

# Gridding of Geological Surfaces based on Equality-Inequality Constraints from Elevation Data and Trend Data

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## Abstract

*In the field of geology, many gridding algorithms have been proposed so far. However, most of all algorithms take into account only equality constraints from elevation data. In this paper, we propose a gridding algorithm taking into account equality-inequality constraints from elevation data and trend data. The algorithm is designed to approximate a surface by bi-cubic B-spline and to determine an optimal surface using the exterior penalty function method. The optimal surface is the smoothest one that satisfies the given constraints. Through griddings for simple data sets, it is confirmed that the algorithm enables us to use elevation data and trend data as equality-inequality constraints on geological surfaces. Additionally, through griddings for practical data, it is confirmed that the algorithm is useful to determine a form of geological boundary surface, and that we can obtain an optimal surface even if we have a large number of constraints. In conclusion, this algorithm is more practicable than the one proposed before.*

## 1. Introduction

In the field of geology, point data obtained from field survey are often scattered randomly. In order to interpret the data accurately and to utilize them in practice, we need to perform a gridding. Gridding is a process of interpolating scattered data and creating a regular grid. The work here is of a gridding algorithm taking into account equality-inequality constraints from elevation data and trend data. So far many studies have been conducted on gridding algorithms (e.g. Pelto et al., 1968, Franke, 1982a, Hutchinson, 1989 and Abbass, 1990). There are two types of popular gridding algorithms. One is a kriging (e.g. Krige, 1951, Matheron, 1963, Burrough, 1986, Oliver and Webster, 1990, Cressie, 1993 and Wackernagel, 1995), the other is a spline-fitting (e.g. de Boor, 1962, Bhattacharyya, 1969, Briggs, 1974, Franke, 1982b, Inoue, 1986 and Wahba, 1990). The correspondence between kriging and spline-fitting has been pointed out in several papers (e.g. Kimeldorf and Wahba, 1970, Matheron, 1981, Dubrule, 1984, Wahba, 1990, Cressie, 1993 and Laslett, 1994). In most of all gridding algorithm of geological surfaces, available scattered data are limited to elevation data obtained from drilling survey or geological reconnaissance. Additionally,

the elevation data are used as equality constraints on a form of geological surface. However, the algorithms taking into account only equality constraints from elevation data are impracticable. The purpose of this study is to develop a more practicable gridding algorithm. In this paper, we propose a gridding algorithm taking into account equality-inequality constraints from elevation data and trend data. This algorithm belongs to the spline-fitting. The algorithm is designed to approximate an objective surface by bi-cubic B-spline, to determine an optimal solution using the exterior penalty function method and to create a regular grid. Through some gridding examples using constraints from elevation data and trend data, an availability of the algorithm is confirmed. We conclude from those examples that the algorithm is more practicable than the one proposed before.

## 2. Formulation of Geological Surface and Constraints

### 2.1 Bi-cubic B-spline Surface

A geological surface often has continuity over a wide range. There are two major method to approximate a geological surface. One is a method

based on geostatistics (kriging). The other is a method based on spline function. In a case of kriging, a result sometimes makes a big change of the surface in a local range. In a case of spline, a result has a continuity over a wide range. For this reason, we approximate a geological surface by a bi-cubic B-spline as taken up by de Boor (1962) and Inoue (1986). Suppose that a surface can be expressed in  $z = f(x, y)$ . Let  $\Omega = \Omega_x \times \Omega_y$  be a rectangular domain in  $x$ - $y$  plane. Let  $M_x$  and  $M_y$  be the numbers of sections that constitute  $\Omega_x$  and  $\Omega_y$ , respectively (Figure 1). The surface  $f(x, y)$  in  $\Omega$  can be expressed in a quadratic form:

$$f(x, y) = \sum_{i=1}^{M_x+3} \sum_{j=1}^{M_y+3} c_{ij} N_i(x) N_j(y)$$

Equation 1

where  $N_i(x)$ ,  $N_j(y)$  are normalized cubic B-spline bases with respect to  $x$ ,  $y$  respectively, and  $c_{ij}$  are the constants. An increase in  $M_x$  and  $M_y$  will lead to an increase in capacity to express surface.

## 2.2 Constraints from Elevation Data and Trend Data

Elevation data and trend data are used as constraints on a form of surface. Suppose that an elevation  $z_p$  is obtained at a point  $(x_p, y_p)$ . A possible constraint from the point is as follow:

$$f(x_p, y_p) - z_p = 0$$

Equation 2a

$$f(x_p, y_p) - z_p < 0$$

Equation 2b

$$f(x_p, y_p) - z_p > 0$$

Equation 2c

Equality constraint (2a) is used in cases that the surface passes through the point. Inequality constraint (2b) is used in cases that the surface passes under the point. Inequality constraint (2c) is used in cases that the surface passes above the point. Let  $\phi$  be an azimuth direction of maximum slope of the surface.  $\phi$  is measured clockwise from north. Let  $\theta$  be a slope angle of the surface. Suppose that the azimuth direction and slope angle  $(\phi_q, \theta_q)$  is obtained at a point  $(x_q, y_q)$ . A possible constraint from the point is as follow:

