parameter q and the scaling ratio of the perpendicular axes (a ratio of axes sizes) is defined by the scale parameter s . These parameters scale distances (i.e. the value of tension as well) in 2 perpendicular directions that should fit the spatial pattern of the anisotropic phenomenon.

Minimum and maximum distances between points control the number of points that are actually used in the interpolation after reading the input data. The maximum distance can be used only for vector data in the GRASS GIS version 5.7. However, this parameter internally influences the effect of the tension, because the tension works as a distance-scaling factor. Therefore, the tension can be set with or without normalisation. The data density does not affect the normalised tension parameter. In this study we use only the normalised tension.

4. Evaluation of Interpolation Accuracy

The interpolation accuracy can be measured by different methods. The most straightforward is to evaluate deviations between interpolated surface and the input points. The overall error, measured e.g. by Root Mean Squared Error (RMSE) then characterises the interpolation accuracy in the given points. However, this approach does not provide information about the accuracy in areas between these points. The interpolation accuracy in areas between the input points is actually a predictive accuracy of the interpolation method. (This contrasts with approximation methods that need not to pass through the given input points.)

One of the options to evaluate the predictive accuracy between points is to use an evaluation dataset that contains data not used in the interpolation. For each evaluation point the deviation between actual and interpolated value are calculated and the overall accuracy is tested. However, in many applications due to a limited number of input points, such independent evaluation dataset is difficult to select. Moreover, the accuracy information is available only for these independent points and they rarely cover the entire area of interest with a sufficient density.

The accuracy assessment by a cross-validation is based on removing one input data point at a time, performing the interpolation for the location of the removed point using the remaining samples and calculating the residual between the actual value of the removed data point and its estimate. The procedure is repeated until every sample has been, in turn, removed. This form of CV is also known as the ‘‘leave-one-out’’ method (Tomczak, 1998).

The CV of this particular form is especially suitable for relatively dense data sets, since removing points from already under-sampled areas can lead to misrepresentation of the surface to be interpolated. Despite the wide use of this technique for assessing interpolation schemes, one should be aware of its shortcomings. Specifically, CV will usually overestimate the interpolation error because the estimate is being computed at a location where data are genuinely available. In addition, the computed surface and hence the cross-validated estimate may be altered by the removal of the point being cross-validated. In practice these issues are unavoidable but with increasing number of input data points they have less impact (Jeffrey et al, 2001).

The overall performance of the interpolator is then evaluated by statistical means such as the Root Mean of Squared Residuals, Mean Absolute Error (MAE) or Mean Error (Tomczak, 1998). Low Root Mean Squared Error (RMSE) indicates an interpolator that is likely to give most reliable estimates in the areas with no data. The minimum RMSE calculated by CV can be used to find the optimum interpolation control parameters (Mitasova et al, 1995). However, Hutchinson (1998) has found that CV does not always represent a reliable estimate of the model error, especially when a short-range correlation in data is present.

Therefore it is appropriate to use additional evaluation methods to ensure the reliability and consistency of the predictions. For example, in the interpolation of precipitation, a comparison with expert hand-drawn precipitation maps (e.g. Custer et al, 1996, Hofierka et al, 2002) and maps of derived hydrological processes can provide some insight into the capabilities of the interpolation algorithms to adequately represent the behaviour of the modelled phenomena, including the features which may not be directly incorporated in the data.

By CV that has been implemented in the GRASS GIS, the user can calculate prediction errors that are saved in the database as a point data set. As the computational demands are high, currently only a few thousands of points can be analysed in a reasonable time. However, the algorithm can be improved by simplifying the matrix calculations and by removing unused points that are located outside the inner interpolation segment.

5. Application to Digital Terrain Modelling

A suitability of CV for optimisation of interpolation control parameters was tested on samples of digital elevation data from Slovakia. The study area is located in the Central Slovakia at the contact of Turiec River floodplain with Veľká Fatra Mountains. The region consists of two parts: a relatively flat area in North-West with gentle slopes and floodplain containing terrain microforms and a mountainous area in South-East with steep slopes and narrow valleys. The size of area is 5.2 x 5.2 km, with the elevation ranging from 465 to 1380 m a.s.l. (Figure 1).

