Dr. Tanner

GRAVITATIONAL POTENTIAL THEORY LECTURES

by

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Introductory remarks

These lectures were given at Queen's University, Kingston, Ontario over a period of three weeks in the winter of 1984 to fourth year students in the Department of Geology. The lectures are intended to provide a foundation for further study to people interested in the geological interpretation of gravity anomalies.

The emphasis is on the mathematical formulation of potential field theory to provide a basic understanding of how the gravity effect of a particular geophysical model is calculated and to see under what conditions we can perform operations on the gravity field, such as in the process of upward continuation. It is also the aim to describe some of the methods available for the "inversion" of gravity data to determine geological structure. There are many papers and books dealing with one aspect or another of gravity interpretation theory. However, only a few selected references are given; the ones named are excellent sources of information and cover the points given in these lectures.

The choice of topics is largely a personal one guided by several years of experience in the interpretation of regional gravity surveys. The material in section 5.2 and the associated overheads should be of interest in other areas of geophysical interpretation. The lectures are guided, in part, by potential theory lectures given in 1971 by Prof. M.H.P. Bott at the University of Durham, Durham City, England. Lectures 1 to 4 set the stage for the material in lectures 5 and 6.The computer programs mentioned in the text are available, on request, from the Division of Gravity, Geothermics and Geodynamics. Reference should be made to this report.

Finally, I should like to especially thank my colleagues Mrinal Paul and Herb Valliant for making helpful comments regarding these notes.

Potential theory lecture 1

1. Review of basic ideas and vector operations

1.1 Newton's law of gravitation

The attractive force, F, between two masses is given by:

$$F = G*m1*m2/(R*R)$$

where $R = ((x'-x)^2 + (y'-y)^2 + (z'-z)^2)^{\frac{1}{2}}$
G is the universal constant of gravitation
and x', y' , z' refer to the position of m1
x, y, z refer to the position of m2 (in a right-handed coordinate system)

The gravitational force per unit mass is F/m1 where m1 is a small, compact test mass.

At any point in space the force of gravity has a magnitude and a direction.

At any point in space the distance from an element of mass in a body to the observer's location has a magnitude, R, and a direction. The direction cosines of this vector are:

(x'-x)/R	(x-direction)
(y'-y)/R	(y-direction)
(z'-z)/R	(z-direction)

The force of gravity is directed from the observer to the mass element.

At a given point x', y' z' the z-component of the force of gravity is:

$$g_z (x',y',z') = - G\, m(x,y,z)*(z'-z)/(R*R*R)$$

the x-component is:

$$g_x (x',y',z') = - G\, m(x,y,z)*(x'-x)/(R*R*R)$$

and the y-component is:

$$g_y (x',y',z') = - G\, m(x,y,z)*(y'-y)/(R*R*R)$$

Note that the quantity (z'-z)/R is the cosine of the angle that the R vector makes with the z-axis, etc.

In vector notation the force of gravity is, for a small, distant mass m(x,y,z):

$$\vec{g}(x',y',z') = -G\,(m(x,y,z)/R*R)*(\vec{R}/R)$$

where $\vec{g}$ and $\vec{R}$ are vector quantities.

The x-component of $\vec{R}$ is (x'-x); the y-component is (y'-y); the z-component is (z'-z).

1.2 The DEL operator

We can perform basic mathematical operations (involving differentiation) on a vector using the DEL operator, ∇'. The DEL operator is a vector operator and has three components:

the x-component is $\frac{\partial}{\partial x'}$;

the y-component is $\frac{\partial}{\partial y'}$;

the z-component is $\frac{\partial}{\partial z'}$.

Note that if the DEL operator operates on the field-point coordinate x',y',z' we write ∇'. If, as we will need later, it operates on a source-point (also termed body-point) coordinate it is written as ∇. For the time being we will be using ∇'.

There are four uses of the DEL operator which will arise in potential field theory: Divergence of a vector field (the result is a scalar quantity)
Curl of a vector field (the result is a vector quantity)
Gradient of a scalar variable (a vector)
Directional derivative of a scalar or of a vector (a scalar or a vector respectively)

1.2.1 Divergence

The divergence of a gravitational field is explicitly

$$\frac{\partial g_x}{\partial x'}(x',y',z') + \frac{\partial g_y}{\partial y'}(x',y',z') + \frac{\partial g_z}{\partial z'}(x',y',z').$$

As will be discussed later, this quantity is zero in free space and equal to $-4\pi G$ times the mass density within a gravitating body.

As an example, suppose the following velocity field exists within a fluid:

$$v_x\,(x',y',z') = (v_o/a)\,x'$$

$$v_y\,(x',y',z') = (v_o/a)\,y'$$

$$v_z\,(x',y',z') = (v_o/a)\,z'$$

where v_o and a are some suitable values of velocity and distance respectively.

The divergence of this field is not zero but equal to $3v_o/a$.

In vector notation we write the divergence of $\vec{v}$ as follows:

$$\nabla' . \vec{v} = 3\, v_o / a \quad \text{where} \quad . \text{ means dot product.}$$

1.2.2 Curl

The curl of a vector field, $\vec{v}$, is defined as:

$$\left(\frac{\partial v_z}{\partial y'} - \frac{\partial v_y}{\partial z'} \right) \text{ is the x-component of the curl}$$

$$\left(\frac{\partial v_x}{\partial z'} - \frac{\partial v_z}{\partial x'} \right) \text{ is the y-component of the curl}$$

$$\left(\frac{\partial v_y}{\partial x'} - \frac{\partial v_x}{\partial y'} \right) \text{ is the z-component of the curl}$$

The curl of the velocity field defined above is zero.

However the curl of the following velocity field is not zero:

$$v_x(x',y',z') = -(v_o/a)\, y'$$

$$v_y(x',y',z') = (v_o/a)\, x'$$

$$v_z(x',y',z') = 0$$

(where v_o and a are suitable constant values of velocity and distance)

and, in fact, the z-component of the curl is equal to $2(v_o/a)$. Note that v_o/a is the angular velocity of the motion.

Note also that the divergence of this latter velocity field is zero.

In vector notation the curl of a vector is written as:

$$\nabla' \times \vec{v} = 2(v_o/a).$$

A vector field which possesses neither divergence nor curl is termed "harmonic". There are many theorems which have been developed concerning harmonic functions (see, for example, "The theory of the potential" by O.D. Kellog).

1.2.3 Gradient

The x-component of the gradient of a scalar function U(x',y',z') is given by:

$$\frac{\partial U}{\partial x'}(x',y',z')$$

the y-component is: $\frac{\partial U}{\partial y'}(x',y',z')$

and the z-component is: $\frac{\partial U}{\partial z}(x',y',z')$.

Temperature is in example of a scalar potential function. The flow of heat at a given point in a solid body with uniform thermal properties is proportional to the temperature gradient at that point.

In vector notation the gradient, $\vec{g}$, of the scalar U is written as:

$$\vec{g} = \nabla U$$

There is a theorem, termed Helmholz's theorem, which states that any physically reasonable vector field can be derived from the gradient of a scalar function U(x',y',z') and the curl of a vector function $\vec{A}$(x',y',z'). U and $\vec{A}$ are termed scalar and vector potentials, respectively. In some cases, such as gravity, we only need a scalar potential to completely describe the gravity field. In magnetics we generally require the use of a vector potential although the magnetic scalar potential is of use in certain cases.

