Numerical method to calculate coal strata surface curvature, predetermined by discreet points of the irregular grid

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Abstract
This article reports on implementation of the numerical method for surface curvature calculation at random point; it is determined by discreet set of points on the irregular grid. The results of this work were used for the research of structural failures of coal strata evidenced by the data obtained from the exploration wells.
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The necessity to calculate the curvature surface *z=F(x,y)* (or radius of curvature, as these notions are reciprocal) occurs, particularly, when we need the solution of the calculation problems for tensile or compressive stresses at the points of the curvature surface. It is known that [1] stresses acting at the instant of the pure bend of the stress within the material are calculated according to the formula below:

$$\left.\begin{aligned} \sigma_x &= Ezk_x, \\ \sigma_y &= Ezk_y, \end{aligned}\right\}, \qquad (1)$$

where

E is the elasticity modulus (Young's modulus) of the material (kg/cm^2);

k_x, k_y – the curvature surface with respect to the directions of X and У axes at the points under study;

z – the distance from the neutral axis at bending (m);

σ_x, σ_y – the stresses on X and У axes (kg/cm^2).

When the calculations are carried out, the numerical value of the material elasticity modulus E is, as a rule, taken as standard reference data, which have been earlier found based on the special laboratory tests, or defined by the appropriate empirical dependence on the mechanical and physical properties.

The value of the distance from the neutral axis is set by the researcher and depends on whether the calculations of the stresses at the point under interest are required or, in other words, it is determined by the certain initial value. The only issue that we need to calculate is the curvature surface at the point under analysis.

Theatrically, the curvature at any point (x_j,y_i) of the surface *z=F(x,y)* is directed by the arrangement of axes and is calculated by formula [2]

$$k_{x_j} = \left| d^2\varphi(x_j)/dx^2 \right| / \left[(1 + d\varphi(x_j)/dx)^2 \right]^{3/2} \qquad (2)$$

or

$$k_{y_i} = \left| d^2\psi(y_i)/dy^2 \right| / \left[(1 + d\psi(y_i)/dy)^2 \right]^{3/2} \qquad (3)$$

where $\varphi(x)$, $\psi(y)$ are the equations of lines, derived from the intersection with the surface by *XOZ* plane at the fixed y_i and YOZ plane at the fixed x_j respectively.

Unfortunately, when the surface is set by the discreet points, there exist the difficulties with the analytic expressions for $\varphi(x)$ line and $\psi(y)$ line, which are to be developed with the objective to calculate the derivatives of the first and second order.

Therefore, for the practical solution of this problem we offered the following procedure. Firstly, we produce the two-dimensional interpolation of the values for points z_{ji} with respect to both directions of X and Y axes with the equal step h (this simplifies the calculations); the interpolation results in the range of numerical values $\{\varphi(x_j)\}=\{z(x_j)\}$ at fixed y_i and $\{\psi(y_i)\}=\{z(y_i)\}$ at fixed x_j. After this, we use the method of numerical differentiation for the function with a constant step by the function values at these points. This method is based on the use of the Lagrange interpolation polynomial formula for equidistant points. The general formula for calculation of the derivative of the first order with Lagrange interpolation polynomial $L_{xz}(x_j)$ for the equidistant points x_j is expressed as [3]:

$$\phi'(x_j)=z'(x_j)\approx L'_n(x_j)=\frac{1}{n}\sum_{j=0}^{n}\frac{(-1)^{n-j}z_j}{j(n-j)}\frac{d}{dq}\left\{\frac{q^{[n+1]}}{q-j}\right\},\ j=0,\dots,n, \quad (4)$$

where $q=(x-x_0)/h$ is the new variable of differentiation.

The similar structure is seen in the formula for the calculation of the first order derivative with the use of Lagrange interpolating polynomial $L_{yz}(y_i)$ for the equidistant points y_i.

From the general formula (3), we can develop the specific formulae for the derivatives of the first and second order for each of n points belonging to x_j (or y_i). The further algorithm is as follows.

Let us consider the case, when with the two-dimensional interpolation of the values belonging to function $z(x_j,y_i)$, we receive NxN matrix of numerical values z_{ji} (without intervention into generality, we assume that the number of the points of interpolation by both axes is identical and equal to N). For calculation of the derivatives and the curve by formulae (3) and (2), it is necessary to define subset $\{n\}\subset\{N\}$, where n is the number of points, for which the derivatives are calculated. Methodically, this implies that by Lagrange interpolating polynomial $L_{xz}(x_j)$ (or $L_{yz}(y_i)$) of degree n, we can make a piecewise approximation of the equation for the flat line, which passes through n of points.

When calculating the derivatives and further the curvature surface, the choice of interpolation step and number of points are essential (the method is used only for the equidistant points). The most important thing here is that this procedure envisages the error, value of which is inevitable due to approximate numerical methods.

