COMPARISON OF APPROXIMATION METHODS FOR PARTIAL DERIVATIVES OF SURFACES ON REGULAR GRIDS

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In many GIS is implemented the approximation of partial derivatives of the 1st and the 2nd order. These derivatives are further used for computation of surfaces of derived morphometrical variables as slope, aspect and different types of curvatures. In geomorphologic researche are often required surfaces of derived morphometrical variables of the 3rd order. It is impossible to approximate the partial derivatives of the 3rd order with sufficient quality by tools offered in a common GIS. In this paper is presented and tested a method for this approximation fulfilling the accuracy requirements.

Key words: partial derivatives of the 3rd order, approximation, GmIS, morphometrical variables

1 PREFACE

Common GIS are not offering approximation of partial derivatives of the 3rd order. High quality partial derivatives of the 3rd order are crucial for computing morphometrical variables of the 3rd order widely used in geomorphometry. For the requirements of Geomorphologic Information System (GmIS) was in PACINA (2008) implemented a robust algorithm for approximation of partial derivatives up to the 3rd order with sufficient quality. This article is focused on testing the accuracy of different methods for approximation of partial derivatives.

Approximated partial derivatives by method described in PACINA (2008), JENCO et al. (2009) and PACINA (2009a) are used for computation of derived morphometrical variables up to the 3rd order. Surfaces of derived morphometrical variables of different orders are further on used for automatic delimitation of elementary forms of georelief (PACINA 2008, PACINA 2009a, PACINA 2009b and PACINA and JENČO 2009).

This algorithm is approximating the partial derivatives from 5x5 neighbourhood by general polynomial of the 3rd order¹, using the weighted least square method. For the least square method were proposed and tested two different weights. Into the process of testing were included methods for approximation of partial derivatives of the 3rd order (based on non-weighted least square method) presented by FLORINSKY (2009), and standard methods available in common GIS.

A polynomial function with variables of topographical surface was chosen for the comparison of results. From this polynomial function we can compute absolutely precise partial derivatives which are further used as the *etalon*.

The accuracy of approximation of the 1st and the 2nd derivatives was tested only by visual control and comparison of isolines, because this approximation is implemented in most of commonly used GIS. The test of approximation accuracy of the partial derivatives of the 3rd order is based on analysing the differences between the etalon and the computed derivatives. For the comparison of these differences were used four statistical indicators.

2 TESTED METHODS

This article is focused on the accuracy of the 3rd derivative approximation. The implemented method for the 3rd order partial derivative is producing the 1st and the 2nd partial derivatives as well. These results are tested only by visual comparison of isolines.

2.1 Methods based on splines

Very powerful and accurate method for computing partial derivatives² is a method called regularized spline under tension (RST). By constructing the spline surface is the whole area divided into segments. For each of the segments of the spline surface is computed parametrical expression. By deriving the parametrical expression we get the partial deriva-

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tives in the direction of x and y. The RST computation is implemented for instance in GIS GRASS. With the use of the RST interpolation, we can get only the first and the second order partial derivatives. For more information about RST see MITÁŠ and MITÁŠOVÁ (1988) and MITÁŠOVÁ and MITÁŠ (1993).

In this case was the RST interpolation applied on the regular grid (Fig. 2) computed by the polynomial (3.1). The input points were reinterpolated using interpolation parameters to preserve the original input surface structure.

2.2 METHODS BASED ON APPROXIMATING POLYNOMIAL

Using these methods, we approximate data on the grid by the polynomial function. The approximate derivatives of data on the grid are computed by derivation of the polynomial function. The order of used polynomial may not to be lower than the order of computed derivative.

This method based on derivation of interpolation polynomial is very common in GIS. Here we compute the derivation of interpolation polynomial just by computing the differences of the neighbouring cells and divided by their distance. This method can compute partial derivatives of any order just by applying the same computation over and over again. From the derivative of the 1^{st} order, we can compute de-rivative of the 2^{nd} order in the same way as the 1st order derivative. This method is very unstable for computing partial derivatives of higher orders and therefore is successfully used only for approximation of the 1st and 2nd partial derivatives.

Approximation based on general polynomial of the 2^{nd} order is shown in CHAPLOT et al. (2006) or MENTLÍK et al. (2006). Polynomial (2.2.1) is used for the approximation of the 1^{st} and the 2^{nd} partial derivative.