1.2.3.1 Example from gravitational theory

Another example of a scalar potential is that of a small mass element, m:

U(x',y',z') = G m(x,y,z)/R

where R is as previously defined

The x-component of the gradient of U(x',y',z') is:

G m(x,y,z)*(x-x')/(R*R*R).

which is equal to the x-component of gravity as previously obtained. The other components of gravity are also correctly obtained in the same way.

The use of a scalar potential is for mathematical convenience. The scalar gravity potential can't be measured directly whereas the acceleration of an object due to gravity can.

How do we calculate the gravitational potential of a body?

We must know the distribution of density throughout the body. This is a scalar function denoted by ρ(x,y,z).

We must know the size and shape of the body.

We then calculate the potential U(x',y',z') at the field point x',y',z' as follows:

$$U(x',y',z') = G \iiint_{x\,y\,z} \frac{\rho(x,y,z)}{R}\, dxdydz \qquad 1.1$$

where $R = ((x'-x)^2 + (y'-y)^2 + (z'-z)^2)^{1/2}$

This is a volume integral with respect to x, y and z and can be carried out analytically for only a limited number of cases. For example, when the density contrast is constant and the body has a simple shape such as a prism or a sphere.

In the case of a sphere of radius a and constant density the gravitational potential is only a function of the distance, r, of the observer from the center of the sphere. It is given by:

$$U(r) = G\, 4\pi\rho(a*a/2 - r*r/6) \qquad r<a$$

$$= G\, 4\pi\rho((a*a*a/3)/r) \qquad r>a$$

The radial component of gravity is given by dU(r)/dr and is equal to:

$$g_r(r) = -\, G\, 4\pi\rho r/3 \qquad r<a$$

$$g_r(r) = -\, G\, 4\pi\rho a*a*a/(3*r*r) \qquad r>a$$

An interesting consequence of Newton's law of gravitation is that the gravitational potential and attraction at an exterior point behave as though all of the mass were concentrated at the center of the sphere.

The divergence of g(r) is obtained from the expression

$$(1/(r*r))\, d(r*r(g_r(r))/dr$$

and is equal to:

$$\begin{cases} -4\pi\rho G & r<a \\ 0 & r>a \end{cases}$$

1.2.4 Directional derivative

The directional derivative of a scalar, t(x',y',z'), is given by

$$a \frac{d\, t(x',y',z')}{dx'} + b \frac{d\, t(x',y',z')}{dy'} + c \frac{d\, t(x',y',z')}{dz'}$$

where a, b and c are the direction cosines of a unit vector, $\vec{n}$, which specifies the direction in which the derivative is taken.

The directional derivative of a vector, $\vec{v}(x',y',z')$, is

$$f_x = a \frac{d\, v_x(x',y',z')}{dx'} + b \frac{d\, v_x(x',y',z')}{dy'} + c \frac{d\, v_x(x',y',z')}{dz'}$$

$$f_y = a \frac{d\, v_y(x',y',z')}{dx'} + b \frac{d\, v_y(x',y',z')}{dy'} + c \frac{d\, v_y(x',y',z')}{dz'}$$

$$f_z = a \frac{d\, v_z(x',y',z')}{dx'} + b \frac{d\, v_z(x',y',z')}{dy'} + c \frac{d\, v_z(x',y',z')}{dz'}$$

where f_x, f_y and f_z are the x-, y- and z-components of the resulting vector $\vec{f}$.

Instead of a unit vector, $\vec{n}$, any vector, $\vec{u}$, can be used but then the result is multiplied by the magnitude of $\vec{u}$.

In vector notation the directional derivative of a scalar, t, is:

$$\vec{n}.\nabla' t(x',y',z')$$

or $$\vec{u}.\nabla' t(x',y',z')$$ (scalar quantities)

and the directional derivative of a vector, v, is:

$$\vec{n}.\nabla' \vec{v}(x',y',z')$$

or $$\vec{u}.\nabla' \vec{v}(x',y',z').$$ (vector quantities)

Potential theory lecture 2

2. Topics related to the gravitational potential

2.1 Derivatives of the potential

The scalar gravitational potential, U(x',y',z') is a function of the coordinates x', y', and z' only. Hence spatial derivatives must be taken with respect to x', y', and z'.

To obtain the vertical component of gravity, for example, we differentiate the integral for U(x',y',z) with respect to z'.

$$\frac{dU(x',y',z')}{dz'} = \frac{d}{dz'} G \iiint_{x\,y\,z} \rho(x,y,z)(1/R)\, dxdydz \qquad 2.1$$

We can take the differentiation in under the integral sign and operate on the quantity 1/R as it is the only part of the integrand which is a function of z'.

We obtain in this way the integral expression for g_z as

$$g_z = -G \iiint_{x\,y\,z} \rho(x,y,z)\ (z'-z)/(R*R*R)\ dxdydz \qquad 2.2$$

We can differentiate g_z with respect to z' again to obtain

$$\frac{dg_z}{dz'} = \frac{d^2U}{dz'^2} = \iiint_{x\,y\,z} \frac{\rho(x,y,z)\ (2(z-z')^2 - (x-x')^2 - (y-y')^2\ )}{R*R*R*R*R}\ dxdydz \qquad 2.3$$

We can differentiate U(x',y',z') any number of times with respect to x' or y' or z' or any combination such as $\frac{d^2U(x',y',z')}{dx'dy'}$

If we calculate $\nabla'.\vec{g}$ we will find that $(\nabla')^2(1/R)$ is equal to zero inside the integrand whenever R is not equal to zero, i.e. whenever at least x or y or z is not equal to x' or y' or z' respectively. When x=x' and y=y' and z=z' simultaneously, the function $(\nabla')^2(1/R)$, when integrated, acts as a delta function and picks up the value of the density at the point in question (times a factor of $-4\pi G$). This proof is given in the book "The Theory of the Potential" by O.D. Kellogg or "Electromagnetic Theory" by J.A. Stratton.

2.2 The change of gravitational potential with time

Consider a fixed mass element m(x,y,z) and a movable observer. At time t1 the observer is at x',y',z' and at time t2 she is at $x'+\Delta x', y'+\Delta y', z'+\Delta z'$. The only change in the expression for the gravity potential

$$U(x',y',z') = G\, m(x,y,z)(1/R)$$

is in the value of the reciprocal distance 1/R. This difference is given by:

$$\frac{1}{((x - x' - \quad x')^2 + (y - y' - \quad y')^2 + (z - z' - \quad z')^2)^{\frac{1}{2}}} - \frac{1}{((x - x')^2 + (y - y')^2 + (z - z')^2)^{\frac{1}{2}}}$$

If we denote the displacement at the observer's point by the vector $\vec{u}'$ which has x- y- and z-components of dx',dy' and dz', respectively, the difference may be written as:

$$- \frac{\vec{u}'.\vec{R}}{R*R*R}$$

or

$$+ \quad \vec{u}'.\nabla'(1/R)$$

where Rx = x'-x; Ry = y'-y; Rz = z'-z.

