

Fixed depth slice illustration of three-dimensional ellipsoid

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1 Introduction

Seismology is the study of the properties of sound waves as they travel through the earth. Seismic waves emanate from a source such as an earthquake or an explosion. These waves are transmitted from the source through the various layers of the earth and are recorded on the earth's surface at monitoring stations or seismometers and the recording is called a seismogram.

The earth is composed of different layers: inner core, outer core, mantle, moho, and the crust. Each of these layers have different properties for seismic wave propagation. The different wave propagation properties of these layers are reasonably described by various physical laws. As a result, when a seismic wave is measured at a seismometer the seismogram contains information about the origin location of the event in question. Key pieces of information are origin time of the source, arrival time at the receiver, and the travel time of the wave to pass through the various media.

There are two main types of seismic waves: P-waves and S-waves. P-waves are compressional waves and are characterized by the material moving back and forth in the direction that the wave is traveling. S-waves are shear waves and are characterized by the material moving orthogonally to the wave path. P-waves travel faster than S-waves and thus the recorded P-wave marks the arrival time.

Location of the event origin or hypocenter is of particular interest. Though seismology provides a great deal of information about the origin of a seismic event, there is much uncertainty when one tries to pinpoint the hypocenter. Thus statistical techniques can be implemented on a set of

seismological data to help improve hypocenter estimation and to quantify the uncertainty of the estimation.

Seismologists are able to compute a point estimate for a source origin as well as a 3-dimensional uncertainty ellipsoid around the point estimate. The uncertainty ellipsoid is usually a 95% confidence region. This report will briefly explain the statistical model for travel time as well as the methods for computing a point estimate and confidence region. Then it will explain how the confidence region is reported in seismological notation and an analysis is described for illustrating slices of the uncertainty ellipsoid at different depths inside the earth.

1.1 Statistical Travel Time Model

The model for the travel time of a P-wave from the hypocenter to the i^{th} seismic monitoring station is a non-linear model of the form

$$t_i = t_0 + T(\mathbf{x}_i; \boldsymbol{\theta}) + \epsilon_i, \quad i = 1, 2, \dots, n, \quad (1)$$

where t_i is the observed travel time to the i^{th} station, t_0 is the origin time, T is a nonlinear function for travel time, \mathbf{x}_i is a vector of the i^{th} station location, and $\boldsymbol{\theta} = (x, y, z)'$ is a vector of longitude, latitude, and depth of the hypocenter. The parameters of interest are t_0, x, y, z . It is also assumed that the error terms are independent and identically distributed as $N(0, \sigma^2)$.

The Location Object Oriented tool (LOCOO) written at Sandia National Laboratory is used to find estimates of t_0 and $\boldsymbol{\theta}$. LOCOO uses a linearized least-squares technique with the Levenberg-Marquardt algorithm to improve performance in highly nonlinear regions of model space. The estimation methods are described in the next section.

1.2 Parameter Estimates: Non-Linear Least Squares

Generally, equation (1) can be written as

$$y_i = f(\mathbf{x}_i; \boldsymbol{\theta}) + \epsilon_i, \quad i = 1, 2, \dots, n, \quad (2)$$

where $\boldsymbol{\theta}$ is a $p \times 1$ vector (p parameters of interest) and ϵ_i 's are *iid* $N(0, \sigma^2)$. For simplicity, denote $f(\mathbf{x}_i; \boldsymbol{\theta})$ by $f_i(\boldsymbol{\theta})$. Equation (2) can be written in vector notation as

$$\mathbf{y} = \mathbf{f}(\boldsymbol{\theta}) + \boldsymbol{\epsilon}$$

where \mathbf{y} is a $n \times 1$ vector, $\mathbf{f}(\boldsymbol{\theta}) = (f_1(\boldsymbol{\theta}), f_2(\boldsymbol{\theta}), \dots, f_n(\boldsymbol{\theta}))'$, and $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$. The least squares estimate of $\boldsymbol{\theta}$, denoted by $\hat{\boldsymbol{\theta}}$, is the minimizer of the sum of squares error for $\boldsymbol{\theta}$, i.e. it minimizes the quantity

$$SSE(\boldsymbol{\theta}) = (\mathbf{y} - \mathbf{f}(\boldsymbol{\theta}))' (\mathbf{y} - \mathbf{f}(\boldsymbol{\theta})).$$