A spatial resolution of the DEM determines its application properties and ability to represent the terrain features in a desired detail (Weibel and Heller, 1991). Therefore samples were chosen from the two original raster DEMs – with resolution 25 and 100 meters, respectively (Figure 1). These two reference DEMs were generated by the *s.surf.rst* method from contour lines with 10-m interval, elevation points and a river network; all representing a scale 1:50 000.

The 25-m DEM represents the original (map) variability of surface with high conformity. The resulting surface is smooth, detailed features fit well with the original contour lines, small differences are visible in very narrow valleys and ridges. The surface represented by the 100-m DEM does not represent all the details of the original elevation structure, especially in the areas of high-frequency variability (slopes), but the overall trend of the terrain fits well. On the other hand, the 100-m DEM holds as much as possible of the original variability, and its smoothness and spatial autocorrelation is lower than in the 25-m DEM.

To assess CV suitability, the samples at different density are randomly taken and evaluated for the DEMs of both resolutions. The sample sets consist of 20, 10, 5, 2, 1, 0.5 % of the total number of cells (43 264) for 25-m DEM and 40, 20, 10, 5% of the total number of cells for 100-m DEM (2 704 cells).

Each random sample set was subject of an iterative interpolation with tension and smoothing parameters varying from 10 to 90 and from 0.1 to 0.9, respectively. For each iteration, the CV procedure was realised and an overall prediction error calculated using minimum, maximum error, mean error, standard deviation and RMSE. The predictive error for each individual sample point was saved into a GIS database. The overall results are compared in order to find the minimum statistical errors.

Generally, the lowest RMSE or MAE (mean absolute error) indicates the optimal parameter combination that should provide interpolation with the lowest prediction error. For each iteration, the prediction errors for individual points were analysed in order to see spatial differences in errors and sensitivity of parameters. The results of CV were also analysed by a visual inspection of the interpolated elevation and other topographic parameters (slope, aspect, profile and tangential curvatures). More information on topographic parameters used in the analysis can be found in Mitasova and Hofierka (1993).

For each combination of tension and smoothing, the CV deviations were compared with deviations between the reference surfaces and surfaces interpolated form random samples (elevation, slope and curvatures) on a per-pixel basis. This approach allows getting detailed information about errors for the entire study area.

6. Results and Discussion

CV provides reasonable results on condition that sampling points sufficiently cover the modelled terrain.

For the 25-m DEM, the results become consistent and reliable when using the 8,653 points (20% of total grid cells). As the optimum parameters, tension = 20 and smoothing = 0.1 were selected. This combination gives the overall RMS error of 1.45 m, which is fairly acceptable for the scale of the original data (Table 1, Figure 2).

While sampling a lower number of points (i.e. in our case 2-10% of grid cells), CV still offers optimum set-up of the interpolation control parameters (tension = 30 and smoothing = 0.1), however the interpolation error becomes worse. This reflects the fact that lower number of sampling points does not represent sufficiently the high variability of the reference surface. The decrease in the accuracy with lower sample density is clearly seen in the Figure 2 where the differences between reference and interpolated surface rapidly increase both in amplitude and extent.

While both 10% and 5% samplings fit the overall surface trend well, the samplings of 2% and less do not represent correctly important features of the reference surface. This is also evident from the derived topographic parameters. As regards the 2% sampling, it is important to note that despite the deviations in the vertical dimension, CV still offers the optimal interpolation parameters in the sense of minimum surface differences.

The CV procedure doesn't work properly when selecting less then 1% of the cells. A number of points in this sampling do not capture representatively the terrain features; therefore the prediction provides results with unacceptably high RMSE. Visual inspection of the results confirms these statements. Visualised slope and curvatures reveal that decreasing number of sampling points increases the surface smoothness and generalisation. The evident leap in the surface smoothness is between the 5% and 2% samplings.