This is the derivative of 1/R with respect to the primed variables in the direction of u and multiplied by the magnitude of u.

The change in potential is given by:

$$U(x',y',z') = G\, m(x,y,z)\ \vec{u}'.\nabla'(1/R) \qquad 2.4.1$$

Now suppose that we keep the observer's location fixed and move the mass element a small distance $\vec{u}$. As above, the the change in potential is:

$$U(x',y',z') = G\, m(x,y,z)\; \vec{u}.\nabla(1/R) \qquad 2.4.2$$

but note that the DEL operator acts on the unprimed coordinates, that is on x,y,z.

Now suppose that we keep the observer's location fixed and the position of the mass element fixed but we change the amount of mass.

This contribution to the change in potential is

$$\Delta U(x',y',z') = G\Delta m(x,y,z)\; (1/R) \qquad 2.4.3$$

If we express the mass element as the product of density contrast $\rho(x,y,z)$ times some small volume element dV (=dxdydz) the total change in mass is:

$$dm(x,y,z) = (d\rho(x,y,z) + \vec{u}.\nabla\rho(x,y,z) + (\nabla.\vec{u})\rho(x,y,z))\; dxdydz$$

and the change in potential is

$$\Delta U(x',y',z') = G\; (d\rho(x,y,z) + \vec{u}.\nabla\rho(x,y,z) + (\nabla.\vec{u})\rho(x,y,z))(1/R)$$

$$*dxdydz \qquad 2.4.4$$

Noting that (1/R) = - (1/R) we can substitute

$-\vec{u}'.\nabla(1/R)$ for $\vec{u}'.\nabla'(1/R)$ in expression (1).

The change in potential U for a gravitating body can be written as:

$$\Delta U(x',y',z') = G \iiint_{x\,y\,z} \rho(x,y,z)\; (\vec{u}-\vec{u}').\nabla(1/R)\; dxdydz$$

$$+\; G \iiint_{x\,y\,z} \frac{d\rho(x,y,z) + \vec{u}.\nabla\rho(x,y,z) + (\nabla.\vec{u})\rho(x,y,z)}{R}\; dxdydz \qquad 2.5$$

If there is no net change in the total mass of the body the second integral is zero.

If, in addition, the observer's position remains fixed in space the net change in gravitational potential is:

$$\Delta U(x',y',x') = G \iiint_{x\,y\,z} \rho(x,y,z)\ \vec{u}.\nabla(1/R)\ dxdydz \qquad 2.6$$

A knowledge of how the gravity potential changes with time is useful in studies of deformation at mine sites.

2.3 The scalar magnetic potential

Imagine a magnetic dipole of pole strength p(x,y,z) with poles separated by a small distance $\vec{l}$ (where $\vec{l}$ is directed from the negative pole to the positive pole). The magnetic moment is p(x,y,z)$\vec{l}$.

The magnetic potential, (V+)(x',y',z'), at the observer's position x',y',z' due to the positive pole is

$$(V+)(x',y',z') = -p(x,y,z)/R$$

(the minus sign is used since like poles repel each other).

The magnetic potential, (V-)(x',y',z'), at the observer's position due to the negative pole is

$$(V-)(x',y',z') = p(x,y,z)/R'$$

(here the primes are used to distinguish between the slightly different distances R and R').

Adding the two potentials to get the scalar potential for a dipole gives

$$V(x',y',z') = p(x,y,z)(\ 1/R' - 1/R\ )$$

By the same sort of argument as before this can be rewritten as

$$V(x',y',z') = - p(x,y,z)\ \vec{l}(x,y,z).\nabla(1/R)$$

where the DEL operator operates on the unprimed coordinates.

Since $-\nabla(1/R) = \nabla'(1/R)$ we can also write

$$V(x',y',z') = p(x,y,z)\ \vec{l}(x,y,z).\nabla'(1/R)$$

For an extended magnetic body the scalar potential is

$$V(x',y',z') = \iiint_{xyz} \vec{m}(x,y,z)\ .\nabla'(1/R)\ dxdydz \qquad 2.7$$

where $\vec{m}(x,y,z)$ stands for magnetic moment per unit volume
($\vec{m}(x,y,z)dxdydz = p(x,y,z)\ \vec{l}(x,y,z)$)

If the direction of magnetization is uniform, that is it does not vary with position, (x,y,z), in the body, then $\vec{m}(x,y,z) = q(x,y,z)\ \vec{n}$ (where q(x,y,z) is a scalar quantity) and the operation $\vec{n}.\nabla'$ can be taken outside of the integral sign to give.

$$V(x',y'z') = \vec{n}.\nabla' \iiint_{xyz} q(x,y,z)\ (1/R)\ dxdydz \qquad 2.8$$

In this special case the magnetic scalar potential is formally the same as the directional derivative of a gravitational potential. This result is attributed to Poisson and is known as Poisson's relation. This relation has been used to determine the direction of magnetization in seamounts.

2.4 Practical shapes of bodies to use in gravity modelling

2.4.1 The gravity field of a right rectangular prism

Right rectangular prisms can be used as building blocks for 3-D gravity models and for modelling topography to do terrain corrections.
They have the disadvantage that they can not easily accommodate sloping contacts. The formula for the vertical component has been published by D. Nagy in GEOPHYSICS in vol 31, 1966 pages 362-371. It should be noted that the formulation in terms of arctan is less troublsome to program than the one which uses arcsine.

2.4.2 The gravity field of a 2-D horizontal slab with a sloping face

This is a useful model because it can be employed to construct a 2-D model with a polygonal cross-section. The integration is complicated by the fact that the x-limit of integration is a function of z cot(A) where A is an angle related to the dip of the face. The integrated result is given in several geophysical textbooks (e.g. "Geophysical Exploration" by C.A. Heiland). We will discuss this model in a subsequent section in more detail. In using a 2-D program to calculate the gravity effect of a body you must remember to close the body i.e. make the last body-point x and z coordinates the same as the first unless the program does this automatically.

Potential theory lecture 3

3. Two-dimensional interpretation; Green's theorem and the equivalent layer

3.1 The 2-D potential

If the gravitating source is essentially two-dimensional in character, it is convenient to use a 2-D formulation for the potential and its derivatives.

To do this we integrate the 3-D potential with respect to (w.r.t.) y from y = - L to y = + L and obtain (for y' = 0):

$$U(x',z') = G \iint_{x\,z} 2\,\rho(x,z)\,[\ln(L + ((L*L) + (x'-x)^2 + (z'-z)^2)^{\frac{1}{2}}) - \ln(-L + ((L*L) + (x'-x)^2 + (z'-z)^2)^{\frac{1}{2}})]dxdz \qquad 3.1.1$$

For large L this may be approximated by:

$$\iint_{x\,z} 2\,\rho(x,z)\,[\ln((L*L)/((x'-x)^2 + (z'-z)^2))^{\frac{1}{2}}]dxdz \qquad 3.1.2$$

Since ln(L*L) is not a function of x' or z', it may be ignored. This is OK from a geophysical point of view but needs mathematical justification! See the book by O.D. Kellogg for a mathematical justification. Therefore, the 2-D potential is given by:

$$U(x',z') = -\,G \iint_{x\,z} 2\,\rho(x,z)\,\ln((x'-x)^2 + (z'-z)^2)^{\frac{1}{2}}dxdz. \qquad 3.1.3$$

Note that the exponent in the argument of the logarithm can be taken outside and cancels out the factor of 2.