One approach to minimizing $SSE(\boldsymbol{\theta})$ involves approximating $\mathbf{f}(\boldsymbol{\theta})$ around the true value $\boldsymbol{\theta}^*$ by a first order Taylor series expansion. This approximation yields some useful results from linear model theory. The Taylor expansion for $\mathbf{f}(\boldsymbol{\theta})$ around $\boldsymbol{\theta}^*$ is

$$\mathbf{f}(\boldsymbol{\theta}) \approx \mathbf{f}(\boldsymbol{\theta}^*) + \mathbf{F} \cdot (\boldsymbol{\theta} - \boldsymbol{\theta}^*) \tag{3}$$

where \mathbf{F} is the Jacobian of $\mathbf{f}(\boldsymbol{\theta})$ evaluated at $\boldsymbol{\theta}^*$. Explicitly,

$$\mathbf{F} = \left. \frac{\partial \mathbf{f}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}'} \right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^*} = \begin{pmatrix} \frac{\partial f_1(\boldsymbol{\theta}^*)}{\partial \theta_1} & \frac{\partial f_1(\boldsymbol{\theta}^*)}{\partial \theta_2} & \dots & \frac{\partial f_1(\boldsymbol{\theta}^*)}{\partial \theta_p} \\ \frac{\partial f_2(\boldsymbol{\theta}^*)}{\partial \theta_1} & \frac{\partial f_2(\boldsymbol{\theta}^*)}{\partial \theta_2} & \dots & \frac{\partial f_2(\boldsymbol{\theta}^*)}{\partial \theta_p} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n(\boldsymbol{\theta}^*)}{\partial \theta_1} & \frac{\partial f_n(\boldsymbol{\theta}^*)}{\partial \theta_2} & \dots & \frac{\partial f_n(\boldsymbol{\theta}^*)}{\partial \theta_p} \end{pmatrix}$$

Now, using the Taylor expansion the sum of squares error for $\boldsymbol{\theta}$ can be approximated:

$$\begin{aligned} SSE(\boldsymbol{\theta}) &= (\mathbf{y} - \mathbf{f}(\boldsymbol{\theta}))' (\mathbf{y} - \mathbf{f}(\boldsymbol{\theta})) \\ &\approx (\mathbf{y} - \mathbf{f}(\boldsymbol{\theta}^*) - \mathbf{F} \cdot (\boldsymbol{\theta} - \boldsymbol{\theta}^*))' (\mathbf{y} - \mathbf{f}(\boldsymbol{\theta}^*) - \mathbf{F} \cdot (\boldsymbol{\theta} - \boldsymbol{\theta}^*)) \\ &= (\mathbf{z} - \mathbf{F} \cdot \boldsymbol{\beta})' (\mathbf{z} - \mathbf{F} \cdot \boldsymbol{\beta}) \end{aligned}$$

where $\mathbf{z} = \mathbf{y} - \mathbf{f}(\boldsymbol{\theta}^*)$ and $\boldsymbol{\beta} = \boldsymbol{\theta} - \boldsymbol{\theta}^*$. Since (4) is a linear form for $SSE(\boldsymbol{\theta})$, linear model theory gives the ordinary least-squares solution for $\boldsymbol{\beta}$, namely

$$\begin{aligned}
\hat{\beta} &= (\mathbf{F}'\mathbf{F})^{-1}\mathbf{F}'\mathbf{z} \\
\Rightarrow \hat{\theta} - \theta^* &\approx (\mathbf{F}'\mathbf{F})^{-1}\mathbf{F}'(\mathbf{y} - \mathbf{f}(\theta^*)) \\
&= (\mathbf{F}'\mathbf{F})^{-1}\mathbf{F}'\mathbf{e}
\end{aligned} \tag{4}$$

where $\mathbf{e} = \mathbf{y} - \mathbf{f}(\theta^*)$ is the residual vector. It can be shown from (4) that, for a large enough n ,

$$\hat{\theta} - \theta^* \sim N_p(\mathbf{0}, \sigma^2(\mathbf{F}'\mathbf{F})^{-1}). \tag{5}$$

