Jour. Korean Inst. Mining Geol.
Vol. 17, No. 3, 1984, p. 163-169

Linear Inversion of Heat Flow Data

Wook Han

ABSTRACT: A linear inversion of heat flow values using heat production data with reliable value is studied in this work. To evaluate 2-D problem, a thin vertical sheet model is considered. Making use of a relation based on potential theory, a new relation between q_{rad} and A_0 is derived. The forward calculations with noise and without noise are shown. The inversion of random search is comparable to that of ridge regression method. The agreements between the computed and best fit after inversion suggest the importance of random search method in the inversion technique.

INTRODUCTION

The interpretation of heat flow values due to the sources of heat production may be complicated by a lot of factors. However, this problem can be alleviated to a certain degree if the accurate information of the heat sources on the typical rock types is available.

I collected the heat production data in the upper crust during the past three years. The heat production data with reliable value can give constraints on the vertical distribution of the heat source. This study is an experiment of the use of heat production and heat flow values.

To evaluate this problem, I chose to consider a thin vertical sheet model. I obtained eight data sets of heat prodction for heat flow values (sedimentary, igneous and metamorphic rocks). I am interested in determining the vertical distribution due to geochemical (isotopic) evolution of the continental crust.

Ridge regression inversion is used to estimate heat production values from heat flow data. The heat flow values are inverted to get the available information on the radioactive elements in the continental upper crust.

* Dept. of Environmental Sci., Korea Military Academy

THEORY

Forward problem

Consider a thin vertical sheet with heat production contrast (A_0) as the Figure 1. Simmons (1967) has shown the relation of the gravity to get theoretical surface heat flow values.

(1) $q_z = F_z A_0 / 2\pi G \rho$

q_z=heat flow at the surface
A_0=heat production
F_z=gravity
ρ=density

This equation is valid for the steady-state conditon of heat production.

The factors contributing to the problem of nonuniqueness are shown by Al-Chalobi (1971) and Hohmann (1982), From their discussion, we are concerned with the effects introduced by two factors because of considering the case of an exact model calculation: (a) heat flow values on some plane may be produced by a lot of possible solutions down so a certain depth; (b) observational errors resulting from measurements, reductions (radioactive part+mantle heat flow) and time (~1975, and 1975~1982) are always present on the field observations.

The difficulty is to determine the separate values for heat flow, time and equipment for

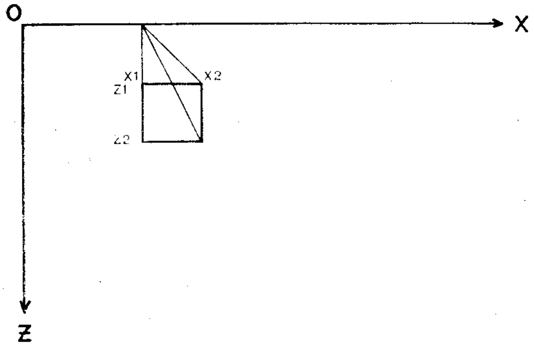

Fig. 1. Very thin vertical sheet

the measurements. But the heat production and the transfer mechanism in the upper crust can be determined with confidence. And to determine depth is another difficulty. However, the problem can be solved by the isotopic evolution in the continental crust and can be linearly dependent.

The considerations about the forward problem are as follows;

(a) potential theory shows a heat flow anomaly on some plane down to a certain depth

(b) isotopic evolution of the continental crust shows the vertical distribution of the radioactive elements.

From Figure 1, the gravity of the model is given by

$$g=-2G\int_s\int\frac{(z-z')}{(x-x')^2+(z-z')^2}\rho dx'dz'$$

where prime shows new coordinate.