We can use the 2-D DEL operator (where the term $\frac{d}{dy'}$ is ommitted) to obtain

$\vec{g}(x',z')$ from $U(x',z')$.

The expression for $g_z(x',z')$ is

$$-\,2G \iint_{x\,z} \rho(x,z)\,\frac{(z'-z)}{(x'-x)^2 + (z'-z)^2}\,dx\,dz \qquad 3.2$$

As in the 3-D case, the potential U(x',z') can be differentiated any number of times w.r.t. x' or z' to obtain the x- and z-components of gravity and any of their spatial derivatives.

3.2 The 2-D slab with a sloping face

In the case of a horizontal, two-dimensional slab with a sloping face, the body can be split up into two parts to take into account the situation that the limit of integration for one coordinate depends upon the other coordinate in the region bounded by the face (see diagram below and Appendix).

For the triangular part we can integrate first w.r.t. z and then w.r.t. x. The upper limit of the z integral is a function of x and given by:

$$\text{upper limit} = \frac{x*(z2 - z1)}{(x2 - x1)} + \frac{(x2*z1 - x1*z2)}{(x2 - x1)}$$

The lower limit is z1.

Integrating w.r.t. z gives (ρ = constant)

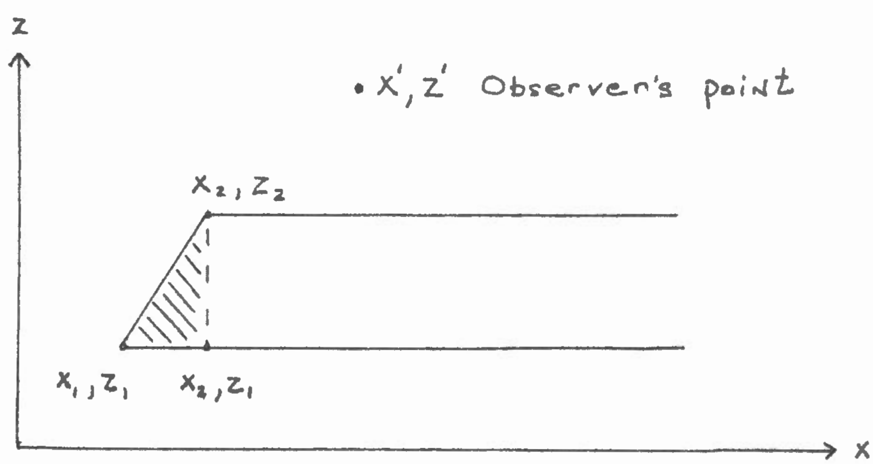
$$g\,(x',z') = G\rho \int_{x_1}^{x_2} \ln((x'-x)^2 + (z'-z)^2)\,\Big|_{z1}^{z=\text{upper limit (as above)}} dx \qquad 3.3$$

To integrate the logarithm w.r.t. x, a change of variable can be made to make the argument of the logarithm of the form (u*u + c*c) where u is the variable of integration and c is a constant.

The rectangular portion can be readily integrated with the aid of integral tables w.r.t. x and then z.

Both portions have terms involving arctangents and logarithms.

A FORTRAN subroutine called GMSTEP has been written to calculate the gravity (and magnetic) effect of a 2-D slab with a sloping face.



3.3 Green's Theorem

This is a very useful theorem; it is proven in many textbooks (e.g. "An Introduction to the Theory of Newtonian Attraction" by A.S. Ramsey or "Foundations of Potential Theory" by O.D. Kellogg). To give some idea of how it is derived we take the 3-D expression for the gravity potential and substitute $(-1/4\pi)\nabla^2 U(x,y,z)$ for $\rho(x,y,z,)$ in the integrand and write the result in the form of three integrals.

$$\frac{-G}{4\pi}\iiint_{xyz}\frac{\frac{d^2U(x,y,z)}{dx^2}dxdydz}{R} \qquad \frac{-G}{4\pi}\iiint_{xyz}\frac{\frac{d^2U(x,y,z)}{dy^2}dxdydz}{R} \qquad \frac{-G}{4\pi}\iiint_{xyz}\frac{\frac{d^2U(x,y,z)}{dz^2}dxdydz}{R} \qquad 3.4$$

We take the first and integrate by parts w.r.t. x; the second by parts w.r.t. y; the third by parts w.r.t. z. We then integrate the first again by parts w.r.t. x., etc. This process (if we think of a rectangular prism) converts the original volume integral into the sum of two surface integrals and another volume integral. In vector notation these are:

$$\frac{-G}{4\pi}\iiint\frac{\nabla^2 U(x,y,z)}{R}\,dV = -\frac{G}{4\pi}\iiint U(x,y,z)\,\nabla^2(1/R)\,dV$$

$$-\frac{G}{4\pi}\iint(1/R)\nabla U(x,y,z).\vec{n}\,dS + \frac{G}{4\pi}\iint U(x,y,z)\,\nabla(1/R).\vec{n}\,dS \qquad 3.5$$

In the surface integrals (x,y,z) refers to a point on the surface, S, which encloses the volume, V. The unit vector $\vec{n}$ is normal to the surface, S, and points outwards, away from the volume , V.

In this case (1/R) is a particular function which has been specified; any function, W(x,y,z), instead of (1/R) could be inserted into the above integrals and this is the form that Green's Theorem is usually given.

(Note: there are other important integral theorems such as Gauss's Theorem and Stokes's Theorem which are described in the books by Ramsey and by Kellogg mentioned above.)

3.4 Green's equivalent layer

When the observer is at an external point (x',y',z') the value of $\nabla^2(1/R)$ is zero so the first integral on the right-hand side of the equal sign in expression (4) above vanishes. If the surface of the body is an equipotential surface, U(x,y,z) at the surface S is a constant, say Uo, and can be taken outside the integral sign in the second surface integral. For a point outside the volume V this second surface integral

$$\frac{GU_o}{4\pi}\iint \nabla(1/R).\vec{n}\ dS$$

vanishes. This can be seen to vanish if we set U(x,y,z) = 1 in expression (4). The left-hand side vanishes because U is constant. The first integral on the right-hand side vanishes because $\nabla^2(1/R)$ is zero and the first surface integral vanishes because U is constant. Therefore, when the surface of the body is an equipotential surface, the surface integral involving $\nabla(1/R).\vec{n}$ is zero.

For the case considered here where S is an equipotential surface and $(+1/4\pi)\nabla^2 U(x,y,z) = -\rho(x,y,z)$ we have at a point exterior to V:

$$G\iiint \frac{\rho(x,y,z)}{R}\ dV \qquad = -\frac{G}{4\pi}\iint (1/R)\nabla U(x,y,z).\vec{n}\ dS = U(x',y',z') \qquad 3.6.1$$

This means that if we know the normal component of the gradient of the potential (in our case $g_z(x,y,z)$) at every point on an equipotential surface (in our case the land surface but this may not be strictly true in most practical situations) we can calculate the potential at some point (x',y',z') above the surface. This means that we can analytically continue a potential function in empty space outside a body without knowing the distribution of mass inside the body. However, we need to know the potential (or its derivative in the direction normal to the surface) at every point of the surface and we have to know the shape and position of the surface.