(2.2.1)

$$z(x,y) = a_0 + a_1x + a_2y + a_3xy + a_4x^2 + a_5y^2$$

We will estimate the approximation from the 3x3 neighborhood. Polynomial (2.2.1) has only six coefficients, therefore the weighted least square method must be applied. We consider that the highest weight has the point in the centre of the 3x3 neighborhood and points further from the center have less influence on the computed partial derivative. For estimating the partial derivatives of the 3^{rd}_{+} order, we need to use the polynomial of the 3^{rd} order.

2.3 APPROXIMATION BASED ON GENERAL POLYNOMIAL OF THE 3RD ORDER

We will approximate the input data by a general polynomial of the 3rd order:

(2.3.1)

 $z_{i,j}(x, y) = a_0 + a_1(x - x_i) + a_2(y - y_j) + a_3(x - x_i)^2 + a_4(y - y_j)^2 + a_5(x - x_i)(y - y_j)$ $+a_6(x - x_i)^3 + a_7(y - y_j)^3 + a_8(x - x_i)^2(y - y_j) + a_9(x - x_i)(y - y_j)^2$

We will use the 5x5 neighbourhood of actually computed point. Let us mark the coordinates of the centre of the 5x5 neighbourhood in which we will approximate the derivatives $(x_i,$ y_i). On **Figure 1** are shown the nods of the 5x5 neighbourhood. Symbols f in each of the nods represents function values in the nod. Value his distance between the nods.



2.3.1 Estimation of derivatives

Let us estimate derivatives of the polynomial in the point (x_i, y_i) . Then $z(x_i, y_i) = a_0$. Partial derivative of z by x will then be:

(2.3.2)

$$\frac{\partial z}{\partial x} = a_1 + 2a_3(x - x_i) + a_5(y - y_j) + 3a_6(x - x_i)^2 + 2a_8(x - x_i)(y - y_j) + a_9(y - y_j)^2.$$

¹ For example the morphometrical variables of the 3^{rd} order: a_{gn} – change of orientation change in the direction of a fall line, A_{Ntt} – change of orientation in the direction of a contour line ² RST is primarily used for interpolating an elevation grid from elevation data

From which results:

$$\left. \frac{\partial z}{\partial x} \right|_{(x_i, y_j)} = a_1. \tag{2.3.3}$$

And the other derivatives:

 $\begin{array}{l} (2.3.4) \\ \frac{\partial z}{\partial y}\Big|_{(x_i,y_j)} = a_2, \frac{\partial z^2}{\partial x^2}\Big|_{(x_i,y_j)} = 2a_3, \frac{\partial z^2}{\partial y^2}\Big|_{(x_i,y_j)} = 2a_4, \frac{\partial z^2}{\partial x \partial y}\Big|_{(x_i,y_j)} = a_5. \\ \frac{\partial z^3}{\partial x^3}\Big|_{(x_i,y_j)} = 6a_6, \frac{\partial z^3}{\partial y^3}\Big|_{(x_i,y_j)} = 6a_7, \frac{\partial z^3}{\partial x^2 \partial y}\Big|_{(x_i,y_j)} = 2a_8, \frac{\partial z^3}{\partial x \partial y^2}\Big|_{(x_i,y_j)} = 2a_8. \end{array}$

2.3.2 Estimation of the derivatives coefficients

We interleave the polynomial (2.3.1) across 25 nods (5x5 neighbourhood), but the polynomial (2.3.1) has got only ten coefficients, so we use the least squares method. To encounter the higher influence of points closer to the center of approximate area, we will use the weighted least square method.

$$\sum_{k=-2}^{2} \sum_{l=-2}^{2} w_{ij} [f_{k,l} - z(x_i, y_j)]^2, \qquad (2.3.5)$$

where $w_{i,j}$ is the weight of x_{i,y_j} point, $f_{k,l}$ is value in the nod and $z(x_i, y_j)$ is the function value of the polynomial (2.3.1) in the point (x_i, y_j) .