Using identities

$$g=-G\rho\Big(\beta\ln(\beta^2+(z_1-z_2)^2-2\beta+2(z-z_2)\tan^{-1}\frac{\beta}{(z-z_2)}\Big)_{x_1}^{x_2}-\Big((\beta\ln(\beta^2+(z-z_1)^2)-2\beta+2(z-z_1)\tan^{-1}\Big(\frac{\beta}{(z-z_1)}\Big)_{x_1}^{x_2}\Big)$$

$$\beta=x-x'$$

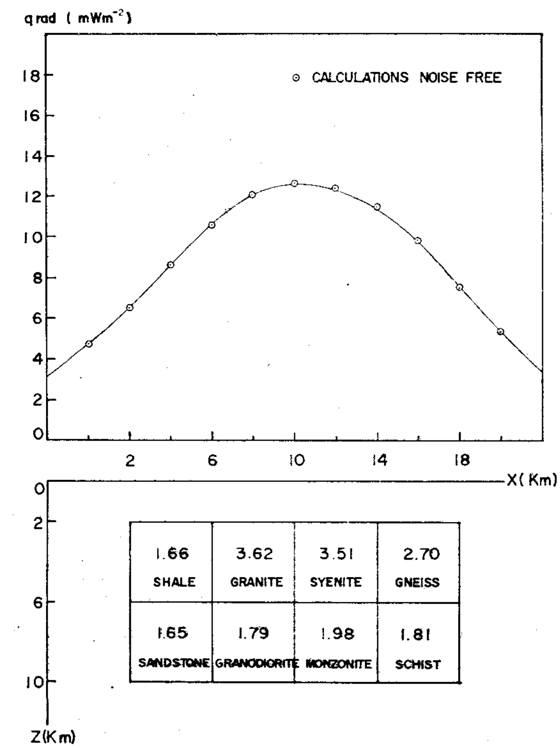

Fig. 2. 2-D calculations using representative values (unit; μWm^{-3})

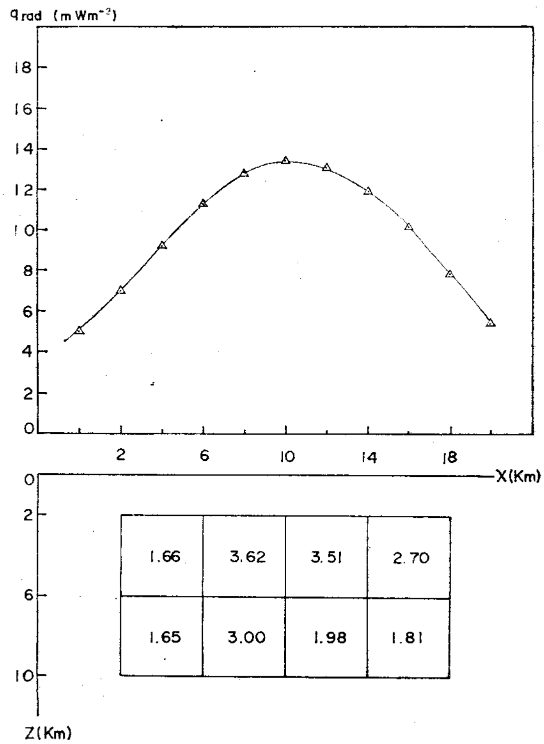

Fig. 3. 2-D calculations with magmatic body (3.0 μWm^{-3})

From (1)

$$q_{rad} = -\frac{A_0}{2\pi}[(x-x_2)[\ln\{(x-x_2)^2+(z-z_2)^2\}$$
$$-\ln\{(x-x_2)^2+(z-z_1)^2\}]$$
$$+(x-x_1)[\ln\{(x-x_1)^2+(z-z_1)^2\}$$
$$-\ln\{(x-x_1)^2+(z-z_2)^2\}$$
$$+2(z-z_2)\ \{\tan^{-1}\frac{(x-x_2)}{(z-z_2)}$$
$$-\tan^{-1}\frac{(x-x_1)}{(z-z_2)}\}$$
$$+2(z-z_1)\ \{\tan^{-1}\frac{(x-x_1)}{(z-z_1)}$$
$$-\tan^{-1}\frac{(x-x_2)}{(z-z_1)}\}]] \qquad (2)$$

where x is the horizontal distance and z is the depth. Using (2) 2-D calculations are shown in Figures 2 and 3.

Inverse problem

For this study, the summary of ridge regression inversion given by Marquardt (1970), Inman (1675) and Hohmann (1982) is reviewed in detail.

Because of the linear condition of the equation, Taylor's series expansion of the first order in the unknown parameters are given as

$$\Delta\bar{q} = A\Delta\bar{P} + \bar{\varepsilon}$$

where A is the $n \times m$ matrix of derivatives. A is a related small change in model parameter ΔP to a small change in data Δq. $\bar{\varepsilon}$ refers to a vector of error in the data points.