A number of useful results may be obtained from (5). One of these is the fact that

$$\frac{(\hat{\theta} - \theta^*)\mathbf{F}'\mathbf{F}(\hat{\theta} - \theta^*)}{ps^2} \sim F_{p,n-p}$$

thus yielding a way to compute an approximate confidence region for θ^* . A $100(1 - \alpha)\%$ confidence region may be found by estimating \mathbf{F}' with $\mathbf{F}'(\hat{\theta})$ (the Jacobian evaluated at $\hat{\theta}$) and then using

$$\left\{ \theta^* : (\theta^* - \hat{\theta})'\mathbf{F}'(\hat{\theta})\mathbf{F}(\hat{\theta})(\theta^* - \hat{\theta}) \leq ps^2 F_{p,n-p}^\alpha \right\}.$$

1.3 Uncertainty Ellipsoids

Uncertainty ellipsoid is a Seismological term that is used in place of a three-dimensional confidence region. The standard confidence level in seismology is 95%. LOCOO will compute the least squares estimate for the hypocenter and then build a 95% confidence ellipsoid around it. The half-lengths of the major axes of the ellipsoid are reported in *trend-plunge* notation. Trend-plunge is a type of spherical coordinate system commonly used for reporting vectors in seismological applications. The definitions for trend and plunge are found below.

Definition: Trend - *A rotation clockwise from the northward axis*

Definition: Plunge - *A rotation downward from the horizontal plane*

1.4 Problem Objectives

The goal of this problem is to take the three-dimensional confidence region reported in LOCOO and plot slices of it at different depths. This can be thought of as taking a horizontal plane and moving it down the z -axis and then plotting the resulting intersection of the plane and the ellipsoid for different depths. This problem will be approached as follows:

1. Describe a three dimensional ellipsoid in matrix form.
2. Find the rotation matrix that will give the desired orientation.
3. Intersect the ellipsoid with a horizontal plane.
4. Derive the equation of the resulting intersection.
5. Use the equation to plot the ellipse-plane intersections.

2 Methods

2.1 Describing the three-dimensional ellipsoid

Consider the general matrix representation of a three dimensional ellipsoid: $\mathbf{t}'\mathbf{R}\mathbf{D}\mathbf{R}'\mathbf{t} = 1$ where the 3×1 vector \mathbf{t} contains the centroid. Thus

$$\mathbf{t} = \begin{pmatrix} x - x_o \\ y - y_o \\ z - z_o \end{pmatrix}$$

and the centroid's coordinates are given by (x_o, y_o, z_o) . \mathbf{D} is a 3×3 diagonal matrix where the entries are the inverses of the half lengths of the ellipsoid axes squared. Then \mathbf{D} can be written as

$$\mathbf{D} = \begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{b^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$

where a is one-half the length of the major ellipsoid axis, b is one-half the length of the intermediate ellipsoid axis, and c is one-half the length of the minor ellipsoid axis. A 3×3 rotation matrix \mathbf{R} can be constructed that will give the desired orientation.

2.2 Constructing the rotation matrix.

Recall that LOCOO gives the half-lengths of the ellipsoid axes as well as their orientations in trend-plunge notation. This information can be used to construct the rotation matrix \mathbf{R} that will give the proper orientation in the Cartesian Coordinate system. The construction involves converting the trend-plunge vectors into Cartesian unit-vectors and then combining these vectors in a matrix. The resulting matrix will be orthogonal as the ellipsoid axes are mutually orthogonal.

Let (t_1, p_1) be the trend and plunge of the major ellipsoid axis respectively. Similarly let (t_2, p_2) be the trend and plunge of the intermediate ellipsoid axis and (t_3, p_3) be the trend and plunge of the minor ellipsoid axis. The conversion formula for the i_{th} ellipsoid axes is given by

$$\begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} = \begin{pmatrix} \sin(t_i) \cos(p_i) \\ \cos(t_i) \cos(p_i) \\ -\sin(p_i) \end{pmatrix}$$

Note that the conversion results in a unit-vector. Computing this quantity for each ellipsoid axes and then combining them as columns of a 3×3 matrix gives \mathbf{R} .