$$f_x(x_q, y_q) + \sin \phi_q \tan \theta_q = 0$$

Equation 3a

$$f_y(x_q, y_q) + \cos \phi_q \tan \theta_q = 0$$

Equation 3b

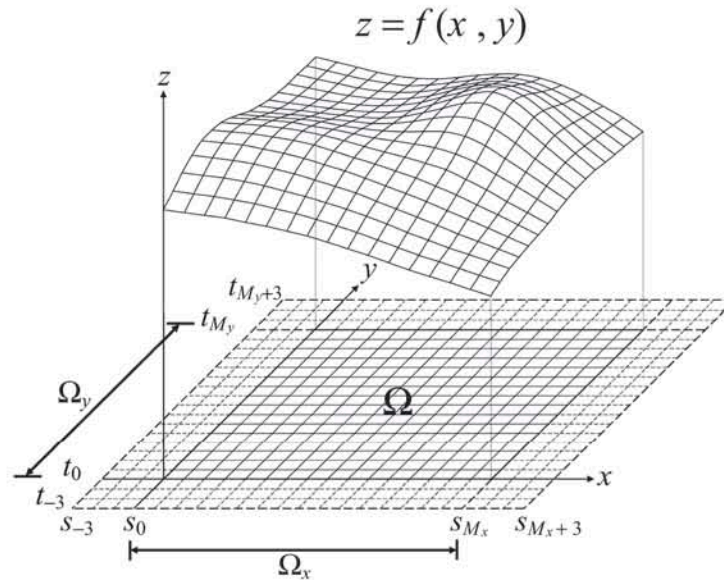


Figure 1: Bi-cubic B-spline function  $f(x, y)$  in domain  $\Omega$



### 3. Methodology for Determining an Optimal Surface

#### 3.1 Constrained Optimization Problem and Criteria for Solution

There may be many feasible solutions that satisfy the equality-inequality constraints. In order to determine an optimal surface, we solve a constrained optimization problem based on the observational data. In general, the constrained optimization problem is defined as follows: Find a vector  $x = (x_1, x_2, \dots, x_n)$  that minimizes a function:

$$J(x) \quad x \in F \subseteq R^n \quad \text{Equation 4a}$$

subject to:

$$g_i(x) = 0 \quad (i = 1, 2, \dots, m_E) \quad \text{Equation 4b}$$

$$h_j(x) \leq 0 \quad (j = 1, 2, \dots, m_I) \quad \text{Equation 4c}$$

where  $J(x)$ ,  $g_i(x)$  and  $h_j(x)$  are all continuously differentiable function and  $F$  is a feasible region.  $J(x)$  is usually called *objective function*.  $m_E$  and  $m_I$  are the numbers of equality constraints and inequality constraints respectively. The objective function and equality-inequality constraints could be linear or nonlinear in the problem. There are two major solution methods to the constrained problem: (1) Lagrange multiplier method (Kuhn and Tucker, 1951, Dubrule and Kostov, 1986 and Kostov and Dubrule, 1986, etc.) and (2) Exterior penalty function method (Zangwill, 1967, Fletcher, 2000 and Yeniyay 2005, etc.). The outlines of each method are summarized below.

#### 3.1 Lagrange Multiplier Method

Lagrange multiplier method is one of the methods that transform the constrained optimization problem into unconstrained minimization problem. For a simple explanation, we describe a solution only taking into account equality constraints. As for a solution taking into account inequality constraints, see Kuhn and Tucker (1951), Dubrule and Kostov (1986), Kostov and Dubrule (1986) and etc.. In this method, a new vector  $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_{m_E})$  called *Lagrange multiplier* is introduced.

Further, a new objective function called *Lagrangian function* is defined as follows:

$$L(x, \lambda) = J(x) + \sum_{i=1}^{m_E} \lambda_i g_i(x) \quad \text{Equation 5}$$

An optimal solution is determined by vectors  $x$  and  $\lambda$  that minimize  $L(x, \lambda)$ . The vectors  $x$  and  $\lambda$  are given as a solution to the equation:

$$\text{grad } L = \left( \frac{\partial L}{\partial x_1}, \dots, \frac{\partial L}{\partial x_n}, \frac{\partial L}{\partial \lambda_1}, \dots, \frac{\partial L}{\partial \lambda_{m_E}} \right) = 0 \quad \text{Equation 6}$$

An advantage of Lagrange multiplier method is that we can obtain an exact optimal solution to the constrained problem. However, in this method, the number of unknowns in (6) depends on not only an order of  $x$  but also the number of constraints  $m_E$ . Thus, we cannot solve the original constrained problem when there is a large number of a constraint.