The ridge regression estimate of $\Delta\bar{P}$, designed to control the instability associated with Ordinary Least Squares (OLS), is

$$(A^TA+\theta^2I)^{-1}A^T\Delta q$$

with in the range $10^{-4}<\theta^2<1.0$ from Hohmann (1982), where I is the identity matrix and θ^2 is added to the diagonal elements to weigh out the very small eigenvalues resulting from poorly determined parameters. The estimator is a function of θ^2.

Perfect data are complete. Completeness depends upon the particular problem. Even though we never have perfect data, analyzing the problem for perfect data provides valuable insight.

In heat flow study we assume a layered model from petrological, geochemical and geophysical evidence and hope the solution may be useful.

So far, I have considered only the case of magmatic body intrusion. Since I am using data set by a un-weight matrix (W), uncorrelated errors and constant variance according to Dr. Hohmann's advice. Three noise levels ($\sigma_y = \pm 1.0$ mWm^{-2}, ± 1.4; 10% of radiogenic heat flow, ± 2.8; 20% of radiogenic heat flow: see Discussion) are added to the data sets. These noise levels are generated by random number generator. Here, noisy data are allowed to have much influence on the inversion in the case of ± 2.8mWm^{-2} noisy data.

The equation for parameter then becomes

$$\bar{P} = (A^TA+\theta^2I)^{-1}A^Tq$$

If standard deviations (σ_y) are known for each data point, the weighting can be selected. In this problem, I use the known standard deviations of the noise levels added to the data ($\sigma_y = \pm 1.0$ mWm^{-2}).

To address how accurately the parameters are calculated, I would like to get the standard deviations of the parameters. Hohman (1982) has shown this may be achieved by the covariance matrix

$$\mathrm{cov}(p) = (A^TA)^{-1}A^T\phi A(A^TA)^{-1}$$

where ϕ is the covariance matrix of error. Assuming uncorrelated errors, ϕ becomes a diagonal matrix with σ_i^2. The square root of the appropriate diagonal element of cov (p) gives an standard deviation.

Random number generation

The subroutine is used for uniform number generator based on the theory and suggestions by G.E. Forshythe et al (1977). The results are followings;

(a) case (± 1.0mWm^{-2}, intervals=2km)

q_{rad}=5.2mWm^{-2}
7.4mWm^{-2}
7.7mWm^{-2}

10.5mWm^{-2}
11.9mWm^{-2}
12.4mWm^{-2}
13.2mWm^{-2}
11.6mWm^{-2}
10.6mWm^{-2}
7.8mWm^{-2}
4.8mWm^{-2}

(b) case (±1.4mWm^{-2})

q_{rad}=4.4mWm^{-2}
5.8mWm^{-2}
8.4mWm^{-2}
10.5mWm^{-2}
12.1mWm^{-2}
13.1mWm^{-2}
12.2mWm^{-2}
10.5mWm^{-2}
11.0mWm^{-2}
8.6mWm^{-2}
5.5mWm^{-2}

(c) case (±2.8mWm^{-2})

q_{rad}=3.0mWm^{-2}
4.7mWm^{-2}
6.6mWm^{-2}
13.2mWm^{-2}
9.5mWm^{-2}
12.2mWm^{-2}
11.0mWm^{-2}
10.7mWm^{-2}
7.0mWm^{-2}
5.9mWm^{-2}
41.mWm^{-2}

To show the effect of heat production data on the interpretation of heat flow values, I considered three cases. In each case, the values are followings:

(1) with free noise

q_{rad}=4.7mWm^{-2}
6.5mWm^{-2}
8.6mWm^{-2}
10.6mWm^{-2}
12.1mWm^{-2}
12.7mWm^{-2}
12.5mWm^{-2}
11.5mWm^{-2}
9.8mWm^{-2}
7.5mWm^{-2}
5.3mWm^{-2}