There are also certain geometrical cases such as the sphere where the surface of the sphere may not be an equipotential surface but it is still possible to calculate the gravitational field at an exterior point knowing only the gravitational field over the surface (e.g. Kellogg, 1953).

We can also reproduce the gravity potential at an exterior point by means of a spread of surface density $\sigma(x,y,z)$ over the surface, S, by making $\sigma(x,y,z) = -(1/4\pi)\, g_z(x,y,z)$. This surface density layer is termed an "equivalent" layer. Surface density has the dimensions of grams/cm^2.

$$U(x',y',z') = \iint \frac{\sigma(x,y,z)}{R}\, dS \qquad 3.6.2$$

We can also calculate any derivative of the potential (taken w.r.t. x',y',z') at the point (x',y',z'). For example we can calculate

$$\frac{dU(x',y',z')}{dz'} = g_z(x',y',z').$$

For a flat surface we have

$$g_z(x',y',z') = (1/2\pi) \int_{y=-\infty}^{y=+\infty} \int_{x=-\infty}^{x=+\infty} g_z(x,y,z) \frac{(z'-z)}{((x'-x)^2 + (y'-y)^2 + (z'-z)^2)^{3/2}}\, dxdy \qquad 3.7$$

So we see that it is possible to continue the gravity field known over a surface upward to any point above the surface.

In practice, the surface gravity values would be given over the x-y plane and z = 0.

In two dimensions the formula is:

$$g_z(x',z') = (1/\pi) \int_{x=-\infty}^{x=+\infty} g_z(x,z) \frac{(z'-z)}{(x'-x)^2 + (z'-z)^2}\, dx \qquad 3.8$$

due to the use of the logarithmic potential (Eqn. 3.1.3)rather than the function (1/R).

The above integral is termed a convolution of $g_z(x,z)$ with another function which, in this case, is

$$\frac{(z'-z)}{(x'-x)^2 + (z'-z)^2}$$

The factor $(1/\pi)$ normalizes the convolution function so that the integral

$$(1/\pi) \int_{x=-\infty}^{x=+\infty} \frac{(z'-z)}{(x'-x)^2 + (z'-z)^2} \, dx$$

$$= (1/\pi) \arctan \frac{(x'-x)}{(z'-z)} \Bigg|_{x=-\infty}^{x=+\infty} = 1$$

This gives the correct scale factor to $g_z(x',z')$.

We can calculate $\frac{dg_z(x',z')}{dz'}$ by convolving the gravity values at ground level with the appropriate function which, in this case, is obtained by differentiating

$$\frac{(z'-z)}{(x'-x)^2 + (z'-z)^2}$$

w.r.t. z' to obtain:

$$\frac{(x'-x)^2 - (z'-z)^2}{((x'-x)^2 + (z'-z)^2)^2}$$

as the desired convolution function.

Potential theory lecture 4

4. Mathematical manipulations of the gravity field

4.1 Fourier methods

Upward continuation is a convolution involving the vertical component of gravity at the surface and a kernel which is a geometrical factor relating the observation point to a surface element. In this case the (two-dimensional) kernel is $(1/R)\cos(A)$ where A is the angle between the $\vec{R}$ vector and the vertical.

$$g_z(x',z'-z) = 1/(\pi) \int_{x=-\infty}^{x=+\infty} g_z(x,z) \frac{(z'-z)}{(x'-x)^2 + (z'-z)^2} dx \qquad 4.1$$

Because the convolution takes place from $x=-\infty$ to $x=+\infty$, we can readily apply Fourier transforms to the problem.

There are different definitions of the Fourier transform but these differ only in the way the normalizing factor is applied. We'll use the following one:

The Fourier transform of g(x) is

$$1/(2\pi)^{\frac{1}{2}} \int_{x=-\infty}^{x=+\infty} g(x) \exp(ik(x))\, dx = H(k)$$

where i is the square root of -1.

We can take the inverse Fourier transform of the Fourier transform and get back the original function, g(x).

$$1/(2\pi)^{\frac{1}{2}} \int_{k=-\infty}^{k=+\infty} H(k) \exp(-ik(x))\, dk = g(x)$$

The inverse Fourier transform uses -i instead of +i.

The Fourier transform of $\quad (1/\pi) \dfrac{(z'-z)}{(x'-x)^2 + (z'-z)^2}$

is $(1/(2\pi)^{\frac{1}{2}})*(\exp(-|k|(z'-z)))*\exp(ikx')$

Note that (z'-z) must be positive otherwise the integral doesn't converge.

The Fourier transform of a convolution involving the product of two functions is equal to the product of the Fourier transform of one function times the Fourier transform of the other function. This and other useful information concerning Fourier transforms and series is contained in "Fourier Analysis" by H.P. Hsu.

Therefore, the Fourier transform of the upward-continued gravity $g_z(x',z'-z)$ is equal to $(1/(2\pi)^{1/2})* \exp(-|k|(z'-z))*\exp(ikx')$ times the Fourier transform of the ground-level gravity, $g_z(x,z)$ (where z= ground-level elevation). We then apply the inverse Fourier transform to obtain the upward-continued gravity field (note that we are upward continuing the vertical component).

If we have regularly spaced data and the number of data points is equal to 2^N, where N is an integer, use may be made of the Fast Fourier Transform. Very often an interpreter will take an observed profile of irregularly spaced data points and join them up by hand and then select 2^N equi-spaced data points for the FFT. However, it is possible to fit a set of sine and cosine functions to a set of irregularly spaced data by evaluating the coefficients using either numerical integration or least-square methods.

To do upward continuation we can use either the convolution method or the Fourier transform method. We can upward-continue any component of the gravity field desired but we need to use the appropriate kernel or its Fourier transform. We can also calculate any derivative of the gravity field at an upper level using the appropriate kernel or its transform. If we make the distance (z'-z) small, we can, in effect, calculate the various components and derivatives at ground level.

These operations on the gravity field can be considered as filtering operations.

4.2 Laplace's equation

In free space where there is no mass, the gravity potential obeys the equation:

$$\nabla'^2 U(x',y',z') = 0 \qquad 4.2$$

This is termed Laplace's equation.

In a rectangular coordinate system the x-, y- and z-components of gravity also obey Laplace's equation but it is not true, in general, for other coordinate systems that any particular component of gravity obeys Laplace's equation.

Solutions of Laplace's equation are given for various coordinate systems in "Solutions of Laplace's Equation" by D.R. Bland.

The following discussion is restricted to a rectangular Cartesian coordinate system.