#### 3.2 Exterior Penalty Function Method

An exterior penalty function method is also one of the transformation methods. In this method, a new constant  $\alpha (> 0)$  called *penalty parameter* is introduced. Further, an *augmented objective function* is defined as follows:

$$Q(x, \alpha) = J(x) + \alpha R(x) \quad \text{Equation 7}$$

where  $R(x)$  is called an *exterior penalty function*.  $R(x)$  is generally formed from a sum of squares of constraint violations:

$$R(x) = \begin{cases} 0 & x \in F \\ \sum_{i=1}^{m_E} [g_i(x)]^2 + \sum_{j=1}^{m_I} [\max(0, h_j(x))]^2 & x \notin F \end{cases} \quad \text{Equation 8}$$

where  $\beta$  is commonly 1 or 2. An optimal solution is determined given by a vector  $x$  that minimizes  $Q(x, \alpha)$ . The vector  $x$  is given as a solution to the equation:

$$\text{grad } Q = \left( \frac{\partial Q}{\partial x_1}, \dots, \frac{\partial Q}{\partial x_n} \right) = 0$$

Equation 9

A parameter  $\alpha$  determines the magnitude of the penalty for the constraint violations. When  $\alpha$  is too small, an optimal vector  $x$  will not be in the feasible region  $F$ . When  $\alpha$  is too large, it prevents to search unfeasible region. Traditionally, in order to find a suitable value of  $\alpha$  and to obtain an  $x$  close to  $F$ , we solve a sequence of unconstrained problems:

$$\text{Minimize } Q(x, \alpha_k) = J(x) + \alpha_k R(x)$$

Equation 10

where  $\{\alpha_k\}$ ,  $k = 0, 1, 2, \dots$  is a sequence of penalties that satisfy  $0 < \alpha_k < \alpha_{k+1}$  and  $\alpha_k \rightarrow \infty$ . Let  $x^{(k)}$  be a solution to the problem:  $\text{Min } Q(x, \alpha_k)$ . When  $\alpha_k \rightarrow \infty$ , the solution  $x^{(k)}$  tends to converge to the optimal solution to the constrained problem. The solution determined by the exterior penalty function method is not as exact as the one determined by Lagrange multiplier method. However, the solution becomes close to exact one when  $\alpha$  is suitably large. The number of unknowns in the equation (9) does not depend on the number of constraints. In contrast to Lagrange multiplier method, we can solve the original constrained problem even if there is a large number of a constraint. In order to improve accuracy of quantitative geological analysis, we will need a large number of data. For this reason, in the present algorithm, the exterior penalty function method is used for optimal surface determination.

### 3.2 Determination of an Optimal Geological Surface

We assume that an optimal surface must be the smoothest one among the feasible solutions and consider a gridding as a constrained optimization problem: Find a surface  $f(x, y)$  that minimizes an objective function:

$$J(f) = m_1 \iint_{\Omega} \left[ \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 \right] dx dy / S$$

$$+ m_2 \iint_{\Omega} \left[ \left( \frac{\partial^2 f}{\partial x^2} \right)^2 + 2 \times \left( \frac{\partial^2 f}{\partial x \partial y} \right)^2 + \left( \frac{\partial^2 f}{\partial y^2} \right)^2 \right] dx dy$$

Equation 11

subject to the constraints (2a), (2b), (2c), (3a) and (3b). In order to solve the problem above, we introduce an augmented objective function:

$$Q(f, \alpha) = J(f) + \alpha R(f)$$

Equation 12

where  $J(f)$  evaluates the smoothness of the surface,  $R(f)$  evaluates the degree of violation of constraints and  $\alpha$  controls a weight balance between  $J(f)$  and  $R(f)$ .  $R(f)$  is defined in a form of residual mean of squares:

$$R(f) = \frac{1}{n_H} \sum_{p=1}^{N_H} \epsilon_p^2$$

$$+ \frac{\gamma}{N_D} \sum_{q=1}^{N_D} \left[ (f_x(x_q, y_q) + \sin \theta_q \tan \phi_q)^2 + (f_y(x_q, y_q) + \cos \theta_q \tan \phi_q)^2 \right]$$

Equation 13

where  $\epsilon_p$  is a residual with respect to elevation data:

$$\epsilon_p = \begin{cases} f(x_p, y_p) - z_p & ; \text{for equality constraint (2a)} \\ \max(f(x_p, y_p) - z_p, 0) & ; \text{for inequality constraint (2b)} \\ \min(f(x_p, y_p) - z_p, 0) & ; \text{for inequality constraint (2c)} \end{cases}$$

Equation 14

$N_H$  is the number of equality-inequality constraints from elevation data,  $n_H$  is the number of constraints that give  $\epsilon_p \neq 0$ ,  $N_D$  is the number of constraints from trend data and  $\gamma$  is another penalty parameter that controls a weight balance between elevation data and trend data. An optimal surface is given by a vector  $c = (c_{11}, c_{12}, \dots, c_{M_x+3}, c_{M_y+3})$  that minimizes  $Q(f, \alpha)$ . Substituting (1) into (12), we obtain a simultaneous equation:

$$\text{grad } Q = \left( \frac{\partial Q}{\partial c_{11}}, \dots, \frac{\partial Q}{\partial c_{M_x+3}}, \dots, \frac{\partial Q}{\partial c_{1, M_y+3}}, \dots, \frac{\partial Q}{\partial c_{M_x+3, M_y+3}} \right) = 0$$