(2) with noise due to magmatic body

q_{rad}=5.0mWm^{-2}
7.0mWm^{-2}
9.2mWm^{-2}
11.3mWm^{-2}
12.9mWm^{-2}
13.4mWm^{-2}
13.1mWm^{-2}
12.0mWm^{-2}
10.2mWm^{-2}
7.8mWm^{-2}
5.6mWm^{-2}

(3) with noise by random number

(a) case (±1.0mWm^{-2})
(b) case (±1.4mWm^{-2})
(c) case (±2.8mWm^{-2})

A large value of θ^2 results in the algorithm which is slow to converge. However it is very stable. Bevington (1969) and Hohmann (1982) show an appropriate values for θ^2 in the inversion process. I have considered the noise level according to high radioactive magmatic rock. In this way, noisy data are not allowed to have much influence on the inversion.

Parameter estimation

Finding a suitable solution to the geophysical parameter estimation usually involves minimizing an objective function. The residuals ($\bar{e}$) from the linearized problem is the misfit.

$$\bar{e}=\bar{Y}-A\bar{x}$$

where $\bar{x}$ is the vector of estimated parameter.

There are $L1$, $L2$ and L_∞ norms for this technique. $L1$ leads to a maximum likelihood estimate when the data contain-independent errors with Laplace distribution. Values more than 2 standard deviations from the mean are much more probabale under Laplace than Gauss distribution.

$L2$ produces a maximum likelihood estimate when the data contain error with Gauss distribution. When the data contain only, this type of noisy, $L2$ estimate is the best to choose. $L1$ may be useful when geologic noise is significant (Claerbout and Muir, 1973). $L_\infty$is senitive to errors in the data points. The largest residual has a minimum value. This is useful when the noise is negligible.

L1 minimization

Parameter estimation by $L1$ minimization and the sophisticated sweepout method is accomplished by the linear programming (Gass, 1969). This study for the positivity, objective function, and constraint equation may be solved by modified simplex algorithm using subroutine zx4LP in the IMSL on the UUCC.

After rewriting,

$$\underset{8\times8}{[A} \,\vdots\, \underset{8\times8}{I} \,\vdots\, \underset{8\times8}{-I} \,\vdots\,] \underset{24\times1}{\begin{bmatrix} \bar{x} \\ \bar{e}^{+} \\ \bar{e}^{-} \end{bmatrix}} \underset{8\times1}{=\bar{y}}$$

And the $L1$ objective functicn can be written

$$\|e\|_1 = [\underset{8\times1}{0} \quad \underset{8\times1}{\bar{1}} \quad \underset{8\times1}{\bar{1}}] \underset{24\times1}{\begin{bmatrix} \bar{x} \\ \bar{e}^{+} \\ \bar{e}^{-} \end{bmatrix}}$$

Thus we can solve the problem as a linear program. But the physical constraints over the model are very important for the obje ctive function and should be appropriate. Otherwise the objective functions are often unbounded.

Random search

The random search method is designed for thoroughness of search rather than for speed of convergence. But this method achieves a reasonable compromise between the conflicting requirements of search and convergence. The position of the global minimum can be found with sufficient confidence. The approximation converges siowly to minimum. However, the search provide the better figures with minimum and maximum values in the crust because simplex method is insensitive to the objective function or the physical constraints about the inverse model.

In practice, 0.1 mWm^{-2} magnitude has little meaning but I would like to use 0.1 magnitude to compare with three cases. The best fit values can be obtained with the range of error (0.1 μWm^{-3}) after the calculation of inversion. The heat production values after inversion are followings:

(1) with free noise

1.65, 3.62, 3.51, 2.70
1.65, 1.79, 1.98, 1.81

—results by random search method

1.83, 3.50, 3.46, 2.68
1.41, 2.01, 2.06, 1.84

This search method converges slowly and it takes about 30 min. by 150 random addresses. The range of heat production values in the continental crust is 1.0μWm^{-3} to 4.0μWm^{-3}. We used these values for minimum and maximum. These are reasonable values in the real earth and heat production values after inversion compare favourably with ridge regression. The search algorithm is simple and efficient. However, the method is not better than ridge regression.

