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Author(s)	YAMAMOTO, Akihiko
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Estimating the Optimum Reduction Density for Gravity Anomaly : A Theoretical Overview

Akihiko Yamamoto

Institute of Seismology and Volcanology, Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan

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Abstract

We need a priori information about gravity reduction density to evaluate Bouguer anomaly value. Bouguer and terrain corrections are made, in general, by using a representative density value for an area of interest. However, estimation of the reduction density has been a major difficulty since there is not a unique solution for the problem.

This paper attempts to introduce and summarize several methods, developed independently during the last sixty years, which furnish an optimum reduction density from surface gravity measurements. A theoretical overview of these methods is also given, where mathematical expressions and their significance are extensively discussed. We formulate an exact mathematical expression of classical methods which have been used in graphical procedure for many years.

A few examples are represented to compare the results by several methods for estimating Bouguer density, and to illustrate the estimation errors introduced by improper assumptions. A modern sophisticated method, using linear statistics and information theory, provides an excellent estimate of Bouguer density, whereas inadequate usage of classical methods leads to a distortion of density estimates.

1. Introduction

Recently a great deal of interest has been expressed in many geophysical papers concerning the interpretations of Bouguer anomaly. The evaluation of Bouguer anomaly value requires knowledges of station height and surface terrain density since free-air, Bouguer and terrain corrections are proportional to height and/or density. To interpret gravity anomalies in an extensive area we need an optimum reduction density as the representative value in the area of interest since the gravity reduction is usually made using a constant density based on the simple assumption that surface and near-surface rocks forming the topography have an average density. Quantitative analysis of gravity anomalies, therefore, relies heavily on the accuracy of Bouguer reduction density

about which we need a priori information. An error of 0.1 g/cm^3 in the reduction density, corresponding to an error of nearly 0.42 mGal in Bouguer anomaly for every 100 m, is not a very large error in itself but an error of 0.1 g/cm^3 in the density may have a large effect on the interpretations of Bouguer anomalies. However, density determinations for gravity reduction have been a major difficulty with inherent uncertainties and center of concern to compute Bouguer anomalies since there is not a unique solution to determine a correction density from gravity data, whereas gravity measurements are usually made at a point where station height is accurately known.

At first (when tortion balance was in use), the laboratory method was used for density estimates where the reduction density for Bouguer anomaly was an average one which was determined from rock samples taken from surface or near-surface outcrops. Presently density determinations on direct rock sampling are still useful for estimating the average density of a rock unit or formation. This method, however, may have some drawbacks because the outcrop may not be truly representative of the strata below. When the gravimeter replaced the tortion balance, Nettleton (1939) made a significant breakthrough in the field method of density determinations from gravity data and developed his own profile method (Vajk, 1956). The field method is characterized by using an extensive gravity data made by surface or sub-surface gravity measurements. Applications of borehole gravimetry also give a good estimate of bulk in-situ rock densities (e.g. Hammer, 1950 ; Gibb and Thomas, 1980 ; LaFehr, 1983) Recently, Sissons (1981) configured a least-squares method for the direct inversion of surface and subsurface gravity measurements to estimate in-situ rock densities. However, these methods associated with subsurface gravity measurements are valid only for quite limited area where the rock unit is reasonably homogeneous in composition. Thereafter, effective and efficient methods for density determinations from surface gravity measurements have been extensively developed (e.g. Parasnis, 1952 ; Rikitake et al., 1965 ; Fukao et al., 1981 ; Murata, 1993). Most of these methods adopted statistical procedures using the correlations among Bouguer anomalies, free-air anomalies, station heights, and reduction density itself from surface gravity data.

On the other hand several methods have been proposed to estimate a variable density of surface and near-surface topography (Vajk, 1956 ; Grant and Elsaharty, 1962 ; Bichara and Lakshmanan, 1983 ; Rimbert et al., 1987 ; Moribayashi, 1990 ; Murata, 1993) since the residual anomalies after gravity reduction using a single constant density still contain density inhomogeneities. They applied the method of overlapping windows and determine a Bouguer reduction

density for each of the windows using the data within each window. More recently, Nawa et al. (1997) proposed a method of inverting gravity data for the variable density distribution over a large region and successfully derived a terrain density map in Southwest Japan, in which the relation of the resulting terrain densities to geological features and the limitations of the method are fully discussed.

The purpose of this paper is (1) to introduce and summarize the widely used methods of estimating a representative density from surface gravity measurements, and (2) to give a sound overview of their theoretical aspects as well as a few examples.

2. Methods

We discuss here the following methods which have been proposed for last sixty years and widely used in gravity analyses:

(a) *Nettleton's method* or *profile method* (Nettleton, 1939; Nettleton, 1976). In this method topographic structure is based on the hypothesis that Bouguer anomalies behave as stochastic quantities which are not correlated with point elevations. Nettleton (1939) suggested that Bouguer anomalies be computed for various densities from closely spaced gravity measurements over some pronounced topography and that an optimum density of near-surface material is that which gives the least correlation between Bouguer anomalies and topography.

(b) *G-H relationship method* or *simple G-H method*. Bouguer anomalies are described as a function of altitude and the density is estimated by the procedure based on a linear fitting scheme. The optimum density is determined from the slope of a best fitting straight line.

(c) *Rikitake et al.'s method* (Rikitake et al., 1965). This is a natural generalization of G-H method. G-H results for variable densities are usually plotted against densities used for terrain correction. The optimum density is determined such that terrain correction density coincides with that by G-H method.

(d) *F-H relationship method* or *simple F-H method* (Parasnis, 1952; Parasnis, 1979). Bouguer anomalies are described as a function of assumed density itself. The optimum density is estimated by minimizing the summations of the difference between the Bouguer anomaly averaged in whole area and each Bouguer anomaly.

(e) *Extended F-H method* (Fukao et al., 1981). This method uses F-H method over subdivided mesh areas of equal size and estimates a reduction density

corresponding to each mesh size. Finally the density is calculated as a function of mesh size and the optimum density is determined such that the calculated density becomes an approximately constant value over various mesh sizes.
(f) ABIC method (Murata, 1990, 1993). The reduction density is estimated by fitting a smooth surface to observed Bouguer anomalies. This is done by an objective trade-off between the minimizations of the sum of the square of the residuals and a penalty to the surface roughness using the objective Bayesian procedure which minimizes *the Akaike's Bayesian Information Criterion* (*ABIC*) (Akaike, 1980).

In this paper we describe theoretical aspects of the above methods and compare the results using these methods.