Equation 15

The optimal vector  $c$  is determined by an iterative calculation with an increasing sequence of penalties  $\{\alpha_1, \alpha_2, \dots, \alpha_{N_{\text{ITR}}}\}$ . The  $k$ -th element of the sequence is given by:

$$\alpha_k = \alpha_1 \times \left( \frac{\alpha_{N_{\text{ITR}}}}{\alpha_1} \right)^{\frac{k-1}{N_{\text{ITR}}-1}} \quad (k = 1, 2, \dots, N_{\text{ITR}})$$

Equation 16





#### 4.2 Calculation using Equality-Inequality Constraints from Elevation Data

Figure 3 shows a gridding example using equality-inequality constraints from elevation data. A down-pointing triangle on the map means a location of the data that provides inequality constraints (2b). An up-pointing triangle means a location of the data that provides inequality constraints (2c). Domain  $\Omega$  for gridding is  $[0, 100] \times [0, 100]$ . Parameters in calculation are as follows:  $M_x = M_y = 10$ ,  $\alpha_{\min} = 1$ ,  $\alpha_{\max} = 10^2$ ,  $N_{\text{ITR}} = 10$ ,  $m_1 = 0$ , and  $m_2 = 1$ . When  $\alpha = 10^2$ ,  $R(f)$  is  $2.79 \times 10^{-4}$  (RMS error of unsatisfied elevation data is  $1.67 \times 10^{-2}$ ). The result shows that inequality constraints control the shape of surface in the east and west part as well as equality constraints in central part.

#### 4.3 Calculation using Constraints from Trend Data

Figure 4 shows a gridding example using constraints from trend data. In this example, the equality constraints from elevation data are only  $z = 50$ . A symbol of dip data is given by a long bar and short spike perpendicular to the long bar. Short spike means the azimuth direction of maximum slope. Numerical value in parenthesis near the symbol of dip data is slope angle. For example, a symbol near the upper-right corner means  $\phi = 275$  and  $\theta = 45$ . Domain  $\Omega$  for gridding is  $[0, 100] \times [0, 50]$ . Parameters in calculation are as follows:  $M_x = M_y = 10$ ,  $\alpha = 10^3$ ,  $\gamma = 10^3$ ,  $m_1 = 0$ , and  $m_2 = 1$ . RMS error of unsatisfied elevation data is  $1.12 \times 10^{-4}$ . RMS

error of unsatisfied trend data is  $1.51 \times 10^{-5}$ . The result shows that the constraints from trend data control the shape of surface as well as the constraints from elevation data.

#### 4.4 Calculation using all Types of Constraints

Figure 5 shows a gridding example using all types of constraints from elevation data and trend data. Domain  $\Omega$  for gridding is  $[0, 100] \times [0, 100]$ . Parameters in calculation are as follows:  $M_x = M_y = 10$ ,  $\alpha_{\min} = 1$ ,  $\alpha_{\max} = 10^2$ ,  $N_{\text{ITR}} = 10$ ,  $\gamma = 10^4$ ,  $m_1 = 0$ , and  $m_2 = 1$ . RMS error of unsatisfied elevation data is  $1.47 \times 10^{-3}$ . RMS error of unsatisfied trend data is  $6.45 \times 10^{-6}$ . The result shows that the optimal surface satisfies all types of constraints in numerically as well as in visually.

### 5. Applications

#### 5.1 Trend Data Derived from Geological Reconnaissance

The algorithm is helpful to determine a form of geological boundary surface. One practical example is a surface fitting to strike-dip data derived from geological reconnaissance. Figure 6 shows a gridding result using constraints only from strike-dip data digitized from a scanned geological map. It is easy to see an outline of folding structure and local variation of strike-dip. Such a result will be useful for geomorphological analyses and hydrological analyses.

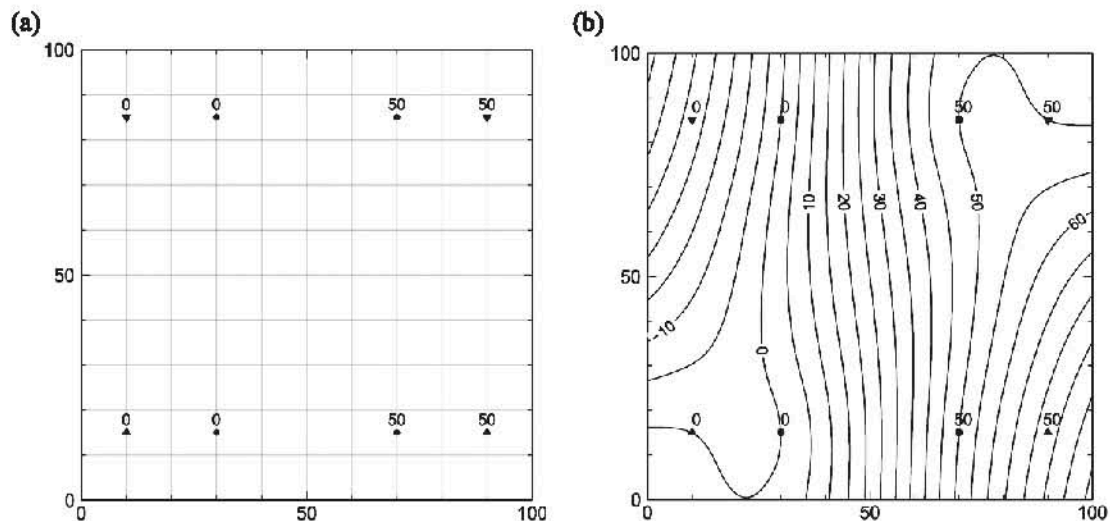


Figure 3: Gridding example using equality-inequality constraints. (a) distribution map of the data, (b) contour map of generated DEM