$$\mathbf{R} = \begin{pmatrix} \sin(t_1) \cos(p_1) & \sin(t_2) \cos(p_2) & \sin(t_3) \cos(p_3) \\ \cos(t_1) \cos(p_1) & \cos(t_2) \cos(p_2) & \cos(t_3) \cos(p_3) \\ -\sin(p_1) & -\sin(p_2) & -\sin(p_3) \end{pmatrix}$$

Verifying that this is the desired rotation matrix is straightforward. Start with unit vectors on the coordinate axes. Arrange these unit vectors in a 3×3 identity matrix, \mathbf{I} , and note that \mathbf{I} defines the usual three dimensional space. The columns of \mathbf{I} would also define the directions of the unrotated ellipsoid axes. Pre-multiplying \mathbf{I} by \mathbf{R}' will then rotate the ellipsoid axes to the desired orientation.

2.3 Intersecting the ellipsoid with a plane

This section explains how to intersect a rotated and translated ellipsoid with a horizontal plane. The following derivation describes the figure that results from the intersection. It also provides a useful result.

First, as the rotation matrix has been found, define the matrix \mathbf{A} as

$$\mathbf{A} = \mathbf{RDR}' = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}.$$

Now the full equation of the ellipsoid may be written as

$$\begin{pmatrix} x - x_o \\ y - y_o \\ z - z_o \end{pmatrix}' \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x - x_o \\ y - y_o \\ z - z_o \end{pmatrix} = 1. \quad (6)$$

Take a horizontal plane and intersect the ellipsoid at the depth of the centroid, i.e. set $z = z_o$ and the equation of the ellipsoid reduces to

$$\begin{pmatrix} x - x_o \\ y - y_o \\ 0 \end{pmatrix}' \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x - x_o \\ y - y_o \\ 0 \end{pmatrix} = 1$$

and multiplication yields

$$\begin{pmatrix} x - x_o \\ y - y_o \end{pmatrix}' \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x - x_o \\ y - y_o \end{pmatrix} = 1.$$

Noting that this is the equation of an ellipse implies that the matrix

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

is symmetric, positive definite and invertible by definition of an ellipse. This result will be used later.

The intersection of an ellipsoid with a plane is empty, a point, or an ellipse for any depth and orientation of the intersecting plane. As this is the case, the goal of the problem is then to plot a two-dimensional ellipse at different depths.

2.4 Equation of the intersection of the ellipsoid with a plane

The size and location of the intersection ellipse will be different for different depths. It is then desirable to derive this equation in terms of an arbitrary but fixed z . So set $z = \tilde{z}$ in equation (6) and the equation for the uncertainty ellipsoid is

$$\begin{pmatrix} x - x_o \\ y - y_o \\ \tilde{z} - z_o \end{pmatrix}^T \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x - x_o \\ y - y_o \\ \tilde{z} - z_o \end{pmatrix} = 1. \quad (7)$$

With the depth of the ellipsoid-plane intersection fixed, an expression for the resulting 2-dimensional ellipse may be found. The approach will be to partition (7) and then manipulate the expression ultimately ending at an equation for an ellipse that will adjust the center and size for different depths. So partition (7) as

$$\mathbf{u} = \begin{pmatrix} x - x_o \\ y - y_o \end{pmatrix} \quad \mathbf{A}_{11} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad \mathbf{A}_{12} = \begin{pmatrix} a_{13} \\ a_{23} \end{pmatrix}$$

$$\mathbf{A}_{21} = \begin{pmatrix} a_{31} & a_{32} \end{pmatrix} \quad \mathbf{A}_{22} = a_{33}.$$

Also set $\tilde{z} - z_o = k$ as it is a constant. Thus equation (7) can be written as

$$\begin{pmatrix} \mathbf{u} \\ k \end{pmatrix}' \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ k \end{pmatrix} = \mathbf{u}'\mathbf{A}_{11}\mathbf{u} + k\mathbf{A}_{21}\mathbf{u} + k\mathbf{u}'\mathbf{A}_{12} + k^2\mathbf{A}_{22} = 1. \quad (8)$$