(2) with noise due to magmatic body

1.66, 3.61, 3.47, 2.69
1.62, 3.01, 2.12, 1.78

(3) with noise level by random number generator

(a) case ($\pm$1.0 mWm^{-2})

1.94, 2.74, 4.34, 3.14
1.86, 2.22, 1.42, 1.13

(b) case ($\pm$1.4 mWm^{-2})

1.41, 4.20, 2.47, 3.81
1.20, 2.30, 1.70, 1.76

(c) case ($\pm$2.8 mWm^{-2})

2.76, 3.34, 2.77, 2.98
1.77, 2.08, 1.84, 1.64

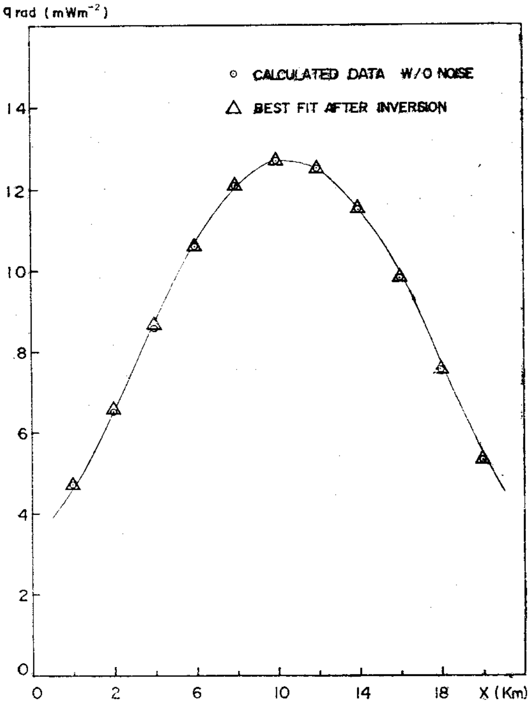

Fig. 4. Case (1) without noise

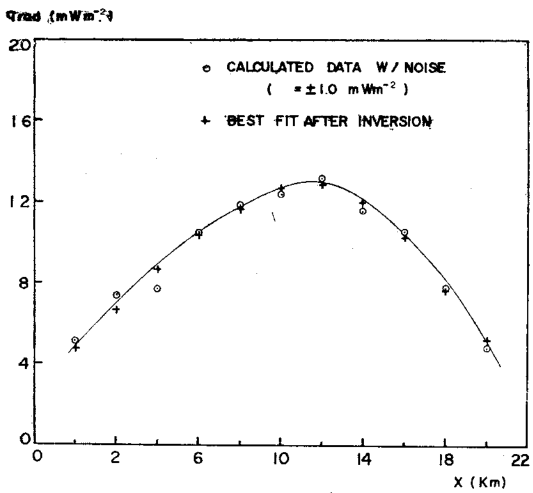

Fig. 5. (a) case with noise

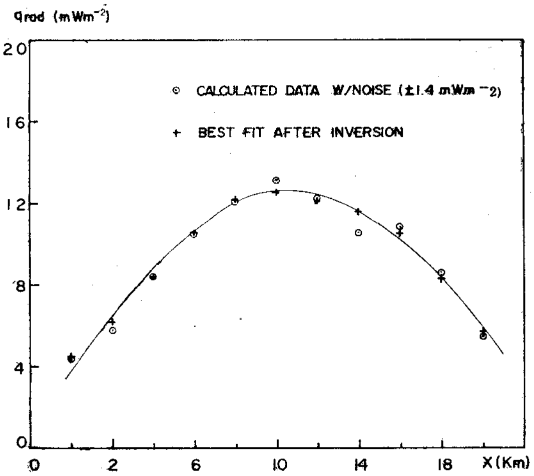

Fig. 6. (b) case with noise

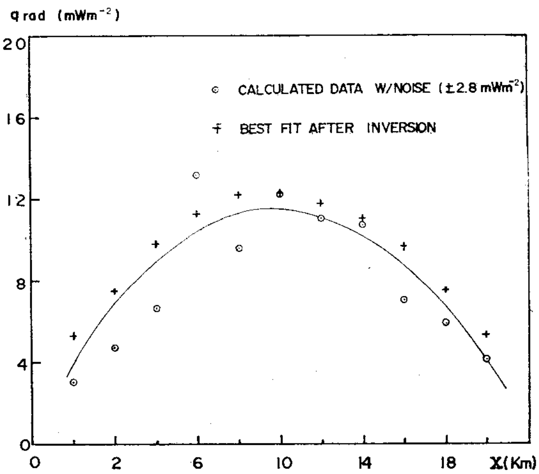

Fig. 7. (c) case with noise

In each case, the parameters of the model are used to calculate radiogenic heat flow (q_{rad}) from the forward model. These heat flow values except the case of ± 2.8 mWm^{-2} are not far from the original points. Both data sets are shown by comparing with different symbols in Figures 4, 5, 6 and 7. In each figure, the original data is plotted along with the best fit values after inversion.