The similar results were obtained from analysing the random samples from the 100-m DEM. While CV procedure gives optimum parameters (tension = 30 and smoothing = 0.1) and acceptable results for input data representing 40% and 20% of the total cells (that is around 2% level in the 25-m DEM), the lower point densities make CV unusable (Table 2, Figure 3).

Despite the high point density in the 40% sample, the RMS predictive error is rather high (12.61 m). This fact relates to the lower smoothness of the reference 100-m DEM that decreases the prediction accuracy of values at missing points. The visual inspection of the results (Figure 3) reveals that even the 40% sampling density significantly smoothes out the resulting surface. In analogy to the 25-m DEM case, the decreasing sampling density smoothes and generalises the original terrain structures. While a surface interpolated from the 20% sampling fits the main structure of the reference surface well, the 10% and less samples fail to capture sufficient information about the terrain forms.

The analysis of the spatial distribution of the predictive error is done from the CV deviations that were calculated for each sample point. The Figure 4 shows an apparent error dependency on the vertical differentiation of the terrain. While the error amplitude is low in the flat area these values become quite high in the mountainous area. This trend is obvious in all samples, and the range of errors increases with decreasing sampling density. In high-density samples, a significant number of points with low deviations can be found in the mountainous area, while the low-density samples contain only few points with acceptable deviation.

The presence of high deviations (more then +/- 10 m) in relatively dense samples (even in 10% sample) indicates that there are local maxima of absolute prediction error that should be treated carefully when evaluating the resulting surface. It is apparent that the frequency of local maxima is high in the area of ridges and valleys, which generally represent the local extremes, typically with high curvature. This imposes a question whether the optimisation of interpolation parameters based on the averaging of CV deviations from all points (such as RMSE) is suitable for each application. In some cases, other criteria such as minimisation of local maximum deviations could be considered.

7. Conclusions

This study has demonstrated that the Regularised Spline with Tension and cross-validation are appropriate and effective tools in digital terrain modelling if density of the input elevation data is sufficient. With optimisation of parameters by CV, the RST method can be fully automated and applicable in various mapping tasks, not only for generation of the DEM, but also for interpolation of other spatially-distributed phenomena. The optimisation of RST control parameters by CV helps to minimise the prediction error and maximise the exploitation of the method. Considering the fact, supported by many studies, that the RST is one of the most accurate interpolation methods, this provides the user a combination of tools that are valuable in many applications. This approach makes the use of advanced interpolation methods such as RST easier to use for less experienced users.

The main drawback of CV is that it does not guarantee optimum parameters in all situations. The reliability of CV depends on density and homogeneity of input points. For lower data densities, the applicability of CV must be assessed by other methods and the CV deviations should be compared with the original values and local variations. The selection of appropriate criteria for parameter optimisation for heterogeneous data still poses a challenge for further study.

The pre-processing of input data may significantly affect the quality of interpolation (see Cebecauer et al 2002) and therefore it should be considered prior to the application of CV. Other task-specific criteria (e.g. preservation of extreme values, surface smoothing and generalisation, hydrological connectivity) should also be taken into account when selecting the optimal parameters. These criteria may be often in a contradiction with the results found by CV.

This study provides an in-depth insight that is one of preconditions for further development of RST in the GRASS GIS. An important task for the future is a spatial analysis of CV deviations. The understanding of the linkage between deviations and the spatial variation of the modelled phenomena is needed for proper sampling strategies and for introduction of spatially variable RST parameters (such as the smoothing and tension in different types of terrain).