Note that the matrix \mathbf{A}_{11} was found to be positive definite in section 2.3. A number of SPD properties will be used. \mathbf{A}_{11} may be factored as $\mathbf{A}_{11} = \mathbf{A}_{11}^{\frac{1}{2}}\mathbf{A}_{11}^{\frac{1}{2}}$ where $\mathbf{A}_{11}^{\frac{1}{2}}$ is symmetric, positive definite, and invertible. Also note that $\mathbf{A}_{12}' = \mathbf{A}_{21}$ by symmetry of \mathbf{RDR}' . Then the two middle terms in the right hand side of (8) may be combined as they are scalars. Factor \mathbf{A}_{11} in the first term and multiply by the identity $\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{A}_{11}^{-\frac{1}{2}}$ in the second term to get

$$\mathbf{u}'\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{u} + 2k\mathbf{u}'\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{A}_{11}^{-\frac{1}{2}}\mathbf{A}_{12} + k^2\mathbf{A}_{22} = 1.$$

In order to pull out the equation of an ellipse, it is necessary to complete the square in terms of the vector $\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{u}$. So set $\mathbf{v} = \mathbf{A}_{11}^{\frac{1}{2}}\mathbf{u}$ and then complete the square with respect to \mathbf{v} . This will give

$$\begin{aligned} \mathbf{v}'\mathbf{v} + 2k\mathbf{v}'\mathbf{A}_{11}^{-\frac{1}{2}}\mathbf{A}_{12} + k^2\mathbf{A}_{22} &= 1 \\ \implies (\mathbf{v} + k\mathbf{A}_{11}^{-\frac{1}{2}}\mathbf{A}_{12})'(\mathbf{v} + k\mathbf{A}_{11}^{-\frac{1}{2}}\mathbf{A}_{12}) + k^2\mathbf{A}_{22} &= 1 + k^2\mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12} \end{aligned}$$

and this result will lend itself to finding the general equation of an ellipse.

What is required now is to resubstitute for \mathbf{v} in terms of \mathbf{u} and then factoring some matrices to get the ellipse equation. These operations are performed below:

$$\begin{aligned} (\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{u} + k\mathbf{A}_{11}^{-\frac{1}{2}}\mathbf{A}_{12})'(\mathbf{A}_{11}^{\frac{1}{2}}\mathbf{u} + k\mathbf{A}_{11}^{-\frac{1}{2}}\mathbf{A}_{12}) &= 1 - k^2(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}) \\ \implies (\mathbf{A}_{11}^{\frac{1}{2}}(\mathbf{u} + k\mathbf{A}_{11}^{-1}\mathbf{A}_{12}))' \mathbf{A}_{11}^{\frac{1}{2}}(\mathbf{u} + k\mathbf{A}_{11}^{-1}\mathbf{A}_{12}) &= 1 - k^2(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}) \\ \implies (\mathbf{u} + k\mathbf{A}_{11}^{-1}\mathbf{A}_{12})' \mathbf{A}_{11}(\mathbf{u} + k\mathbf{A}_{11}^{-1}\mathbf{A}_{12}) &= 1 - k^2(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}) \end{aligned} \quad (9)$$

Noting that (9) fits the general form $(\mathbf{x} - \boldsymbol{\mu})'\boldsymbol{\Sigma}(\mathbf{x} - \boldsymbol{\mu}) = c$, the general equation for an ellipse, the desired result is achieved. It now helps to substitute back in for \mathbf{u} and k to see how to plot the ellipses for different depths \tilde{z} . The final result is found in equation (10).

$$\left(\begin{pmatrix} x \\ y \end{pmatrix} - \boldsymbol{\mu} \right)' \mathbf{A}_{11} \left(\begin{pmatrix} x \\ y \end{pmatrix} - \boldsymbol{\mu} \right) = 1 - (\tilde{z} - z_o)^2 (A_{22} - \mathbf{A}_{21} \mathbf{A}_{11}^{-1} \mathbf{A}_{12}) \quad (10)$$

where the vector

$$\boldsymbol{\mu} = \begin{pmatrix} x_o \\ y_o \end{pmatrix} - (\tilde{z} - z_o) \mathbf{A}_{11}^{-1} \mathbf{A}_{12}$$

provides an adjustment to the center of the ellipses at different depths. The right hand side of (10) provides an adjustment to the size of the ellipse at different depths. It is also easy to see that the matrix \mathbf{A}_{11} contains information on the orientation of the ellipses. Results of slicing a confidence region are found in the next section. Note, it is imperative that the entries of \mathbf{A}_{11} , \mathbf{A}_{12} , and \mathbf{A}_{21} are first converted to the proper units measured on the x and y axes so that the relative size of the ellipses is correct.