We assume that

$$U(x',y',z') = F(x')*G(y')*H(z')$$

insert this into Laplace's equation and obtain three separate equations, one in F, one in G and one in H.

$$\frac{d^2F(x')}{dx'^2} - a\,F(x') = 0; \quad \frac{d^2G(y')}{dy'^2} - b\,G(y') = 0; \quad \frac{d^2H(z')}{dz'^2} + (a+b)\,H(z') = 0 \qquad 4.3$$

It can be seen that depending upon whether a and b are real or complex, and positive or negative, a given solution involves sine, cosine and exponential terms. Any linear combination of solutions also will satisfy Laplace's equation.

For the two dimensional case we want to eliminate the y-dependence so we set b=0. We then set a= $-m^2$ and ontain the following solution for U(x,z):

$$U(x',z') = + Am*\cosh(mz')*\cos(mx') + Bm*\cosh(mz')*\sin(mx')$$

$$+ Cm*\sinh(mz')*\cos(mx') + Dm*\sinh(mz')*\sin(mx')$$

$\sinh(mz')=(1/2)*(\exp(mz') - \exp(-mz'))$; $\cosh(mz')=(1/2)(\exp(mz)' + \exp(-mz'))$

etc.

For the gravity potential at x',z' (we are returning to the primed coordinates) we can expand the potential in a Fourier series

$$U(x',z') = \sum_{m=0}^{\infty} (Am\,\sin(mx') + Bm\,\cos(mx')).\,\exp(-mz')$$

We normally set z' = 0 corresponding to being at the surface of the Earth in which case exp(-mz') = 1.

To obtain the potential at a distance h above the surface we can take the Fourier series at z'= 0 and multiply it term by term by exp(-mh) to obtain a new series that gives the potential U(x',h).

We again see the role of

(a) exp(-mh) in the case of a Fourier series representation of the gravity potential

or (b) $\exp(-|k|(z'-z))$ in the case of the Fourier transform of the potential

in the process of upward continuation.

If we differentiate the series for the potential term by term w.r.t. z', we obtain a new series for the z-component of gravity, namely $g_z(x',z')$. In practice, we would fit this new series to the observed gravity and then upward-continue the z-component.

4.3 Upward continuation of the gravity field over a semi-infinite, horizontal slab with a sloping face

The face is defined by a plane which extends upwards into space. If we confine our attention to the value of gravity on this plane and actually substitute for z' the value

$$\frac{x'(z2-z1)}{(x2-x1)} + \frac{(x2*z1 - x1*z2)}{(x2-x1)}$$

in the integral for $g_z(x',z')$, M.K. Paul has shown that if the density is only a function of z

the value of gravity anywhere on this plane above the body is a constant equal to:

$$2\,A\,G \int_{z=-\infty}^{z=\text{surface level}} \rho(z)\,dz$$

where $\rho(z)$ is the density
A is the angle of the fault plane (in radians)
and $\tan(A) = \frac{(z2 - z1)}{(x2 - x1)}$

This is a very interesting result. If we believe that we have a geological situation which can be approximated by such a model (such as faulted, flat-lying sedimentary formations) we can upward-continue the gravity over the presumed fault and contour the results in the upper half-plane. If we find a straight-line contour, this could indicate the position and dip of the fault plane (see Figure in Appendix). The method has been described by M.K. Paul and A.K. Goodacre in GEOPHYSICS Vol. 49, pp.1097-1104,1984.

4.4 Downward continuation of the gravity field

We can expand the vertical component of the gravity field in a Fourier series and multiply the the individual terms by exp(md) where d is the distance we wish to continue the field downward and then sum the new series to get the gravity field at a lower level. The theoretical problem is that m goes, in general, to infinity and exp(md) becomes infinitely large. If the coefficients Am and Bm go to zero as rapidly as the function exp(-md) does as m goes to infinity, the new series will converge. However, it is doubtful that any realistic potential field will behave this way. In geophysical practice we just truncate the series and hope for the best.

One can also develop a convolution function for downward continuation that behaves as $\exp(|k|\,d)$ for values of k not too large and apply this to a profile at the Earth's surface. In either case it is assumed that there is no mass between the surface of observation and the deeper surface. If there is mass the potential field is no longer harmonic (obeying Laplace's equation) and the procedure is not valid.

Downward continuation can still be used as a interpretational technique if we are prepared to represent a volume distribution of mass by a series of point sources in three dimensions or a series of line sources in two dimensions. We can attempt to find the depths of sources by continuing the gravity field downward until we obtain a very large peak. This large peak will represent the first point or line source to be encountered. This is because the gravity anomaly due to a point or line source becomes more and more narrow the closer the plane of observation is to the source (the area under the curve stays the same, however).

We then remove this large peak from the anomaly and continue the field further downward (how this removal is actually done is never explained but a suitable way might be by hand).

4.5 Regional-residual separation

The idea of regional-residual separation is to isolate an anomaly of interest. One way to attempt this is to filter out the long wavelength components. The theoretical uncertainty in this approach lies in the fact that, although short wavelength anomalies must be due to shallow sources, long wavelength anomalies can be due to either deep or shallow sources. This latter uncertainty arises as a result of the fact that (if the surface in question is an equipotential surface) we can represent any volume distribution of density by an equivalent layer of surface density so we can always represent deep sources by sources that are more shallow.

To continue an anomaly upward we select a particular rectangular (square) grid (if we are working in a Cartesian coordinate system) and then, selecting a particular point (x',y',z') at which we want to calculate the result, we have to multiply the gravity anomaly value at that point and the other points in the vicinity by an appropriate weighting function based on the expression

$$(1/R^2)\cos A \qquad \text{(3-D kernel)}$$

where $R = ((x-x')^2 + (y-y')^2 + (z-z')^2)^{1/2}$ and $\cos(A) = \frac{(z-z')}{R}$

Here (x,y,z) refers to the grid location of the surface gravity value.

We can calculate our own weights and then normalize them by dividing each one by the sum of all the weights used (or better yet by integrating the kernel w.r.t. x and y to obtain the factor).

We then do a two-dimensional convolution by "sliding" our "filter" around from one grid point to another. At each point we multiply the gridded gravity values by the corresponding weights and then add up the numbers to obtain the upward continued gravity value for that point. This can be done by computer but it is more instructive to do it at least once for a few points by hand using a map with a grid drawn on it and a "filter" constructed on a piece of transparent plastic.

There is a method of regional-residual separation described by G. Simmons (in the Geological Society of America Bulletin, vol 75, 1964 pages 81-98) which involves drawing several intersecting profiles by hand and manually drawing in and adjusting the regional profiles to agree at intersections. Although subjective, it gives results that are difficult to criticize and, in fact, which seem to be very good.

Potential theory lecture 5

5. "Inversion" of gravity data to obtain the causative density distribution

5.1 General remarks

Note that, due to the equivalent layer theorem, a unique solution is not possible. This non-uniqueness is also seen in the expression for the gravity field due to a homogeneous sphere (page 5). In this latter case the radial component of gravity is proportional to the total mass and inversely proportional to the square of the distance from the center of the sphere. Hence there is a trade-off between density and the radius of the sphere that is impossible to determine from a knowledge of the gravity field alone at some distance away from the sphere.

However, if we specify that the source has a uniform density contrast, some progress can often be made. For example, in the case of a sphere the radius may be calculated.

Suppose we know through geological or other geophysical information the sizes and shapes of the bodies that are producing a particular gravity anomaly. In this case we are able to solve the linear problem of gravity inversion to find the densities of the compartments and then make some judgement as to the compositions of the rocks in the various compartments.