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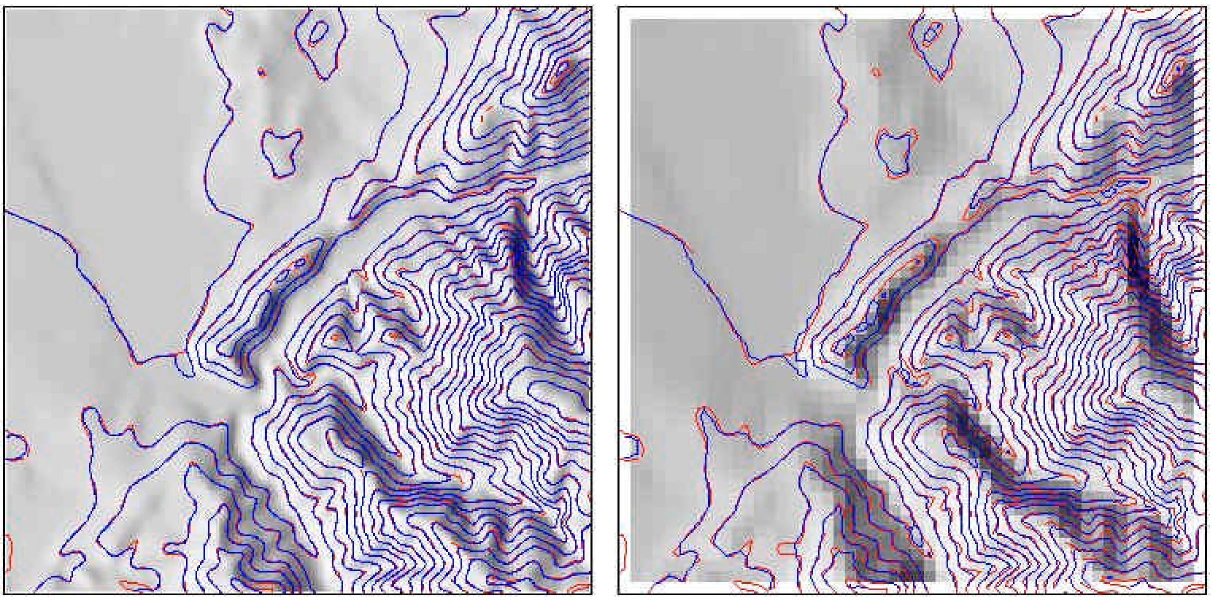

Figure 1 Comparison of the two reference DEMs with spatial resolution of 25 m (left) and 100 m (right). The red lines represent original contours from topographic maps that were used for generation of both reference DEMs; the blue lines represent contours that were derived from the created DEMs (contour interval 50 m).