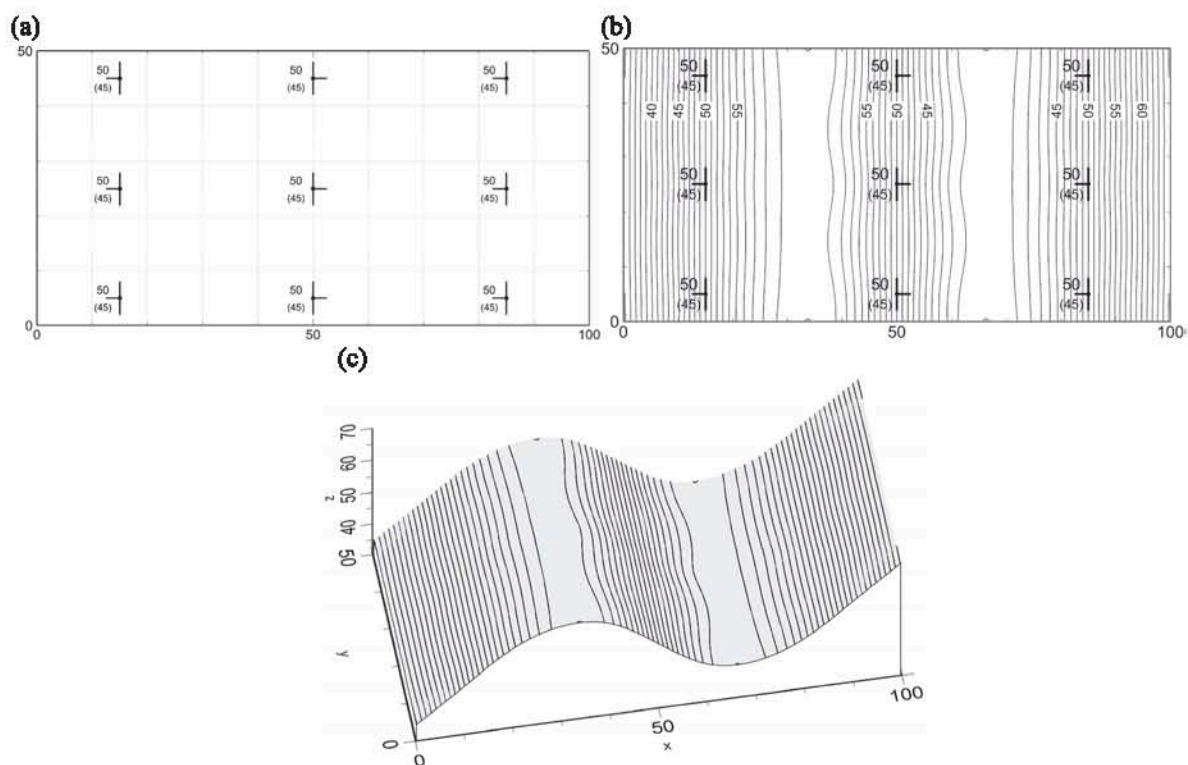


Figure 4: Gridding example using constraints from trend data. (a) distribution map of the data, (b) 2D visualization of generated DEM, (c) 3D visualization of generated DEM