For the right choice of the weight is important to take into account the influence of the surrounding nods, which should be decreasing with the increasing distance from the middle. For the computation was used the following weight:

$$w_{i,j} = \frac{2h\sqrt{2}}{\delta + h\sqrt{i^2 + j^2}},$$
(2.3.6)

where $\delta \ge 0$ (for example 0.1), which influences the importance of the points further from the center.

The system of linear equations for computing the unknown coefficients can be overestimated hence in general must not have any solution. We will then estimate the unknown coefficients by the least square method³.

The unknown coefficients $a_0,...,a_9$ of the polynomial (2.3.1) are given by

$$\mathbf{a} = \mathbf{B}_{\mathbf{w}} \mathbf{f},\tag{2.3.7}$$

and $\mathbf{B}_{\mathbf{w}}$ is computed by this formula.

$$\mathbf{B}_{\mathbf{w}} = inv(\mathbf{Q}^{\mathrm{T}}\mathbf{W}^{\mathrm{T}}\mathbf{W}\mathbf{Q})\mathbf{Q}^{\mathrm{T}}\mathbf{W}^{\mathrm{T}}\mathbf{W}.$$
 (2.3.8)

Size of matrix \mathbf{Q} is 25 x 10, size of \mathbf{a} is 10 x 1 (vector of unknown coefficients) and f is 25 x 1 (vector of the nods).

The computation made in this way is very fast. The matrix is computed only once during the first computation. We do not have to compute all the coefficients of, but only those we need for computation of the partial derivatives of the desired order. The matrix was computed analytically (with the help of symbolic computations in Matlab). This helped to avoid the rounding error during computation of matrix, which made the computation even more precise.

FLORINSKI (2009) introduced similar method for approximations of partial derivatives of the 3rd order based on Taylor approximating polynomial and standard least square method (without weights). The partial derivatives of the 3rd order along FLORINSKI (2009) are computed in the following manner:

$$\begin{aligned} \frac{\partial^3 z}{\partial x^3} &= \frac{z_5 + z_{10} + z_{15} + z_{20} + z_{25} - z_1 - z_6 - z_{11} - z_{16} - z_{21}}{10w^3} + \\ &+ \frac{2(z_2 + z_7 + z_{12} + z_{17} + z_{22} - z_4 - z_9 - z_{14} - z_{19} - z_{24})}{10w^3}, \end{aligned}$$

(2.3.9)

where z_i are the values from 5x5 neighborhood and w is the cell size.

3 THE METHOD OF TESTING

The approximation accuracy was tested on a testing polynomial function with the character of topographical surface. This function was formerly used in BENOVÁ (2005).

$$z = 150 + 0.2y - 1.5 \cdot 10^{-4}y^2 - 2 \cdot 10^{-7}y^3 + 0.1x + + 1.6 \cdot 10^{-4}xy - 1.2 \cdot 10^{-6}xy^2 + 10^{-4}x^2 + + 3.2 \cdot 10^{-6}x^2y + 2 \cdot 10^{-12}x^2y^3 - 10^{-6}x^3 - 10^{-12}x^3y^2 - 10^{-14}x^3y^3 + 2.5 \cdot 10^{-17}x^3y^4 - 5 \cdot 10^{-17}x^4y^3 - 10^{-19}x^4y$$

The polynomial (3.1) is designed with the following properties:

- Graph of the polynomial is a continuous surface. At each point $A_i(x_i, y_i, z_i)$ of this surface are continuous partial derivatives up to the 3^{rd} order.
- At each point $A_i(x_i, y_i, z_i)$ it is possible to express the values of required morphometrical variables.
- The area must contain at least one saddle point and one peak.

To fulfill the presented requirements for values of x and y of the polynomial (3.1) should be valid:



 $x \in (-300, 300), y \in (-200, 600)^4$.

Partial derivatives in the direction of x and y up to the 3^{rd} order were computed by the methods described above. As the *etalon* we use the functional values of the particular derivatives in the direction of x and y.

The accuracy of partial derivatives of the 1st and the 2nd order was tested in many other papers (see MITÁŠ and MITÁŠOVÁ 1988)), we will only visually evaluate the isolines of derived morphometrical variables computed from these derivations.

The accuracy of the partial derivatives of the 3^{rd} order is tested by evaluating the following parameters:

• Equivalence rate = In ideal case should the resulting value equal 100 %.