3. Theoretical approach

First we define Bouguer anomaly as,

$$B=g-\gamma+\beta h-2\pi G\rho h+\rho T, \tag{1}$$

where g: observed gravity value, γ: normal gravity value, β: free-air gradient, h: station height, G: gravitational constant, ρ: Bouguer correction density, and T: terrain correction per unit density, respectively. In this paper we assume that Bouguer correction is made by an infinite slab supposed to lie between the station and the sea level. We also ignore spherical and atmospheric effects for the sake of simplicity.

3.1 Nettleton's method

Nettleton's method (Nettleton, 1939; Vajk, 1956; Nettleton, 1976; Torge, 1989) was the first to evaluate reduction density where surface features should be eliminated as much as possible, based on the assumption that any correlations can be applied for gravity profiles and areas of interest. The measurements are reduced with different elevation factors to find the one which minimize the correlation of gravity with topography. Thus the optimum reduction density is determined such that the correlations between gravity anomaly and topography are totally absent. This method has been widely used for many years since 1940s. Usually graphical evaluations for correlations between topography and Bouguer anomalies for various densities have been used. A good example is illustrated in Figure 1 which schematically compares the density profiles with local topography. The several gravity profiles are reduced with elevation factors corresponding to the densities shown. Note that the optimum reduction

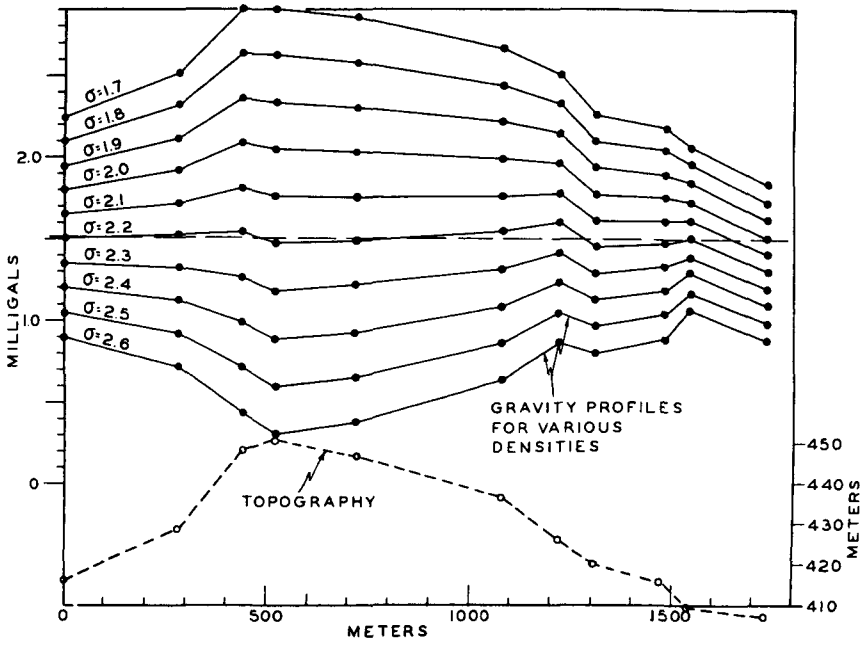

Fig. 1. Density profile over local topographic feature (Nettleton, 1976). The several gravity profiles are reduced with elevation factors corresponding to the densities shown. The optimum density is 2.2 g/cm^3, as that profile has minimum correlation with topography.

density is 2.2 g/cm^3 in this case.

It is essential for the success of Nettleton's method that topography is not correlated with surface structure. So it is necessary to select a topographic profile over a hill rather than a valley to avoid the effect of light sediments. Also, it is preferable to select a profile over rugged topography rather than a one-sided rise or fall. In this sense Nettleton's method should be limited to use only if the gravity anomalies are smooth compared to the topographic relief which is not correlated with subsurface structures. Torge (1989) suggested that the following assumptions should be made for applications of Nettleton's method:

- A density distribution which does not depend on the topography. The Nettleton's estimate fails if the topography is dominated by deeper geological structures;
- A homogeneous density distribution in the area of interest;
- Sufficient large (>100 m) elevation differences and a uniform distribution

of gravity measurements with respect to horizontal positions and elevations;

• A sufficient model of the regional field to be separated from the data.

Jung (1953, 1959) and Linsser (1965) have pointed out that the Nettleton's method can be translated into exact mathematical language by putting the correlation coefficient between Bouguer anomaly and elevation equal to zero. Assuming approximate Bouguer density ρ_0, we can compute the Bouguer anomaly B_0 from (1). Comparison with the "true" anomalies B with Bouguer density

$$\rho=\rho_0+\delta\rho, \tag{2}$$

yields

$$B = B_0-2\pi Gh\delta\rho-\frac{T_0}{\rho_0}\delta\rho, \tag{3}$$

where T_0 is the terrain correction calculated with ρ_0. After subtraction of the regional fields (an average value) the residual anomalies become approximate random quantities. Nettleton's procedure requires that these quantities not be correlated with topography. Let N be the number of gravity stations in the area of interest. The condition for the correlation coefficient r becomes,

$$r=\frac{\sum_{i=1}^{N}(h_i-\bar{h})\,(B_i-\bar{B})}{\sqrt{\sum_{i=1}^{N}(h_i-\bar{h})^2(B_i-\bar{B})^2}}=0, \tag{4}$$

where $\bar{B}$ and $\bar{h}$ are average values of Bouguer anomalies and heights, respectively. Inserting (3) into (4) and assuming that the approximation ρ_0 is sufficient for the terrain correction, that is, we neglect the difference of the terrain correction term of the RHS of (3), lead to

$$\delta\rho=\frac{\sum_{i=1}^{N}(h_i-\bar{h})\,(B_i-\bar{B})}{2\pi G\sum_{i=1}^{N}(h_i-\bar{h})^2}. \tag{5}$$

From equations (2), (3) and (5), we finally obtain the optimum density ρ_N by the Nettleton's method as,

$$\rho_N=\frac{\sum_{i=1}^{N}(h_i-\bar{h})\,(F_i-\bar{F})}{2\pi G\sum_{i=1}^{N}(h_i-\bar{h})^2}, \tag{6}$$

where

$$\begin{cases} F_i = g_i - \gamma_i + \beta h_i \\ \bar{F} = \dfrac{\sum_{i=1}^{N} F_i}{N} \end{cases} . \tag{7}$$

Linsser (1965) proposed another approach to formulate a generalized form of Nettleton's density estimate. He introduced a general formula for the Bouguer anomaly using a non-specified linear operator. By choosing special definition for this operator, he obtained the formulae of several mathematical forms of Nettleton's method. He also pointed out that the determination of the density by Nettleton's profile method using graphical approach gives less reliable results than the statistical investigation of the whole area covered by gravity surveys.