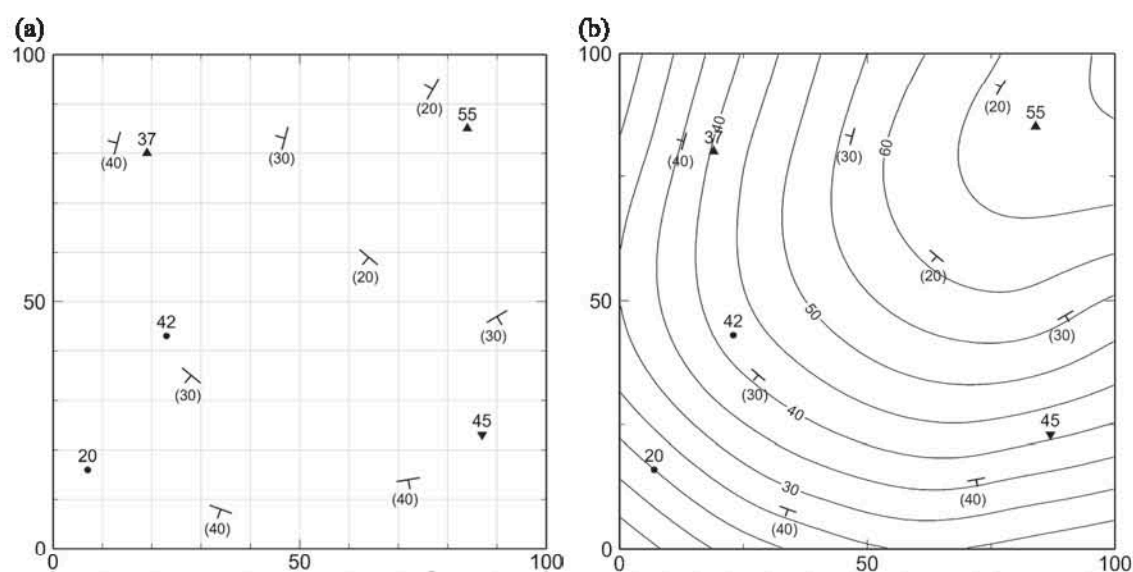


Figure 5: Gridding example using constraints from elevation data and trend data. (a) distribution map of the data, (b) contour map of generated DEM

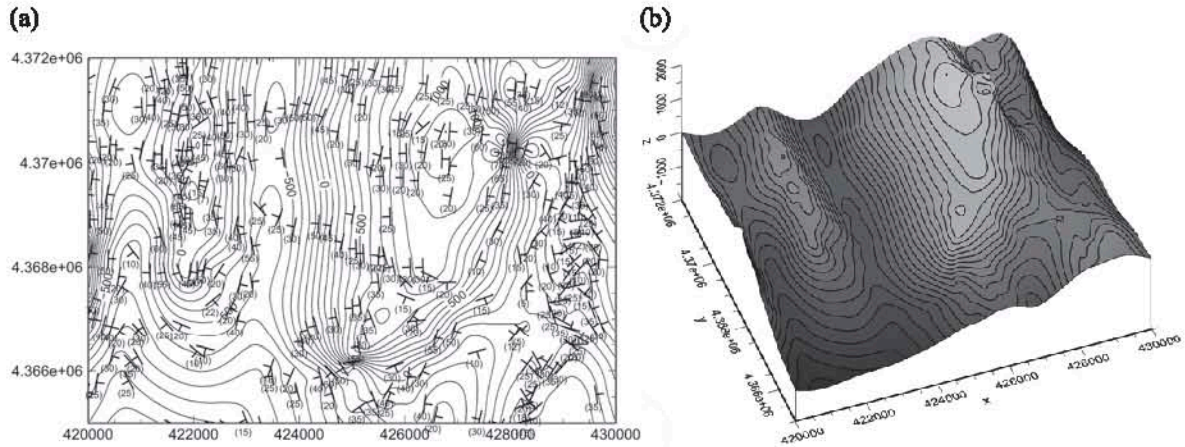


Figure 6: Utilization of strike-dip data digitized from a geological map.  
(a) 2D visualization of generated DEM, (b) 3D visualization of generated DEM

### 5.2 Elevation Data Derived from Drilling Cores

Drilling cores are quite helpful to understand a subsurface condition, especially a form of geological boundary surface. There are many drilling cores in urban area. However, most of all cores do not reach so deep part. In an analysis of deep part, there is a limit to the number of available cores. In such a case, we should use the drilling cores in shallow part as inequality constraints (2b). Figure 7 shows an example of geological surface determined by the constraints derived from drilling cores. In the figure 7(b) and 7(d), there are enough differences between two surfaces around dashed circles. This result shows that the drilling cores in shallow part are effectively used as well as the ones in deep part. The algorithm has a capability of using existing drilling cores more effectively than previous algorithms. Further, combination of inequality constraints from drilling cores and strike-dip data from geological reconnaissance must be quite useful for 3D geological modeling based on geological boundary surfaces.

### 5.3 Topographic Map

Another practical application is the STRIPE method (Noumi, 2003). The STRIPE method is a way to generate DEM from a scanned topographic map. In general, inter-contour areas constitute a large portion of a topographic map. An elevation  $f(x_p, y_p)$  at a point  $(x_p, y_p)$  within an area between two

successive contours  $z = z_1$  and  $z = z_2$  ( $z_1 < z_2$ ) must satisfy inequality constraints:

$$z_1 < f(x_p, y_p) < z_2.$$

Thus, we can create a large number of inequality constraints on  $f(x, y)$  from a scanned topographic map. The number of constraints depends on a density of contours and on a pixel size of the map. Based on this concept, we generated a DEM from a scanned schematic topographic map (Figure 8). The pixels size of the map is  $3000 \times 3000$ . The number of inequality constraints created from the map is 14,691,658. The contour interval is 10m. Domain  $\Omega$  for gridding is  $[0, 3000] \times [0, 3000]$ . Parameters in calculation are as follows:  $M_x = M_y = 200$ ,  $\alpha_{\min} = 1$ ,  $\alpha_{\max} = 10^{10}$ ,  $N_{\text{ITR}} = 500$ ,  $m_1 = 0$ , and  $m_2 = 1$ . Figure 8(b) and 8(c) are contour maps of the generated DEM when  $\alpha = 6.16 \times 10^4$ . The result clearly shows that the calculated contour maps reproduced the original scanned topographic map accurately. In this case, RMS error of unsatisfied constraints is 1.33m. As stated in chapter 3.1, in the exterior penalty function method, the number of unknowns in the simultaneous equation (15) does not depend on the number of constraints. This enables us to determine an optimal solution even if there is a large number of a constraint.