- Arithmetic average = arithmetic average of data differences (etalon vs. computed).
- Standard deviation = quadratic average of values variation from their arithmetic average. For the computation are again used the data differences.
- RMSE Root Mean Square Error.

To make the description of the results easier, let entitle the tested methods in the following manner:

- *etalon* partial derivatives approximated using the functional values of the derivatives in the *x* and *y* direction,
- *method_1* approximation from the RST function,
- *method_2* neighbourhood differences based approximation,

³ For the whole derivation of the weighted least square method see PACINA (2008)

⁴ The input surface was transformed into fictional coordinate system for easier processing in GIS GRASS and Matlab



- *method*_3 approximation based on the polynomial of the 2^{nd} order,
- *method* <u>4</u> approximation based on the polynomial of the 3rd order,
- *method* <u>5</u> approximation along FLORINS-KY (2009).

3.1 TESTING RESULTS

3.1.1 1st partial derivatives

The preciseness of partial derivatives of the 1^{st} order in the direction *x* and *y* was tested on the morphometrical characteristic of the 1^{st} order – slope (γ_N). By visual control of γ_N isolines computed by *method_2*, *method_3* and *method_4* was claimed, that all the results are identical to the etalon.

3.1.2 2nd partial derivatives

The accuracy of the partial derivatives of the 2^{nd} order was tested using one of the normal curvatures $(K_N)_n^5$ (profile curvature). On

the **Figure 3** is presented the $(K_N)_n$ *etalon*. Resulted surface of $(K_N)_n$ computed by *method*_2 and *method*_3 is very similar to the *etalon* and is not shown in this paper.

On **Figure 4** is computed by *method*_1 and *method*_4. At the result of *method*_4 we see the differences from the *etalon*. This may be caused by the approximation method, using the 5x5 neighbourhood of actually computed cell. At the result of *method*_1 are visible the RST interpolation artifacts – deformations along the boundary of the testing area.

3.1.3 3rd partial derivatives

The accuracy of the partial derivatives of the 3^{rd} order was tested by the values of the *equivalence rate* of the *etalon* and the surfaces computed by one of the tested methods. Three other parameters were used as well – *arithmetical average* of differences of these two surfaces, *standard deviation* and RMSE of these differences.

⁵ For detailed description of this curvature see KRCHO (1990) or KRCHO (2001)



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The computed values of the *equivalence* rate, arithmetical average, standard deviation and RMSE are presented in the following tables. For the *method_4* were tested two different weights:

where $\varepsilon > 0$,

$$w_{i,j} = \frac{(\varepsilon + 2h\sqrt{2} - h\sqrt{i^2 + j^2})}{2h\sqrt{2}},$$
(3.1.1)

where $\delta > 0$.

$$w_{i,j} = \frac{2h\sqrt{2}}{\delta + h\sqrt{i^2 + j^2}},$$
(3.1.2)

In the following **Tables 1** – **4** is weight (3.1.1) called *method_4b* and weight (3.1.2) *method_4a*.

If we compare the values in **Tables 1** to 4, we my claim that the preciseness of the partial derivatives of the 3^{rd} order is for all tested methods acceptable. Methods based on the 5x5 neighbourhood approximation are approximately two orders more precise then the *method_2*. The results are overall very precise.

This may be caused by the fact, that the testing function is a polynomial – and we approximate the polynomial by another polynomial.

4 CONCLUSIONS

In this article were presented and tested methods for approximation of the partial derivatives up to the 3^{rd} order. The task of approximating partial derivatives of the 3^{rd} order is very crucial for geomorphometry, as the approximation is very sensitive to computation errors. For this reason was implemented method based on approximation of the input data by a general polynomial of the 3^{rd} order using the 5x5 cell-neighbourhood. This approximation method uses the weighted least-square method implemented in Matlab, where the possible rounding errors are avoided by the analytical computation of matrix **B**_w (with the help of symbolic computations in Matlab).