3 Results

The ellipse derivation was tested using an earthquake event off the east coast of Japan. LOCOO provided a hypocenter estimation along with a 95% confidence region. It was desired to plot slices of the confidence region at different depths inside the earth.

The estimate for the hypocenter is at 36.3° latitude, 141.2° longitude and a depth of 58 km. A plot of the hypocenter estimate and the seismic monitoring station locations is found in Figure 1. The station locations are solid dots and the hypocenter estimate is an open circle. LOCOO provided the lengths of the ellipsoid axes. The major axis orientation is a trend of 247.2485° , a plunge of 58.6309° and a half length of 51.9415 km. The intermediate axis has a trend of 154.1015° , a plunge of 1.9170° with a half length of 14.7086 km. Finally, the minor axis has a trend of 62.9354° , a plunge of 31.3010° with a half length of 11.1682 km. This orientation will make the ellipse slices appear to travel from the north-east to the south-west as the depth increases.

The ellipse equation (10) was programmed in a loop in R. The loop could only be indexed over depths that contained the confidence region because the \mathbf{A}_{11} is not invertible outside this region.

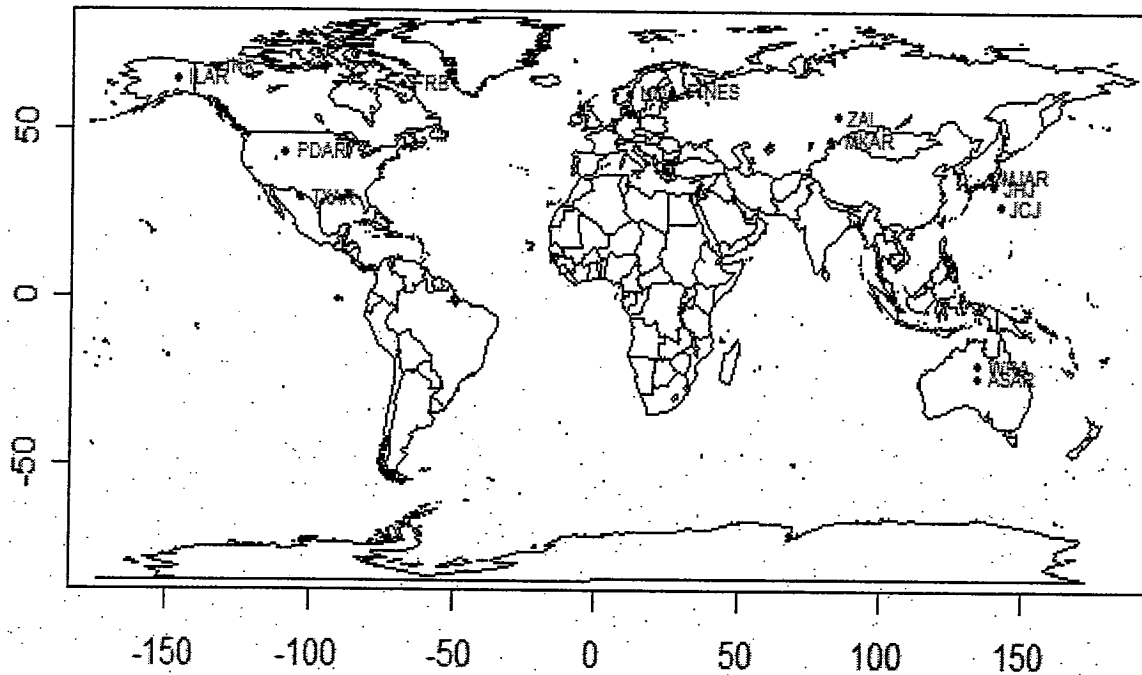


Figure 1: Station Locations and Hypocenter Estimate

The plottable depth for the ellipses is from 37 to 81 km beneath the earth's surface. Some examples of the ellipse slices are included in Figure 2 (page 12). Note the point estimate of the hypocenter is at a depth of $z = 58$ km.