For points x_0, x_1, x_2, x_3, x_4 (n=4), positioned in the succession with the step h, the derivative of the first order at midpoint x_2 is calculated by approximation formula as follows:

$$z'_2\approx\left(z_0-8\cdot z_1+8\cdot z_3-z_4\right)/12\cdot h, \quad (5)$$

while the derivative of the second order – by formula [6]:

$$z''_2\approx\left(-2\cdot z_0+32\cdot z_1-60\cdot z_3+32\cdot z_4\right)/24\cdot h^2 \quad (6)$$

where z_0, z_1, z_3, z_4 are the values of the function at points x_0, x_1, x_3, x_4.

If the number of points is uneven (n - even) and the derivative is taken from the midpoint, then the appropriate formula for the numerical differentiation is expressed much simpler and is highly accurate. For such central points, the first derivative is calculated by formula [7]. In order to observe the symmetry, the indices are enumerated in this order: -2, -1, 0, +1, +2:

$$z'(0)\approx\frac{2}{3h}\left(z_1-z_{-1}\right)-\frac{1}{12h}\left(z_2-z_{-2}\right) \quad (7)$$

Moreover, the calculation of the derivatives by the numerical method always bears the possibility of an error existence and the general expression of this error for the first derivative is written as:

$$R_n(x_j)\approx(-1)^{n-j}h^n\frac{j(n-j)}{(n+1)}z^{(n+1)}(\xi),\ \xi\neq x_j, j=0,\ 1,\ 2,\ \dots n \quad (8)$$

Furthermore, for central point x_2 at n=4 (we take the subset of 5 points) the error expression is the following:

$$R_5(x_2) \approx \frac{h^4}{30} z^{(5)}(\xi) \quad (9)$$

It becomes obvious from formula (9) that the error value is influenced by the distance between the points or the interpolation step and the choice of point ξ from interval (x_0....x_5), provided that point ξ does not coincide with any of points x_0....x_5. If the value of the interpolation step h can be given with quite high accuracy in a definite way, then the choice of point ξ is not so explicit and as the practice shows it is reasonable to take it in the vicinity of the central point.

Eventually, the method we described above finds the application for processing on exploration wells and the authors use it for detecting tectonic fractures in coal strata, caused by accumulation of stresses as a result of abrupt changes of stratum hypsometry [4]. The algorithms of the method are implemented in the medium of integrated mathematical package MATLAB 7.01, which has the predefined functions of two-dimensional interpolation. The techniques applied for this are the methods of nearest neighbor, cubic and linear. We would like to note here that well-developed software programming language is suitable for the matrix data processing and EXCEL system spreadsheet is a convenient way of information exchange.

Since the well network is irregular, we first develop the two-dimensional interpolation with 25 m step on both X and Y coordinates, which stand for the values of depths from the surface to the stratum top and stratum bottom. This results in the matrix of depth values in the interpolation nodes. Leaving aside the issues of determining the physical and mechanical properties of different rocks, namely the elasticity modulus values, in each exploration well and the areas chosen for the stresses analysis (these are distances from the stratum top and the stratum bottom), let us concentrate our attention on the details how the calculations for surface curvature of the coal stratum are to be performed with the objective to calculate further the stresses at the interpolation points.

The calculations for the derivatives of the first and second order by formulae (5) and (6) are made with respect to the 5-point scheme (n = 4), at that the derivatives are calculated only for central point. The first five neighboring points x_j (j = 0,1,2,3,4) are selected with the fixed coordinate value y_i (i = 1, .., N) while the derivatives at point (y_i,x_2) are calculated by function values at point (y_i,x_2). Then, the set of 5 points is shifted with one interpolation step forward and the derivatives for another central point are calculated. With the help of this "shifting" method, we calculate the derivatives at all the points of a matrix row at the fixed coordinate y_i. After that, coordinate y_{i+1} is fixed and the above described is repeated for the new values of function $z(x,y)$.

A similar procedure is performed for fixed values x_j with the 5-point subsets y_j (i=0,1,2,3,4). Thus, with the completion of the cyclic procedures, we obtain the calculated numerical curvature values at all points of interpolation $k_{j,i}$, except the two outermost columns and two outer rows of the matrix created by interpolated values of functional $z(x_j,y_i)$.

Eventually, based on the data of exploration of wells irregular grid and physical and mechanical properties of the rocks in them, the calculations performed by the described method allow us to predict zones of tectonic curvature or stratum strains for the conditions of d_6 strata of Karaganda basin mines and with strain stress calculations to determine the locations of possible discontinuity of tectonic faults.

Conclusions

On condition that the analytical formula is applied to calculate the curvature at any point of the surface and this curvature is defined by a discrete set of points, then there is no need to write an explicit expression of interpolation polynomials, which approximate the surface intersections by the planes parallel to reference axis.

The derivatives of the first and second order in the formula of the curvature line at arbitrary points can be calculated by the numerical differentiation methods, based on the Lagrange's interpolation formula for equidistant points by the function values at these points.

The implementation of the described numerical method has proved its suitability for applicative calculations on the rupture stress of strain in coal strata under the influence of tectonic forces.

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