If we introduce $H=(2\pi Gh-T)$, (1) becomes

$$B=F-H\rho_R, \tag{8}$$

where ρ_R is a true Bouguer density. From equations (6) and (8) we obtain

$$\rho_N = \left\{ \frac{\sum_{i=1}^{N}(h_i-\bar{h})(H_i-\bar{H})}{2\pi G\sum_{i=1}^{N}(h_i-\bar{h})^2} \right\}\rho_R + \left\{ \frac{\sum_{i=1}^{N}(h_i-\bar{h})(B_i-\bar{B})}{2\pi G\sum_{i=1}^{N}(h_i-\bar{h})^2} \right\}. \tag{9}$$

Since we neglect T here, (9) reduces to

$$\begin{aligned} \rho_N &= \rho_R + \frac{\sum_{i=1}^{N}(h_i-\bar{h})(B_i-\bar{B})}{2\pi G\sum_{i=1}^{N}(h_i-\bar{h})^2} \\ &= \rho_R + \delta\rho. \end{aligned} \tag{10}$$

The second term $\delta\rho$ of the RHS of (10) is a deviation of estimated density ρ_N from a true density ρ_R and includes the term of correlations between Bouguer anomalies and topography in the numerator. If the correlations are negative, Nettleton's estimate gives lower value since the denominator of the fluctuation is always positive, and vice versa. Nettleton (1939) suggested that the density by his graphical procedure gives, instead of the true density, an apparent density which corrects for both the anomalous vertical gradient and a possible erroneous constant of gravimeters.

3.2 G-H method

Next we consider the simple G-H method where, in general, terrain corrections are not taken into account. We modify the RHS of (1) as,

$$B=(g-\gamma)+(\beta-2\pi G\rho)h$$

$$= Q + ah. \tag{11}$$

We plot $Q(=g-\gamma)$ against h and draw the best fitting straight line in a least squares sense. The optimum density can then be obtained from its slope.

This can also be translated into the exact mathematical formula. To obtain an optimum density we minimize the summation of the difference between the representative $\bar{B}$ of the smoothed profile of Bouguer anomaly averaged over the area of interest and each Bouguer anomaly value. This least squares minimization can be represented by

$$S = \sum_{i=1}^{N}\{Q_i + ah_i - \bar{B}\}^2 \Longrightarrow minimum\left(\bar{B} = \frac{\sum_{i=1}^{N} B_i}{N}\right) \tag{12}$$

$$\frac{\partial S}{\partial \bar{B}} = \frac{\partial S}{\partial a} = 0 \Longrightarrow Solution. \tag{13}$$

This condition yields the estimates ρ_{gh} as,

$$\rho_{gh} = \frac{\sum_{i=1}^{N}(h_i - \bar{h})(F_i - \bar{F})}{2\pi G \sum_{i=1}^{N}(h_i - \bar{h})^2}. \tag{14}$$

Note that this is equivalent to Nettleton's estimate in (6). This solution by the simple G-H method can be extended to the generalized G-H method where terrain corrections are taken into account. In this case we should use,

$$\begin{aligned} B &= (g - \gamma + \rho T) + (\beta - 2\pi G\rho)h \\ &= Q + ah, \end{aligned} \tag{15}$$

instead of (11). From similar conditions in equations (12) and (13), we obtain the solution ρ_{GH} for the generalized G-H method as,

$$\rho_{GH} = \frac{\sum_{i=1}^{N}(h_i - \bar{h})(F_i - \bar{F})}{\sum_{i=1}^{N}(h_i - \bar{h})(H_i - \bar{H})}, \tag{16}$$

where

$$\begin{cases} F_i = g_i - \gamma_i + \beta h_i \\ H_i = 2\pi G h_i - T_i \\ \bar{F} = \dfrac{\sum_{i=1}^{N} F_i}{N} \\ \bar{H} = \dfrac{\sum_{i=1}^{N} H_i}{N}. \end{cases} \tag{17}$$

Equation (16) can be rewritten as,

$$\rho_{GH} = \rho_R + \frac{\sum_{i=1}^{N}(h_i-\bar{h})(B_i-\bar{B})}{\sum_{i=1}^{N}(h_i-\bar{h})(H_i-\bar{H})}. \tag{18}$$

We also note that the difference of estimated density ρ_{GH} from a true density ρ_R in (18) includes the term of correlations of Bouguer anomalies with topography in the numerator. Positive correlations lead to a larger estimate of density in the generalized G-H method, and vice versa.

3.3 Method of Rikitake et al.

In the method of Rikitake et al. (1965), which is essentially the same as the generalized G-H method, we first define a terrain density ρ_T and we plot $Q'(= g-\gamma+\rho_T T)$ against h similarly in G-H method. Note that T is the terrain correction per unit density. Drawing a best fitting line in a least squares sense also yields the optimum density ρ_B. Finally the optimum reduction density can be determined when ρ_T is equal to ρ_B after some iterations (Rikitake et al., 1965 ; Hagiwara, 1978).

This method can also be translated into similar mathematical languages as in G-H method (Takakura and Hanaoka, 1988). As described above, we separate Bouguer density from terrain correction density in (1) as,

$$\begin{aligned} B &= (g-\gamma+\rho_T T)+(\beta-2\pi G\rho_B)h \\ &= Q'+\alpha' h. \end{aligned} \tag{19}$$

We can formulate the minimization condition similarly in (12),

$$S = \sum_{i=1}^{N}\{Q_i'+\alpha' h_i-\bar{B}\}^2 \Longrightarrow \textit{minimum}\left(\bar{B} = \frac{\sum_{i=1}^{N}B_i}{N}\right) \tag{20}$$

$$\frac{\partial S}{\partial \bar{B}} = \frac{\partial S}{\partial \alpha'} = 0,\ \rho_T = \rho_B \Longrightarrow \textit{Solution}. \tag{21}$$

This minimization condition gives the solution ρ_{RI} as,

$$\rho_{RI} = \frac{\sum_{i=1}^{N}(h_i-\bar{h})(F_i-\bar{F})}{\sum_{i=1}^{N}(h_i-\bar{h})(H_i-\bar{H})}. \tag{22}$$

Note that this is equivalent to the estimate of the generalized G-H method in (16), and the difference of estimated density ρ_{RI} from a true density ρ_R in (22) also has the same form of (18).