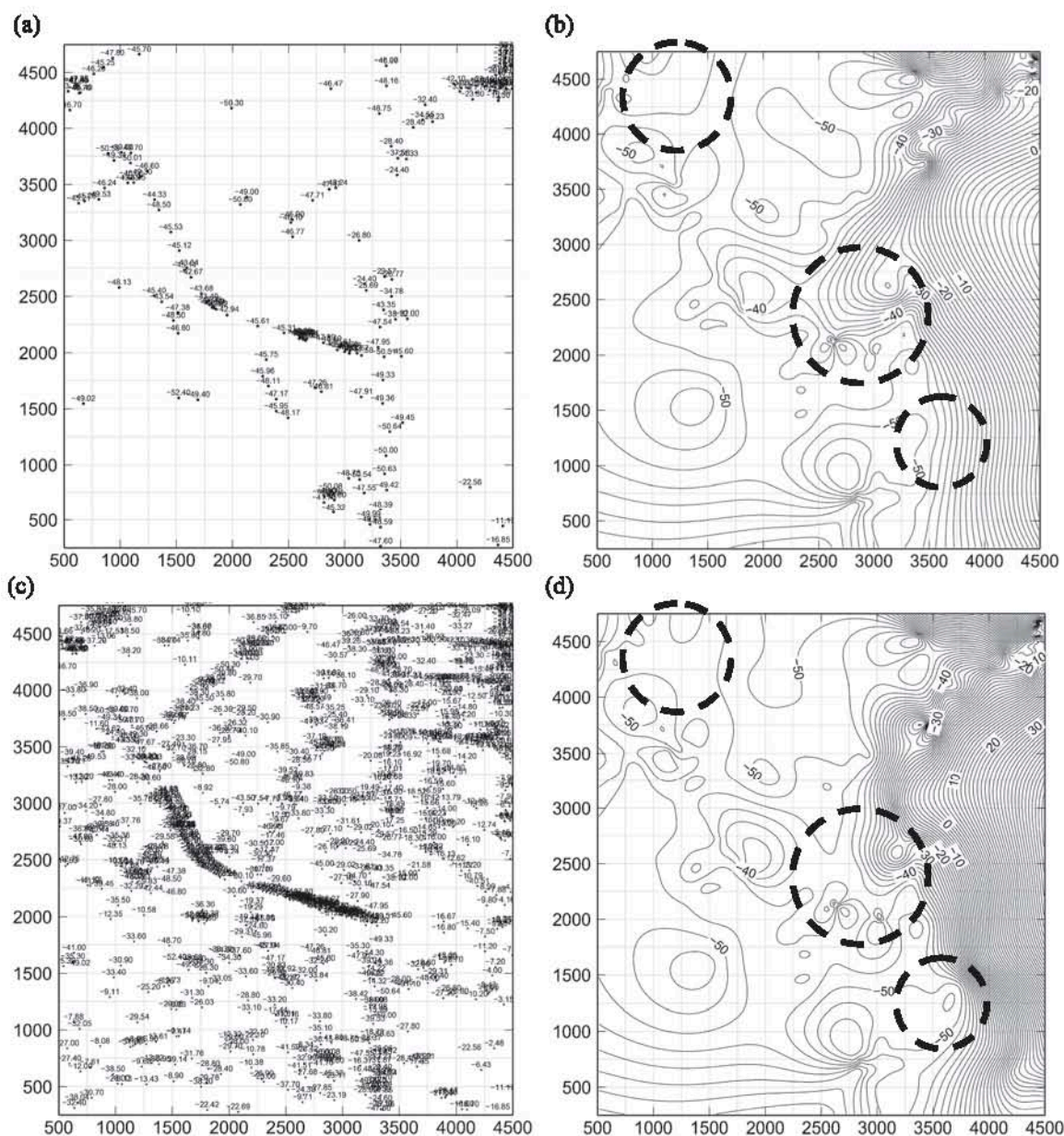


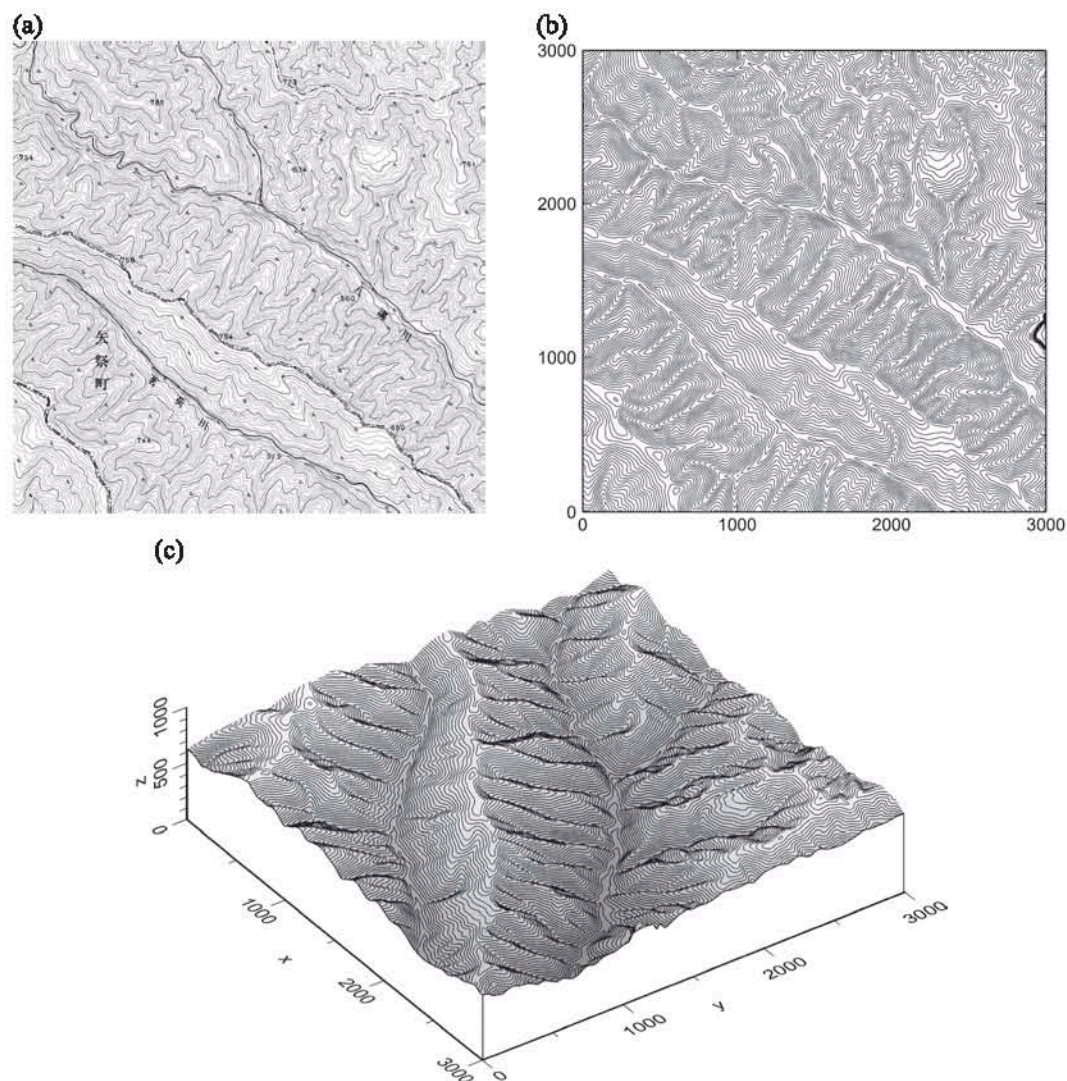
Figure 7: Effectiveness of the inequality constraints. (a) distribution map of drilling cores in deep part, (b) surface determined only by equality constraints from drilling cores in deep part, (c) distribution map of drilling cores in shallow part and deep part, (d) surface determined by equality-inequality constraints from drilling cores in shallow part and deep part

## 6. Conclusion

We presented a gridding algorithm taking into account equality-inequality constraints from elevation data and trend data. The presented algorithm is designed to approximate a surface by a bi-cubic B-spline, to determine a optimal surface based on the exterior penalty function method and to create a regular grid.

In order to confirm an availability of the algorithm, we carried out calculations for several types of input data. Through four examples for elevation data and trend data, it is confirmed that all types of data are available as expected.





**Figure 8: Generation of DEM using a large number of constraints. (a) scanned topographic map (Geospatial Information Authority of Japan, 2001), (b) contour map of generated DEM and (c) 3D visualization of generated DEM.**

Through calculations using geological reconnaissance data and drilling core data, it is confirmed that the algorithm is useful to determine a form of geological boundary surface. Through calculation using topographic map, it is confirmed that we can obtain an optimal surface even if we have a large number of constraints. From these results, we conclude that the presented algorithm is more practicable than the one proposed before. At this moment, available input data are limited to elevation data and trend data. However, two types of input data are insufficient to determine a form of

geological boundary surface with a high accuracy and to understand a subsurface condition. The topic of further study is to increase types of available data, especially to make cross-section data available. As for output, a calculated surface can be saved in two types of files. One is a file for bi-cubic B-spline function of the optimal surface. The file includes information for giving the equation (1). The other is a file for DEM. Both files have unique formats. The use of unique formats will be a big limiting factor in interoperation with other systems such as GISs, Web-GISs, and 3D geological modeling systems.



In order to solve this problem, we need to prepare some major types of files for output data. In addition, the developed FORTRAN program is operational only in CUI (Character User Interface). It will be a limiting factor in dissemination of the program. Another topic of further study is to code the algorithm in more popular language and to enhance interfaces of the program.

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