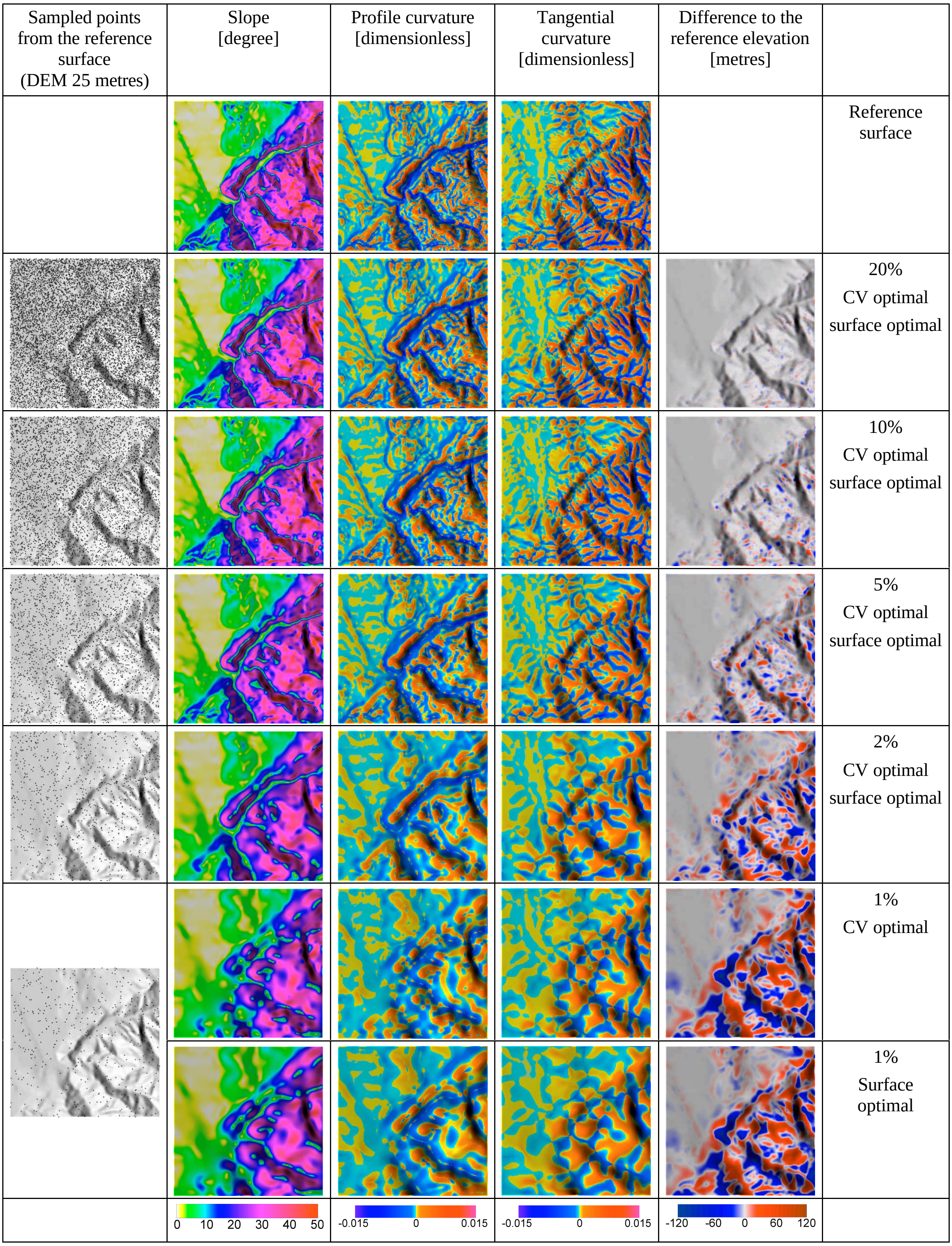

Figure 2 Comparison of the reference and interpolated surfaces (for random samplings taken from the DEM with 25 m resolution) using the optimised parameters from CV and from the comparison of interpolated surfaces with the reference. The values of optimal parameters are presented in the Table 1.