3.4 *F-H method*

In the F-H method proposed by Parasnis (1952, 1979), $(g-\gamma+\beta h)$ in (1) is plotted against $(2\pi Gh-T)$ and the slope of the straight line (determined by least squares method) is adopted as the optimum reduction density. This is equivalent to assuming Bouguer anomaly to be a random error. We shall hereafter denote this "the simple F-H method".

This method mathematically minimizes the summation of the difference between the representative $\bar{B}$ of the smoothed profile of Bouguer anomaly averaged over the area of interest and each Bouguer anomaly value. We modify the RHS of (1) as,

$$\begin{aligned} B &= (g-\gamma+\beta h)-(2\pi Gh-T)\rho \\ &= F-H\rho, \end{aligned} \tag{23}$$

where F is a free-air anomaly and H simply means a topography term. Similarly in G-H method we can formulate a minimization condition as,

$$S=\sum_{i=1}^{N}\{F_i-H_i\rho-\bar{B}\}^2 \Longrightarrow minimum\left(\bar{B}=\frac{\sum_{i=1}^{N}B_i}{N}\right) \tag{24}$$

$$\frac{\partial S}{\partial \bar{B}}=\frac{\partial S}{\partial \rho}=0 \Longrightarrow Solution. \tag{25}$$

We can then obtain the estimated density of ρ_{FH} from the condition (25),

$$\rho_{FH}=\frac{\sum_{i=1}^{N}(H_i-\bar{H})(F_i-\bar{F})}{\sum_{i=1}^{N}(H_i-\bar{H})^2}. \tag{26}$$

Takakura and Hanaoka (1988) showed that the density estimate (26) can be rewritten as,

$$\rho_{FH}=\rho_R+\frac{\sum_{i=1}^{N}(H_i-\bar{H})(B_i-\bar{B})}{\sum_{i=1}^{N}(H_i-\bar{H})^2}. \tag{27}$$

In this case the difference of estimated density ρ_{FH} from a true density ρ_R in (27) also includes the term of correlations of Bouguer anomalies with topography in the numerator. If Bouguer anomalies are negatively correlated with topography, F-H method yields a lower estimate of density, and vice versa.

Parasnis (1979) pointed out that simple F-H method is essentially a generalization of the method due to Siegert (1942) in which the terrain correction is neglected. Note that equations (16), (22) and (26) are identical at $T=0$ and

reduce to Nettleton's estimate in (6). Legge (1944) has described a method neglecting T in which Bouguer anomaly, instead of being treated as a random error, is developed as a power series in the distance of a station from the base.

If the area of interest is so large that the topographic relief is on the whole in isostatic equilibrium, there is no correlation between free-air anomaly and topography. In this case the following formula would hold.

$$\sum_{i=1}^{N}(H_i-\bar{H})(F_i-\bar{F})=0. \tag{28}$$

Substituting (28) into (26) yields a density estimate $\rho_{FH}=0$. This means that a larger area is associated with a lower estimate of reduction density. This would also hold in all methods described so far and we should limit to use the former methods in a smaller area.

3.5 Extended F-H method

In a larger area, topography tends to be in isostatic equilibrium or supported by a dynamic force within the earth, and therefore must be correlated with the long-wavelength components of Bouguer anomalies. Taking these correlations into account, Fukao et al. (1981) proposed a new method, based on Parasnis's F-H method, in which Bouguer anomalies are approximated by a piecewise step function in a two dimensional space.

Fukao et al. (1981) considered a smoothed profile of Bouguer anomaly which would be virtually obtained by dividing the area of interest into a series of meshes of equal size. Let rewrite (1) in the form of a two-dimensional space,

$$\begin{aligned} B_{ij} &= g_{ij}-\gamma_{ij}+\beta h_{ij}-2\pi G\rho h_{ij}+\rho T_{ij} \\ &= (g_{ij}-\gamma_{ij}+\beta h_{ij})-(2\pi G h_{ij}-T_{ij})\rho \\ &= F_{ij}-H_{ij}\rho, \end{aligned} \tag{29}$$

and assuming the number of meshes M, the number of stations N_j within the Jth mesh, we obtain the minimization condition,

$$S=\sum_{j=1}^{M}\sum_{i=1}^{Nj}\{F_{ij}-H_{ij}\rho-\overline{B_j}\}^2 \Longrightarrow minimum\left(\overline{B_j}=\frac{\sum_{k=1}^{N_j}B_{jk}}{N_j}\right) \tag{30}$$

$$\frac{\partial S}{\partial \overline{B_j}}=\frac{\partial S}{\partial \rho}=0 \Longrightarrow Solution. \tag{31}$$

Similarly in F-H method, this minimization condition yields the optimum density ρ_{EF}

$$\rho_{EF}=\frac{\sum_{j=1}^{M}\sum_{i=1}^{Nj}(H_{ij}-\overline{H_j})\,(F_{ij}-\overline{F_j})}{\sum_{j=1}^{M}\sum_{i=1}^{Nj}(H_{ij}-\overline{H_j})^2}. \tag{32}$$

Note that the density estimate thus obtained is in general dependent on mesh size. If the area of interest is sufficiently large where the topographic relief is in isostatic equilibrium on the whole, (32) gives an estimated density $\rho_{EF}\approx 0$ since (28) would hold. Thus a larger mesh size is in general associated with a lower estimate of density. We will examine how estimated density ρ_{EF} changes over mesh sizes in a few examples later.

A reduction of mesh size, on the other hand, may lead to a threshold mesh size at which Bouguer profile loses any correlation in each mesh with the corresponding topographic profile. In this method the threshold mesh size and the optimum reduction density may be obtained by plotting an estimated density as a function of mesh size. Note that the above way of density determination automatically generates sets of correctly estimated Bouguer anomalies in mesh form which are easily subject to machine contouring. If we set $M=1$, (32) becomes identical to Parasnis's estimate in (26). If we set $M=1$ and $T=0$, (32) reduces to Nettleton's estimate (6).

Since the "true" Bouguer anomaly can be represented by $(F_{ij}-H_{ij}\rho_R)$ from (29), where ρ_R is a "true" reduction density, (32) can be easily rewritten as,

$$\rho_{EF}=\rho_R+\frac{\sum_{j=1}^{M}\sum_{i=1}^{Nj}(H_{ij}-\overline{H_j})\,(B_{ij}-\overline{B_j})}{\sum_{j=1}^{M}\sum_{i=1}^{Nj}(H_{ij}-\overline{H_j})^2}. \tag{33}$$

In this case we also recognize that the difference of estimated density ρ_{EF} from a true density ρ_R in (33) includes the term of correlations between Bouguer anomalies and topography in the numerator. Negative correlations lead to a lower estimate of density in F-H method, and vice versa.