5.2 General remarks about least-square fitting

Before discussing the general problem of least-square fitting let's consider the linear problem of fitting a polynomial to a set of points in the x,y plane. For simplicity we will consider a straight-line fit.

We want to represent the set of points by the equation

$$y_j = a + bx_j$$

where x is the independent variable
y is the dependent variable
j refers to the jth point
and a and b are constants to be determined

The standard procedure is to minimize the quantity $\sum_j (y_j - a - bx_j)$ by differentiating the quantity w.r.t. a and w.r.t. b to obtain two simultaneous equations which are then solved for a and b (see Appendix).

Another way to view the procedure is to write out the equation in terms of vectors and matrices.

$$X \vec{u} \cong \vec{y}$$

where $\vec{y}$ is the column vector of y-values

$\vec{u}$ is the column vector of unknown constants (in this case a and b)

and X is the matrix of x-values.

Multiply both sides from the left by the transpose of X (i.e. X^T)

$$X^T X \vec{u} = X^T \vec{y}$$

Now, assuming that the inverse of $X^T X$ exists, multiply both sides from the left by $(X^T X)^{-1}$ to obtain:

$$\vec{u} = (X^T X)^{-1} X^T \vec{y}$$

This is the least-squares solution for $\vec{u}$.

In general we may have matrices of known values and unknown parameters.

Using capital letters for matrices the least-square solution to:

$$X U = Y$$

is

$$U = (X^T X)^{-1} X^T Y$$

In the cases considered subsequently, we will deal with a matrix, M, of theoretically derived quantities, a vector of unknown parameters, $\vec{u}$, and a vector, $\vec{g}$, of observations which are to be modelled in the least-squares sense.

$$\vec{u} = (M^T M)^{-1} M^T \vec{g}$$

As another example of least-squares fitting, suppose we want to describe a set of points plotted on an x,y graph by means of a constant, a sine wave of wavelength L and a cosine wave of wavelength 2L. Each point has a value (x_i, y_i) and there are ten values.

We construct the M matrix as follows:

1	sine $(2\pi x_1/L)$	cosine $(2\pi x_1/2L)$
1	sine $(2\pi x_2/L)$	cosine $(2\pi x_2/2L)$
1	sine $(2\pi x_3/L)$	cosine $(2\pi x_3/2L)$
	etc.	
1	sine $(2\pi x_{10}/L)$	cosine $(2\pi x_{10}/2L)$

The M matrix is a 3 by 10 array of numbers.

There are three unknowns:(i) the constant value c,(ii) the coefficient of the sine $(2\pi x_i/L)$ terms which we'll denote by a and (iii) the coefficient of the cosine $(2\pi x_i/L)$ terms which we'll denote by b.

Denoting an element of M by m_{ij} we can write

$$\begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \\ m_{41} & m_{42} & m_{43} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ m_{10,1} & m_{10,2} & m_{10,3} \end{pmatrix} \quad \begin{pmatrix} c \\ a \\ b \end{pmatrix} \qquad \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ \cdot \\ \cdot \\ \\ \cdot \\ \cdot \\ g_{10} \end{pmatrix}$$

This is the set of equations that we wish to solve in a least-squares sense.

Normally we do not actually find the inverse of $M^T M$ but use other methods to solve the system of equations. The IBM scientific subroutine LLSQ is a good one to use.

It is worthwhile to note that when we expand a function in terms of sines and cosines and their wavelengths fit an integer number of times into the interval over which the data are specified and the data points are equi-spaced, the off-diagonal elements of the matrix

$$(M^T M)$$

are zero and the inverse is easy to compute. In addition, we can add or delete sets of sine and cosine waves of a particular wavelength and the values of the remaining coefficients do not change. In general, when we change the number of coefficients to be determined in a least-squares problem, their derived values also change. It is only when the functions are orthogonal over the data interval that the off-diagonal elements of

$$(M^T M)$$

are zero.

The book "A handbook of numerical matrix inversion and solution of linear equations" by J. R. Westlake is instructive to read. Also highly recommended is "Applied regression analysis" by N. R. Draper and H. Smith.

5.3 Application to gravity problems

Let us now consider the problem of calculating the density contrast of each of three bodies. These are two-dimensional in character and the size and shape of each body is already determined by a seismic survey. The (vertical component of) gravity has been measured at 10 points (g_1 to g_{10}).

Using the above notation for the time being, we can calculate at each of the ten observation points the gravity effect for body number one assuming a density contrast of unity. These will be the matrix elements $m_{1,1}$ to $m_{10,1}$. The matrix elements for body number two (with unit density contrast) are $m_{1,2}$ to $m_{10,2}$ and similarly for body number three.

The unknown densities, represented by a, b and c, are then solved for by the least-squares method (here we are using a,b,c instead of u_1, u_2, etc.).

The least-squares solution also gives the standard deviation of each coefficient a,b and c. If the geometry of the bodies and the observation points is such that the problem is ill-conditioned, this will (or should) be reflected in large values of the standard deviation w.r.t. the corresponding coefficient. The quotient of the coefficient divided by its standard deviation is termed the t-value. The higher this is the more statistically reliable the coefficient is. A t-value of less than about 2 suggests that the value of the coefficient is not significantly different from zero.

5.3.1 Equivalent layer representation

Suppose we don't know the sizes and shapes of the bodies. We can still invert the gravity data to obtain the equivalent layer of surface density which would also reproduce the gravity data. It is understood, however, that the procedure assumes that there is no mass lying between the observer and the equivalent layer. In a practical case we ignore this proviso if we think we are dealing with a homogeneous layer of material lying between the observer and the equivalent layer.

The equivalent layer can be made up of 3-D rectangular prisms in the case of areally distributed gravity data (3-D source) or 2-D rectangular bodies in the case of linearly distributed data (2-D source). These prisms or rectangles generally have a small vertical extent.

Changing our notation somewhat, we can set up the problem as

$$\vec{d} = (M^T M)^{-1} M \vec{g}$$

where $\vec{d}$ is the vector of unknown density values

M is the matrix of values of attraction of each prism at at each observation point

and $\vec{g}$ is the vector of observed gravity values

It is normally useful to add an additional column of 1's to the matrix M to take into account any constant regional (non-zero) value present in the gravity data. This is particularly important to do to avoid "end-effects" or other instabilities which arise in trying to model a long wavelength anomaly with only a limited number of prisms. To model a long wavelength anomaly requires an extended body of similar lateral dimension.

Once the densities have been calculated and the interpreter ensures that a good representation of the vertical component of the gravity field has been achieved, the gravity potential or any other component or any derivative of the field can be calculated because we know the appropriate analytical expressions for these based on a prism. It should be pointed out, however, that just because we have obtained a good fit to the gravity anomaly using the least squares method is no guarantee that we have obtained a good fit in a least squares sense to a particular derivative.

Just how well the procedure outlined above works depends upon the geometrical relationship between the observation points and the equivalent-layer prisms. Generally speaking, the depths of the prisms below the observation points should be about equal to the spacing of the observation points to avoid ill-conditioning of the mathematical process.