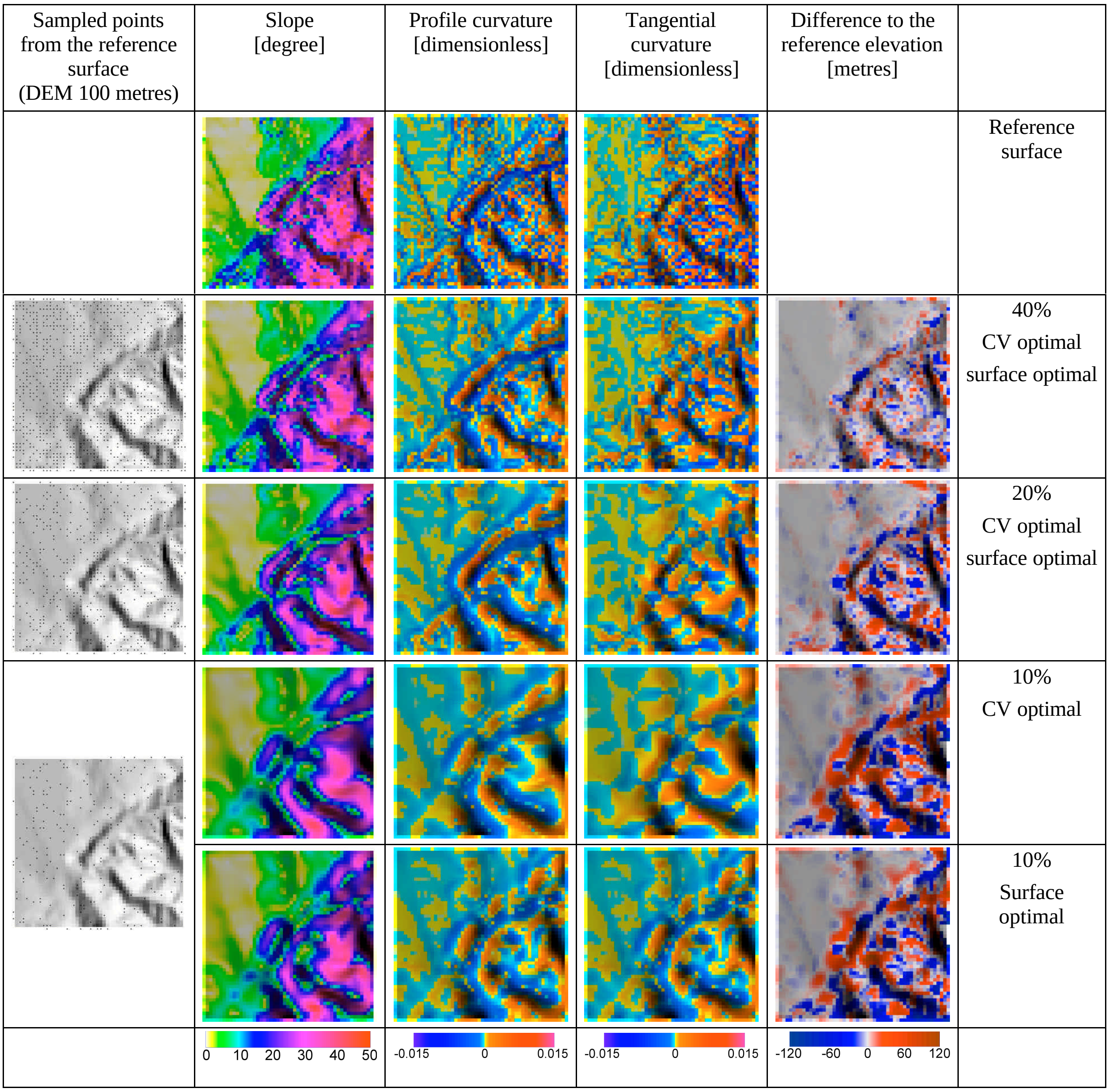

Figure 3 Comparison of the reference and interpolated surfaces (for random samplings taken from the DEM with 100 m resolution) using the optimised parameters from CV and from the comparison of interpolated surfaces with the reference. The values of optimal parameters are presented in the Table 2.