Takakura and Hanaoka (1988) suggested that extended F-H method may lead to an incorrect estimate when gravity data have a quite limited distribution in some meshes over a whole region of interest since (32) incorporates weighted mean of the data included in each mesh. They simply modified (32) and obtained another estimate as,

$$\rho_{TH}=\frac{1}{M}\sum_{j=1}^{M}\left\{\frac{\sum_{i=1}^{Nj}(H_{ij}-\overline{H_j})\,(F_{ij}-\overline{F_j})}{\sum_{i=1}^{Nj}(H_{ij}-\overline{H_j})^2}\right\}. \tag{34}$$

Note that this estimate means the representative value averaged over

subdivided meshes. Takakura and Hanaoka (1988) also showed another possibility that we may adopt weighted average procedure in (34).

3.6 ABIC method

More recently Murata (1990, 1993) proposed another approach based on the assumption that the Bouguer anomaly varies smoothly as compared to topography and approximated the Bouguer anomaly by a smooth function. Assume here that free-air anomaly F_i and topographic correction term H_i are given at points (x_i, y_i) $(i=1, \ldots, N)$. In his method an optimum terrain density is calculated by minimizing the following function,

$$\sum_{i=1}^{N}\{F_i-\rho H_i-f(x_i, y_i|\mathbf{s})\}^2+\sum_{k=1}^{2}\omega_k\int_V\int_V\|\nabla^k f\|^2 dxdy \Longrightarrow \textit{minimum} \qquad (35)$$

where f: the cubic B spline function fitted to the observed Bouguer anomalies $(F_i-\rho H_i)$, $\mathbf{s}$: a vector of spline parameters, $\nabla^k f$: k-th differentiation of the function f, and ω_k: trade-off parameters, respectively. There is a trade-off in this minimization problem between the roughness of the curved surface fitted to the Bouguer anomalies and the residual of the Bouguer anomalies from the fitted surface. The trade-off parameters ω_1 and ω_2 control the first-order roughness (gradient of f) and the second-order roughness (curvature of f) of the Bouguer anomaly surface, respectively. A suitable choice is made for ω_1 and ω_2 by minimizing *ABIC* (Akaike, 1980). Equation (35) can be reduced in a matrix form as,

$$\|\mathbf{F}-\rho\mathbf{H}-\mathbf{Es}\|^2+\|\mathbf{D}_\omega\mathbf{s}\|^2 \Longrightarrow \textit{minimum} \qquad (36)$$

where $\mathbf{s}$: M parameters of the function f, $\mathbf{F}$: vector which denotes free-air anomalies, $\mathbf{H}$: vector which denotes terrain and Bouguer corrections per unit density, and $\mathbf{D}_\omega$ is an $N\times M$ matrix containing the trade-off parameters ω_1 and ω_2, respectively.

$\mathbf{E}$ is an $N\times M$ matrix such that $\mathbf{Es}$ stands for spline values at stations; $\mathbf{s}=[s_1, \ldots, s_M]^T$. T denotes transposition. $\|\cdot\|$ denotes the norm, and $\mathbf{D}_\omega$ is an $N\times M$ matrix calculated from

$$\sum_{k=1}^{2}\omega_k\int_V\int_V\|\nabla^k f\|^2 dxdy = \|\mathbf{D}_\omega\mathbf{s}\|^2. \qquad (37)$$

If the number of spline knots is M_x in the x direction and M_y in the y direction, we obtain $M=(M_x+3)(M_y+3)$. Minimizing (36) reduces to solve the equation

$$\mathbf{a} = \mathbf{Zv}, \qquad (38)$$

where $\mathbf{a}=[F_1, \ldots, F_N, 0, \ldots, 0]^T$ and $\mathbf{v}=[s_1, \ldots, s_M, \rho_1, \ldots, \rho_K]^T$. $\mathbf{Z}$ is an $(N+M)\times(M+K)$ matrix;

$$\mathbf{Z}=\begin{bmatrix} E_{11} & \cdots & E_{1M} & H_{11} & \ldots & H_{1K} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ E_{N1} & \cdots & E_{NM} & H_{N1} & \ldots & H_{NK} \\ D_{11} & \cdots & D_{1M} & 0 & \ldots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ D_{M1} & \cdots & D_{MM} & 0 & \ldots & 0 \end{bmatrix}. \tag{39}$$

$\mathbf{D}$ involves the trade-off parameters ω_1 and ω_2. Once preferable sets of trade-off parameters are obtained, (38) can easily be solved. These preferable sets of ω_1 and ω_2 can be determined by *ABIC* (Akaike, 1980). A mathematical expression of *ABIC* is given by

$$\begin{aligned} ABIC=&N\log(2\pi\hat{\sigma}^2)-\log(\det|\overline{\mathbf{D}^T\mathbf{D}}|) \\ &+\log(\det|\mathbf{Z}^T\mathbf{Z}|)+N+2\times(2K+4), \end{aligned} \tag{40}$$

where $\hat{\sigma}^2$ is defined by

$$\hat{\sigma}^2=\frac{1}{N}\|\mathbf{a}-\mathbf{Z}\mathbf{v}\|^2. \tag{41}$$

$\overline{\mathbf{D}^T\mathbf{D}}$ is the cofactor matrix of $\mathbf{D}^T\mathbf{D}$ with respect to the last diagonal element. The standard error of the parameter vector $\mathbf{v}$ is given by

$$\widehat{\mathbf{c}_v}=\hat{\sigma}^2(\mathbf{Z}^T\mathbf{Z})^{-1}. \tag{42}$$

Equations (36)~(40) are a generalization of the original equations in Murata (1993) (Nawa et al., 1997). The Bouguer density is estimated by iterating the following steps:

(*i*) Set initial values to the trade-off parameters ω_1 and ω_2.

(*ii*) Calculate the matrix $\mathbf{D}^T\mathbf{D}$ and its determinant.

(*iii*) Solve the least squares problem $\|\mathbf{a}-\mathbf{Z}\mathbf{v}\|^2$ by the Householder transformation and calculate the $\hat{\sigma}^2$ from the residual.

(*iv*) Calculate the determinant λ of the matrix $\mathbf{Z}^T\mathbf{Z}$ by

$$\log\lambda=2\sum_{i=1}^{M}\log R_{ii}, \tag{43}$$

where $\mathbf{R}=(R_{ii})$ is the upper triangular matrix such that $\mathbf{Z}=\mathbf{Q}\mathbf{R}$, and the orthogonal matrix $\mathbf{Q}$, is a byproduct of the Householder transformation of step (*iii*).