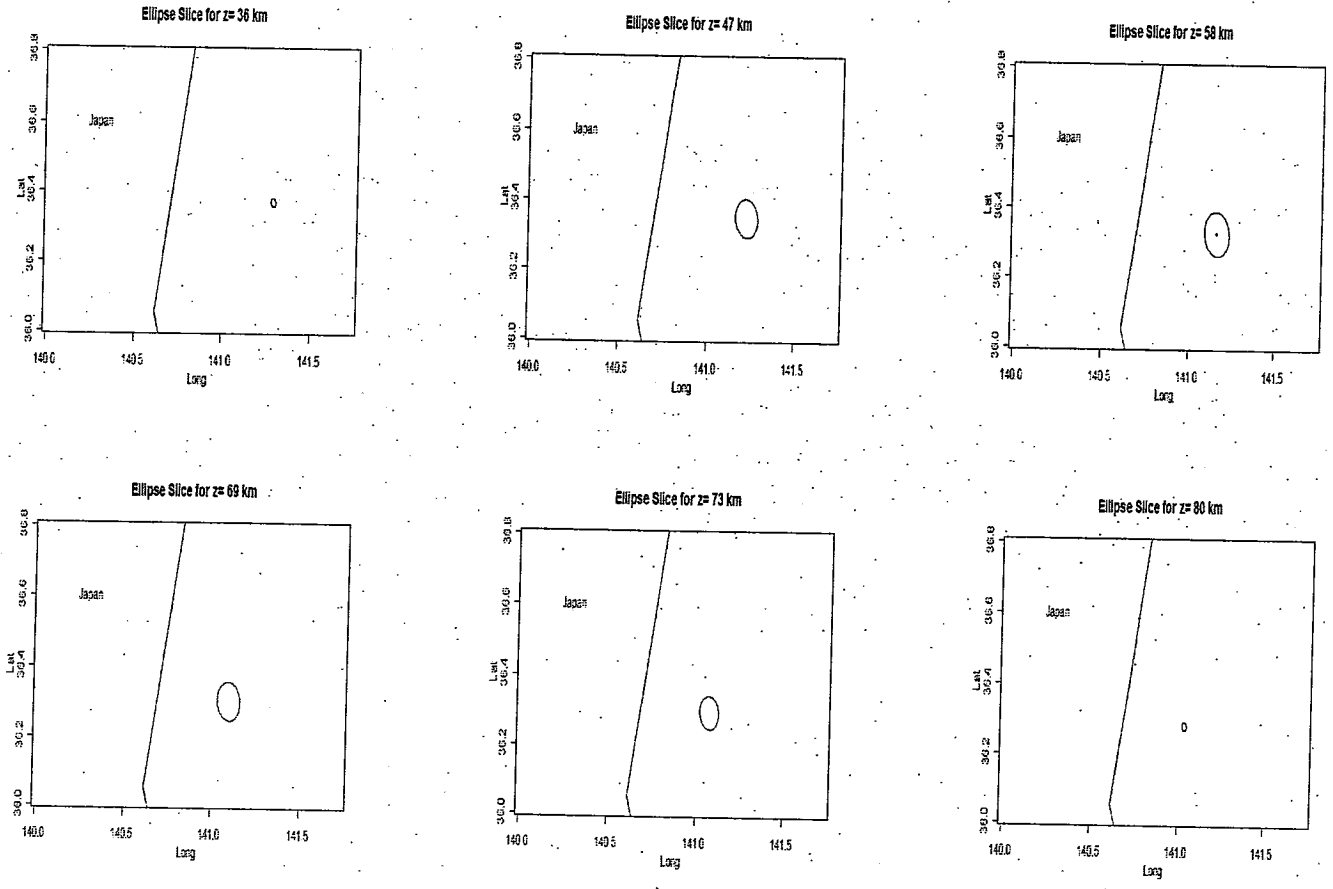


Figure 2: Confidence Region Slices

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