It may be computationally more convenient and quicker to replace the prisms by point sources (in the 3-D case) or by line sources (in the 2-D) case.

5.3.2 Other applications of the method

It can be seen that we can manipulate magnetic anomalies in the same way.

These can be total field anomalies as long as the direction of the field doesn't change appreciably as we cross the anomaly. If the anomaly amplitude is some small fraction of the Earth's main field, the direction will remain sensibly constant.

Various electrical measurements might be treated using the equivalent-layer method.

If we assume that the ratio of magnetization contrast to density contrast is constant throughout a source and that the direction of magnetization is uniform, it is a straight forward procedure to convert a gravity anomaly into a magnetic anomaly and vice-versa (see Poisson's relation in section 2.3).

We can, in effect, do a downward continuation by placing an equivalent layer at progressively deeper and deeper depths and seeing at what level the density of one element becomes extremely large.

Note that we could equally well use combinations of functions, such as sines, cosines and exponentials, which are solutions of Laplace's equation to do the same things. However, in my opinion, the equivalent-layer method gives a better physical significance to what is being done.

We can also arrange to have two or more layers of blocks lying vertically one above the other and, using the whole set of blocks, find what combination of densities will reproduce the observed anomaly. This procedure tends to be unstable when a large, finely subdivided network of blocks is employed but when applied cautiously can be useful.

Potential theory lecture 6

6. "Inversion" of gravity data to obtain the causative density distribution (continued)

6.1 The non-linear problem

When we inspect the formulae for the gravitational attraction of a homogeneous prism and a semi-infinite slab, for example, we notice that gravity anomaly is not a linear combination of the body point coordinates but instead these quantities are raised to various powers (as can be seen by expanding log and arctan in their respective power series). This means we can not directly use the method of least-squares to solve for them. To amplify the point, we can use least-squares to solve for the coefficients a,b and c in the expression:

$$y_j \hat{=} a\, x_j + b\, x_j * x_j + c\, x_j * x_j * x_j$$

because they appear raised only to the first power and do not appear in combination. However, if when we set up the problem of finding a,b and c in the least-square sense for

$$y_j \hat{=} (a-b)*(a-b)\, x_j + (c*c*c + b)\, x_j * x_j + c*a\, x_j * x_j * x_j$$

by forming

$$\sum_j \left(y_j - (a-b)*(a-b)\, x_j - (c*c*c + b)\, x_j * x_j - c*a\, x_j * x_j * x_j \right)^2$$

and differentiating w.r.t. a, b and c to obtain three equations, these equations are not linear in a, b and c.

In such a case, we have a non-linear system of equations to solve.

In the same way, even when we specify that a (2-D) body has a polygonal shape and fix its density contrast at a specified value, the problem of determining the positions of the corner points involves the solution of a set of non-linear equations. To do this we generally need to use some sort of of iterative method to solve the problem.

6.2 Non-linear optimization

6.2.1 Background ideas

The first published utilization of non-linear optimization for potential field modelling that I am aware of was by M. Al-Chalabi in 1970 (Interpretation of two-dimensional magnetic profiles by non-linear optimization, Bull. Geof. Teor. Appl. 12, pp. 3-20)

The general problem of non-linear optimization involves finding the minimum (or maximum) of a function of several variables i.e.,

$$f(x_1, x_2, x_3, \ldots\ldots, x_n)$$

As an example, let us consider topographical height, h, which is a function of two variables, x and y i.e. h=h(x,y). Suppose we are in fairly mountainous terrain and wish to go to the highest peak within a given area (say 100 square miles)but it is foggy and we only have a compass and a barometric altimeter to guide us. We have no map and no prior knowledge of the area. We could walk ten paces in one direction, say north, and see whether the altimeter recorded an increase or a decrease in elevation and note the result in our fieldbook. We could then walk ten paces to the east and see if there were an increase or a decrease in this direction and note the result in our book. Our next sequence of steps wuold be guided by the initial results. For example, if our elevation decreased in a northerly direction we would go south by twenty paces the next time. If our elevation had increased in an easterly direction, we would go another ten paces in this direction the next time. Continuing on in this manner we would eventually arrive at a topographical peak. BUT would it be the highest peak or just one of the lower ones? This is the main difficulty in non-linear optimization. We are never sure if we have achieved a global maximum (or minimum) or merely a local one.

6.2.2 Application to gravity interpretation

In our case the function we wish to minimize is the r.m.s. difference between the observed and calculated gravity anomalies. Restricting ourselves without loss of generality to a 2-D case, this is a function of the density contrast of the body and the positions of its corner points. We can have as many or as few body points variable as we please as long as we have sufficient data points. We must not have more unknowns than observations!

The non-linear optimization program that we use (PQRS) calculates the derivatives of the function (the r.m.s. difference) w.r.t. the variable parameters numerically. It works well and is very useful to use in those cases where these derivatives are tedious to obtain analytically. It should be noted however that in our case we can derive the analytical expressions and there are other non-linear optimization routines which might be faster (since it is not necessary to evaluate the function at two different points to obtain a derivative). Nevertheless, the subroutine PQRS generally works well.

Two FORTRAN programs have been written for the interpretation of (i) gravity anomalies that are essentially two-dimensional in character and (ii) anomalies that exhibit circular symmetry. These are named POLY and CYLIN respectively. In either program the non-linear optimization subroutine is linked to the gravity subroutines AUX and GMSTEP through the subroutine CHANGE. The variable parameters in the subroutine AUX have to be fed back to AUX by FORTRAN statements of the form U(2,1)=V(1), etc. In this case whatever number is in location one of the variable parameter array V is transferred into location 2,1 of the horizontal body coordinate array. Each time PQRS cycles around, a new value from V(1) is entered into U(2,1). If density is a variable we might have a statement RHO(3)=V(7). This means that the density contrast of the third body is variable and that AUX receives the latest updated value from the seventh location of the variable parameter array in PQRS.

In addition to the vertical and horizontal body point coordinates, the density contrast can be allowed to vary at the same time. It is better to fix the density and run the program and then specify a new value of density and run the program again. Letting the density and shape vary at the same time may lead to unreasonable values. It has been shown that a body in which the density is variable can be replaced by an "ideal" body in which the density is uniform. Assuming that the density is uniform, it can be demonstrated numerically that there is a minimum value below which it is not possible to obtain a good fit to the observed anomaly. This happens because, as the density contrast is lowered, the body becomes larger and larger and finally generates an anomaly which is too broad too fit the observed data. This may be a useful technique to distinguish between low-density granites and sedimentary basins as the source of a gravity low.

It is also possible to specify that the regional gravity has the form of a low-degree polynomial and use the non-linear optimization routine to simultaneously solve for the coefficients of the polynomial and, say, the body point coordinates. In POLY a straight-line may be fitted; in CYLIN only a constant regional level (REG in the program) is allowed for.

The non-linear optimization routine is very powerful and can be used in many geophysical applications other than that of gravity modelling.

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Appendix

Copies of illustrations used on overhead projector

Illustrations	1 to 12	are for lecture #1
	13 to 25	2
	26 to 35	3
	36 to 46	4
	47 to 59	5
	60 to 65	6