(*v*) Calculate the *ABIC* using (40).

(*vi*) Test the convergence of the *ABIC* value. When it reaches a minimum, the iteration is complete. Otherwise, update the hyperparameters by the algo-

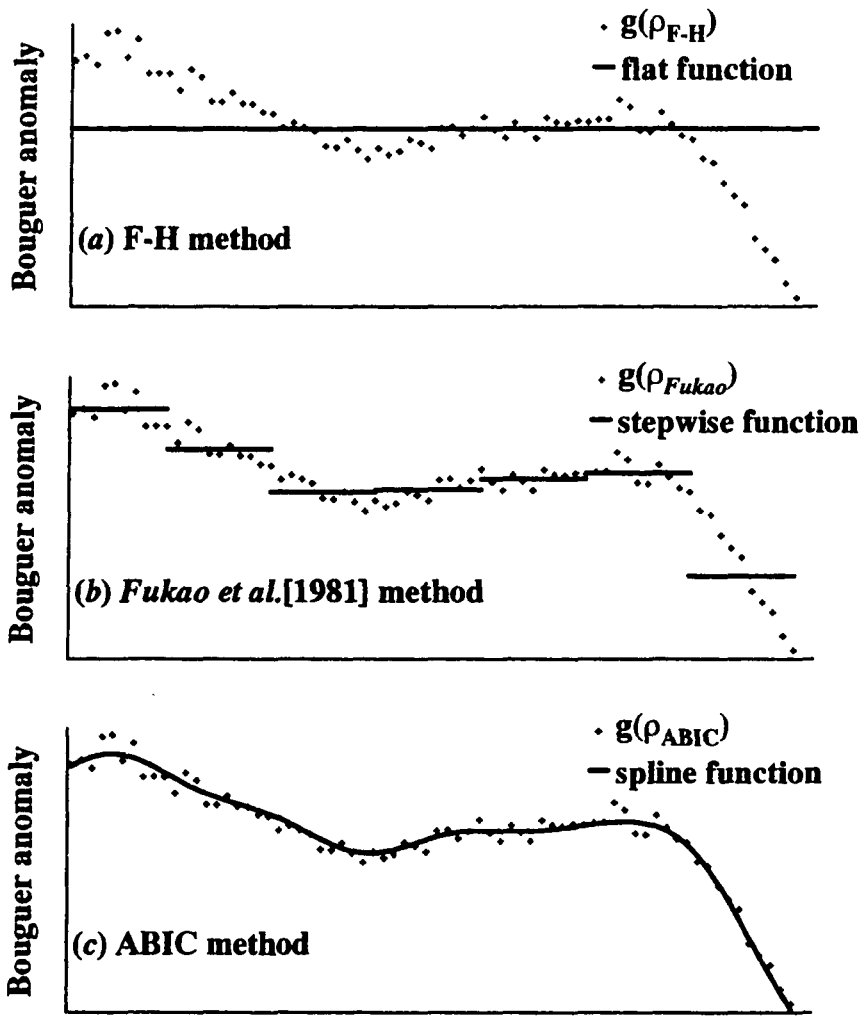

Fig. 2. Cross sections of Bouguer anomaly map for schematic description of estimation of gravity reduction density (Murata, 1990). Three methods estimate Bouguer density by the minimization of the sum of the square of the residuals between observed Bouguer anomalies and fitted surface. Note that the difference of the fitted surface, (a) the F-H method fitting Bouguer anomalies to a horizontal flat surface, (b) the extended F-H method fitting to stepwise surfaces, and (c) the *ABIC* minimization method fitting to a spline surface whose optimum smoothness is determined by *ABIC* (Akaike, 1980).

rithm of the simplex method and return to step (*ii*) for further iteration.

Figure 2 demonstrates the cross sections of Bouguer anomaly for schematic description to understand the features of the above three methods (simple F-H method, extended F-H method and *ABIC* method) which minimize the sum of the square of the residuals between observed Bouguer anomalies and fitted surface (Murata, 1993). In this figure we can examine how the minimization differ on these three methods. In Figure 2(a) the minimization of simple F-H method reduces to determine a single flat surface in a least squares sense. In Figure 2(b) extended F-H method minimizes the residuals by fitting Bouguer anomalies to stepwise surfaces where an area of interest is subdivided into a series of meshes of equal size. In the minimization of *ABIC* method in Figure 2(c) the fitted function is a smooth spline function whose optimum smoothness is determined by minimizing the *ABIC* (Akaike, 1980).

4. Results and Discussions

In this section we compare a few results of calculations by several methods presented in the previous sections. Fukao et al. (1981) and Yamamoto et al. (1982) applied Nettleton's method, Rikitake's method and extended F-H method to gravity data in the Central Ranges, Japan and compared the results of estimated densities. The study area is a typical mountainous region which consists of the three largest mountain ranges (Akaishi, Kiso and Hida) in Japan, having the width of $2^\circ \times 2^\circ$ ($\sim$200 km $\times$ 200 km). All mountains, except Mt. Fuji, whose altitude exceeds 3,000 m in Japan gather in this area.

Figure 3 demonstrates a sample plot of an optimum density as a function of mesh size (Fukao et al., 1981). Calculated density shows an approximately constant value of 2.64 g/cm^3 for mesh size 2′ ($\sim$3.4 km) to 10′ ($\sim$17 km). This can be adopted as the optimum reduction density in the area of interest. For larger mesh sizes estimated density decreases rapidly with increasing mesh size although it is still of a finite value of 1.49 g/cm^3 even at the largest mesh size. This result is in good agreement with earlier theoretical considerations that a larger area is associated with a lower estimate of reduction density. For mesh sizes of less than 2′ we can see a tendency of further increase in estimated density with decreasing mesh size. This can be interpreted as an instability phenomenon arising at the virtual end of the reduction process of mesh size. They obtained the density 1.50 g/cm^3 by Nettleton's method and Rikitake's method. This value is almost identical to the optimum density 1.49 g/cm^3 by extended F-H method for the largest mesh size in Figure 3.