DISCUSSION

The ridge regression method is a curve matching algorithm which minimizes the least squares error between the observed and calaulated data. This requires finding the minimum. Heat flow measurements in a geothermal environment can be uncertain to within as $\pm 20\%$ and the uncertainty in the inter-laboratory is about $\pm 10\%$. In this case, statistical significance can be gained by weighting the data from the uncertainty of the measurements.

We have utilized an inversion for estimating heat sources. The field test from data collection suggests that for the geologic and geochemical settings, the forward model is adequate for matching the observed heat flow profile. The model ignores hydrologic problems with contamination and heat refraction. However, this modelling makes it practical for preliminary evaluation in several heat flow provinces (Bohemian massif, Superior province, Brazilian highland, etc.).

CONCLUSION

The interpretation of heat flow data on the continental crust due to the vertical distribution of radioactive elements with depth through random search can be greatly enhanced by the good fit small error ($0.1 \mu Wm^{-3}$), and reasonable range θ^2 ($10^{-3} \sim 10^{-1}$).

From this study I can confirm the physical model of the continental upper crust. A measure of enhancement depends upon the accuracy of the radioactive elements in the lower crust and mantle heat flow. There is a benefit to understand the thermal state of the lithosphere.

Further studies may be continued as follows;

(a) effects of the distribution of heat sources in the lower crust and upper mantle.

(b) comparison with other geophysical models (magnetic, gravity).

REFERENCES

Al-Chalabi, M. (1971) Some studies relating to nonuniqueness in gravity and magnetic inverse problems. Geophysics, v. 36, p. 835-855.

Bevington, P.R. (1969) Data reduction and error analysis for the physical sciences. McGraw-Hill.

Claerbout, J.F. and Muir, F. (1973) Robust modeling with erratic data. Geophysics, v. 38, p. 826-844.

Forshythe, G.E., Malcolm, M.N., and Moler, C.B. (1977) Computer methods for mathematical computations. Prentice Hall Inc.

Gass (1969) Linear programing method and application. McGraw-Hill.

Goodman, A.W. and Ratti, J.S. (1971) Finite mathematics with applications. MacMillan, p. 39-75.

Hanson, R.J. and Wisniewski, J.A. (1979) A revised simplex code for LP, SAND. p. 78-2322.

Hohmann, G. (1982) Lecture note. Univ. of Utah.

Inman, J.R. (1975) Resistivity inversion with ridge regression. Geophysics, v. 40, p. 798-817.

Jackson, P.D. (1972) Interpretation of inaccurate, insufficient and inconsistent data. Geophys. J.R. A. Soc., v. 28, p. 97-107.

Marquardt, D.W. (1970) Generalized inverses, ridge regression, and nonlinear estimation. Technometrics, v. 12, p. 591-623.

Price, W.L. (1976) A controlled random search procedure for global optimization. The computer J., v. 20, p. 367-370.

Simmons, G. (1967) Interpretation of heat flow anomalies. Reviews of Geophysics, v. 5, p. 43-52.

Telford, et al. (1976) Applied geophysics. Cambridge Univ.

地殼熱流量의 線型 反轉

韓　　郁*

요약: 암석의 대표적 熱源値를 사용하여 지각 熱流量의 反轉을 연구하였으며 2-D 모델은 아주 얇은 正方形板이 고려되었다. 포텐샬 이론을 기초로 하여 지각 열류량과 열원 사이의 새로운 관계를 도출하였으며 두가지 경우의 계산결과가 도시되어 있다. Random search 방법과 ridge regression방법이 비교되었으며 지각열류량의 反轉 연구에서는 random search 방법의 중요성이 발견되었다.

* 陸士 環境學科