The aim of this article was not to test to preciseness of the 1st and the 2nd partial derivatives as many papers have been written on this topic, thus we have only visually compared the isolines of selected morphometrical variables com-

$\frac{\partial z^3}{\partial x^3}$	Eq. rate	Ar. average	Std. deviation	RMSE
$method_2$	100.5621	$1.3845 \cdot 10^{-7}$	$2.1260 \cdot 10^{-7}$	$2.5370 \cdot 10^{-7}$
$method_4a$	99.9954	$-5.1298 \cdot 10^{-11}$	$6.6149 \cdot 10^{-10}$	$6.6347 \cdot 10^{-10}$
$method_4b$	99.9937	$-7.1432 \cdot 10^{-11}$	$9.1008 \cdot 10^{-10}$	$9.1288 \cdot 10^{-10}$
$method_5$	99.9928	$-8.1379\cdot 10^{-11}$	$1.0361 \cdot 10^{-9}$	$1.0393 \cdot 10^{-9}$

Tab.1 Approximation preciseness of $\delta z^3 / \delta x^3$

$\frac{\partial z^3}{\partial y^3}$	Eq. rate	Ar. average	Std. deviation	RMSE
method_2	100.4094	$-5.4159 \cdot 10^{-9}$	$1.1298 \cdot 10^{-8}$	$1.2529 \cdot 10^{-8}$
method_4a	100.0070	$1.4788 \cdot 10^{-10}$	$2.3948 \cdot 10^{-10}$	$2.8146 \cdot 10^{-10}$
method_4b	100.0104	$2.1592 \cdot 10^{-10}$	$3.3582 \cdot 10^{-10}$	$3.9924 \cdot 10^{-10}$
$method_5$	100.0118	$2.4660 \cdot 10^{-10}$	$3.8275 \cdot 10^{-10}$	$4.5531 \cdot 10^{-10}$

Tab. 2 Approximation preciseness of $\delta z^3 / \delta y^3$

$\frac{\partial z^3}{\partial x^2 \partial y}$	Eq. rate	Ar. average	Std. deviation	RMSE
method_2	100.7735	$-3.1177 \cdot 10^{-8}$	$2.1486 \cdot 10^{-7}$	$2.1711 \cdot 10^{-7}$
method_4a	99.9967	$3.7259 \cdot 10^{-10}$	$4.3921 \cdot 10^{-10}$	$5.7596 \cdot 10^{-10}$
method_4b	99.9965	$3.9209 \cdot 10^{-10}$	$4.6218\cdot 10^{-10}$	$6.0609 \cdot 10^{-10}$
$method_5$	99.9964	$4.0043 \cdot 10^{-10}$	$4.7203 \cdot 10^{-10}$	$6.1899 \cdot 10^{-10}$

Tab. 3 Approximation preciseness of $\delta z^3 / \delta x^2 \delta y$

$\frac{\partial z^3}{\partial x \partial y^2}$	Eq. rate	Ar. average	Std. deviation	RMSE
$method_2$	99.4957	$-3.2169 \cdot 10^{-8}$	$7.7610 \cdot 10^{-8}$	$8.4013 \cdot 10^{-8}$
$method_4a$	99.9981	$5.9091 \cdot 10^{-11}$	$5.3963 \cdot 10^{-10}$	$5.4285 \cdot 10^{-10}$
method_4b	99.9980	$6.3364 \cdot 10^{-11}$	$5.8677 \cdot 10^{-10}$	$5.9018 \cdot 10^{-10}$
$method_5$	99.9979	$6.5319 \cdot 10^{-11}$	$6.0900 \cdot 10^{-10}$	$6.1250 \cdot 10^{-10}$

Tab. 4 Approximation preciseness of $\delta z^3 / \delta x^2 \delta y$

puted from partial derivatives approximated by the described methods. The accuracy tests were focused on the 3^{rd} partial derivatives – here we have tested several statistical indicators describing the differences of the tested surface and the etalon. The results have shown that methods based on the approximating polynomial of the 3^{rd} order are giving the best results. These two methods uses for approximation the least square method – the method based on the weighted least squares introduced in this article is even more precise.

The further process of testing will be focused on real terrain data. Here the accuracy of partial derivatives will be tested (within the GmIS) in the process of automatic delimitation and recognition of elementary forms of georelief. The partial derivatives used for computation of desired morphometrical variables (further used for elementary form delimitation) will be computed using above described methods. Then we will test the accuracy of delimited elementary forms borders. Accuracy test on a non-polynomial testing function is suggested as well.

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