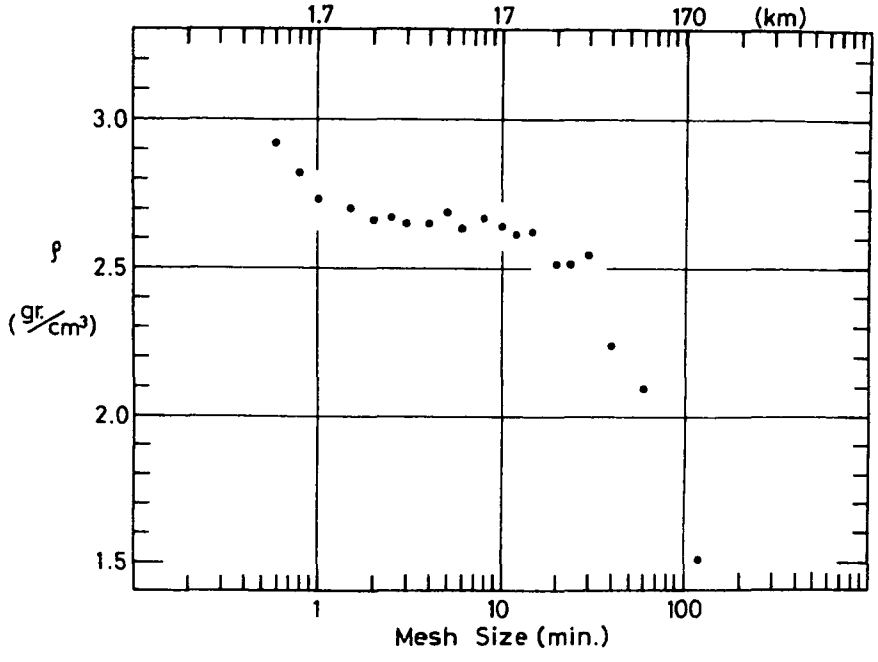

Fig. 3. Plot of an optimum density as a function of mesh size (Fukao et al., 1981). The mesh size is changed from 0.6′×0.6′ to 120′×120′ where 1′~1.7 km. Calculated density shows an approximately constant value of 2.64 g/cm³ for mesh size 2′ (~3.4 km) to 10′ (~17 km). This can be adopted as the optimum reduction density for surface or subsurface terrains in the area.

Next we show another example in which simple F-H method, extended F-H method and *ABIC* method are applied to three regions for comparison. The study areas in this example are: Large area (Abukuma ~50 km×70 km), Middle area (Kirishima ~25 km×20 km), and Small area (Oya~0.75 km×0.85 km), respectively. Abukuma area is located in Yamizo-Abukuma mountain region (Ibaraki and Fukushima Prefecture), Japan, where granitic rocks and metamorphic rocks are dominantly distributed. Kirishima area is characterized by a Kirishima volcano zone located in the southern part of Kyushu District (Kagoshima and Miyazaki Prefecture), Japan. This area mainly consists of andesitic rocks. Oya area is located in Utsunomiya city, Tochigi Prefecture, Japan, where Neogene pumice-tuff named "Oya rocks" is dominant. Average density determined from rock sampling in Oya area is about 1.8 g/cm³ (Murata, 1990). Maximum elevation difference of these three regions is 1,060 m, 1,559.58 m and 11.18 m, respectively.

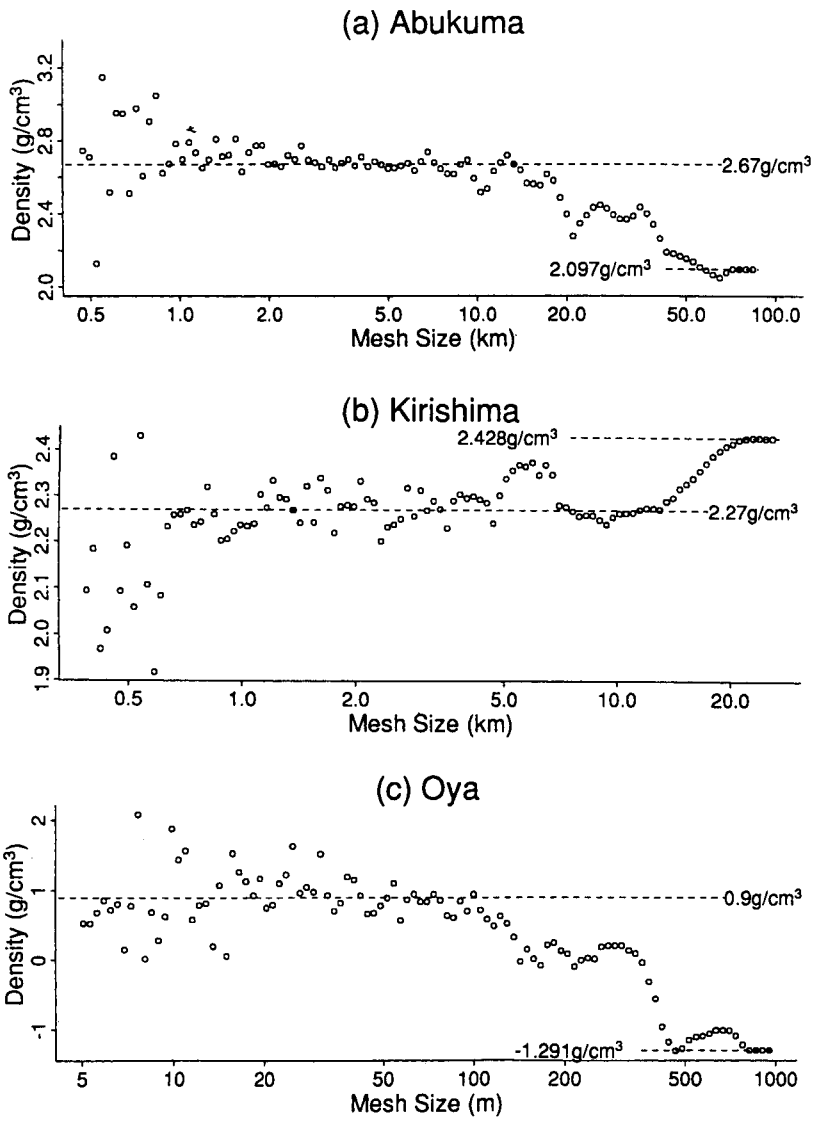

Fig. 4. Plots of optimum densities as a function of mesh size (Murata, 1990) in (a) Large area (Abukuma ~50 km×70 km), (b) Middle area (Kirishima ~25 km×20 km), and (c) Small area (Oya~0.75 km×0.85 km), respectively. Dashed lines are the average densities. In the large area Bouguer density is estimated at about 2.67 g/cm³. In the middle area Bouguer density is not stable and optimum value is about 2.27 g/cm³. In the small area the optimum Bouguer density is estimated at about 0.9 g/cm³.