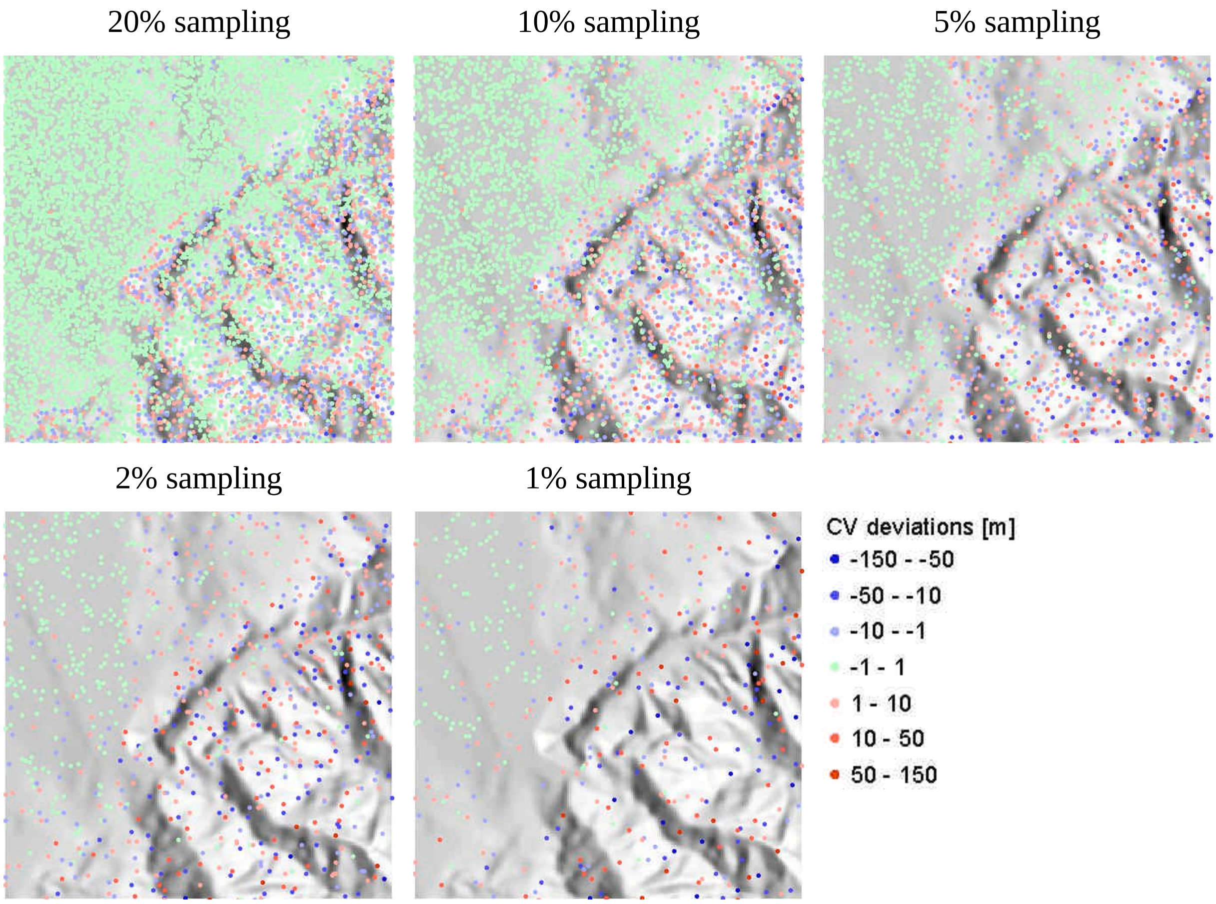

Figure 4 Spatial distributions of the CV deviations for CV-optimized interpolation parameters, for 20%, 10%, 5%, 2% and 1% sampling (for the reference DEM with 25 m resolution)

Table 1 The RST parameters optimised by the cross-validation and by the statistical comparison of surfaces for different samplings and the reference 25-m DEM. The last row presents optimum parameters and RMSE for vertexes of contours used to interpolate a reference surface.

Percentage of 25-m DEM cells	# of points	CV			Surface comparison (reference vs. interpolated)		
		Tension	Smoothing	RMSE	Tension	Smoothing	Standard dev.
20%	**8653**	20	0.1	1.45	20	0.1	1.26
10%	**4326**	30	0.1	3.36	30	0.1	3.35
5%	**2136**	30	0.1	6.69	30	0.1	5.95
2%	**865**	30	0.1	13.92	30	0.1	13.68
1%	**433**	45	0.1	26.54	*30*	*0.1*	*20.08*
0.5%	**216**	25	0.1	26.63	*35*	*0.1*	*31.96*
contours	**10216**	30	0.2	3.77			

Table 2 The RST parameters optimised by the cross-validation and by the statistical comparison of surfaces for different samplings and the reference 100-m DEM.

Percentage of 100-m DEM cells	# of points	CV			Surface comparison (reference vs. interpolated)		
		Tension	Smoothing	RMSE	Tension	Smoothing	Standard dev.
40%	**1082**	30	0.1	12.61	30	0.1	9.51
20%	**541**	30	0.1	19.20	30	0.1	15.66
10%	**270**	25	0.1	28.63	*40*	*0.1*	*26.62*
5%	**135**	20	0.1	43.91	*55*	*0.1*	*40.78*