Figure 4 demonstrates the results using extended F-H method for these three regions (Murata, 1990). Dashed lines are the average densities. Solid lines show regression lines. Estimated reduction densities and standard errors for the above three regions by the three method (F-H method, extended F-H method and *ABIC* minimization method) are also summarized in Table 1. In *ABIC* method various variations of spline knots are used. In-situ densities measured from sample rocks are also shown in large and middle area.

As shown in Figure 4(a) Bouguer density tends to be much stable for mesh sizes of 0.5 km~15 km in the large area and is estimated at about 2.67 g/cm^3. This values shows a good agreement with results obtained from rock sampling (see Table 1). In the middle area shown in Figure 4(b), Bouguer density is not stable and optimum value is about 2.27 g/cm^3. It is intriguing that a large estimate (2.428 g/cm^3) is obtained for the largest mesh size in this case. The estimated value 2.27 g/cm^3 is slightly lower than the mean density of actual rock sampling results of about 2.47 g/cm^3 (see Table 1). Kirishima area is characterized by the existence of volcanic rocks. The presence of pore space resulting from joints, fractures, cleavage and other penetrative structure distorts density determination of (extended) F-H method and may give lower estimate. In Oya area, the optimum Bouguer density is estimated at about 0.9 g/cm^3 as shown in Figure 4(c). This is an unreasonably lower estimate. Furthermore, the densities for larger mesh sizes ($>\sim$150 m) show negative values in which the lowest one is -1.291 g/cm^3. This suggests that negative correlations between Bouguer anomalies and topography are larger than vertical gradients of free-air anomalies.

Various variations of spline knots are used for *ABIC* method (see Table 1). In large area estimated densities by extended F-H method (2.67 g/cm^3) and *ABIC* ($\sim$2.69 g/cm^3) method are very close whereas simple F-H method gives a considerably lower estimate of Bouguer density 2.097 g/cm^3. This means that the estimation errors (the second term of the RHS of equation (27)) of reduction density by F-H method have negative values since the correlations between Bouguer anomalies and topography in this area show negative.

In middle area the estimated density 2.27 g/cm^3 by extended F-H method for mesh sizes of 1 km~5 km shows a good agreement with the density 2.47 g/cm^3 determined from sample rocks. Simple F-H method also gives a good result of 2.428 g/cm^3. *ABIC* method, however, gives a slightly lower estimate $\sim$2.16 g/cm^3. Murata (1990) pointed out that total porosity with volcanic rocks is not reflected in actual densities on rock samples since this middle area is a volcanic region where porous rocks are dominant. Therefore, taking the

Table 1. Estimated reduction densities and standard errors (Murata, 1990) by three methods (F-H method, extended F-H method and ABIC minimization method). In ABIC method several variations of spline knots are used. Actually densities measured from sample rocks are also shown in large and middle area.

Method	Large area survey (Abukuma)		Middle area survey (Kirishima)		Small area surver (Oya)	
	Knots	Density (g/cm³)	Knots	Density (g/cm³)	Knots	Desity (g/cm³)
ABIC minimization	5×7	2.693±0.020	5×4	2.104±0.032	4×4	1.469±0.063
	10×14	2.709±0.017	10×8	2.111±0.032	8×8	1.553±0.063
	15×21	2.710±0.018	15×12	2.139±0.035	12×12	1.651±0.065
	20×28	2.701±0.018	20×16	2.156±0.037	16×16	1.628±0.067
	25×35	2.692±0.018	25×20	2.158±0.037	20×20	1.661±0.068
	30×42	2.694±0.018	30×24	2.163±0.038	24×24	1.661±0.068
	35×49	2.696±0.018	35×28	2.182±0.038	28×28	1.661±0.068
	40×56	2.699±0.018	40×32	2.175±0.038	32×32	1.661±0.067
F-H relation		2.097		2.428		−1.291
FUKAO *et al.* (1981)		2.67		2.27		0.9
Rock sample	Granite 5 samples	2.642±0.050	Andesite 104 sample	2.470±0.217		
	Granodiorite 15 samples	2.643±0.024				
	Metamorphic 9 samples	2.886±0.119				

average porosity in the area into account, Murata (1990) concluded that the estimated densities in Kirshima area by *ABIC* method are reasonable, and that F-H and extended F-H methods yields slightly larger estimates of density. Again, remember equation (33) which describes estimation errors in reduction density. In Kirishima area the correlations between Bouguer anomalies and topography (the numerator of the second term of the RHS of equation (33)) are definitely positive which consequently lead to a larger estimate of reduction density.

In small area simple F-H method shows a quite unreasonable estimate of density $-1.291\ g/cm^3$. This suggests that negative correlations between Bouguer anomalies and topography are larger than vertical gradients of free-air anomalies. Extended F-H method also shows a lower estimate of Bouguer density $0.9\ g/cm^3$ which is still undesirable result. This means that there still remains negative correlations between Bouguer anomalies and topography even in smaller mesh sizes applied in extended F-H method. However, estimated density by *ABIC* method is $1.661\ g/cm^3$ which is reasonable value since the results of rock sampling show about $1.8\ g/cm^3$ (Murata, 1990).

This result convincingly demonstrates that *ABIC* method has led to a success even in a small area where elevation difference is inevitably small, whereas classical methods (Nettleton's method, simple F-H method and extended F-H method) do not furnish a reasonable estimate of reduction density. Presumably, this is due to a fact that the maximum difference of altitude is about only 11 m in a narrow region (Oya area). Note that estimated densities using various spline knots in *ABIC* method do not show any fluctuations in all three cases. This means that *ABIC* method gives quite stable density estimates which do not depend on the number of spline knots.

5. Conclusions

We have summarized several methods of density determinations from surface gravity measurements for gravity reduction, and their theoretical overview was extensively demonstrated. It is suggested that the classical Nettleton's or F-H methods should be used under some assumptions and limited to use only if the gravity anomalies are smooth compared to the topographic relief which is not correlated with subsurface structures. On the contrary, modern methods such as extended F-H and *ABIC* methods are quite useful and powerful even for large areas where the topographic relief is on the whole in isostatic equilibrium as well as for sufficiently small areas where negative

correlations between Bouguer anomalies and topography are larger than vertical gradients of free-air anomalies. We also conclusively demonstrated the effectiveness of the *ABIC* method for a sufficiently small area where the difference of maximum altitude is ~10 m. As shown by Nawa et al. (1997), *ABIC* method can be applied for Bouguer correction with a variable density which is important for understanding geologically meaningful Bouguer anomalies. These facts clearly suggest that extended F-H and *ABIC* methods are very powerful tools to estimate optimum densities from gravity data and to interpret Bouguer anomalies for every geophysical fields.

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