Journal of Uncertain Systems
Vol.10, No.1, pp.61-67, 2016
Online at: www.jus.org.uk

How to Estimate Accuracy of Different Models: Non-Gaussian Case

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Received 1 May 2015; Revised 13 June 2015

Abstract

In geophysics, we usually have several Earth models based on different types of data: seismic, gravity, etc. Each of these models captures some aspects of the Earth structure. To properly combine these models, it is important to know the accuracy of different models. In our previous papers, we showed how this accuracy can be estimated under the assumption that the inaccuracy of these models is normally distributed. In practice, however, the distribution of the model inaccuracy is often non-Gaussian. In this paper, we describe how accuracy estimation methods can be extended to the non-Gaussian case.

Keywords: accuracy of a model, geophysics, non-Gaussian distributions

1 Formulation of the Problem

Need to estimate accuracy of different geophysical models. One of the main objectives of geophysics is to determine the density $\rho(x, y, z)$ at different depths z and at different geographical locations (x, y). There exist several methods for estimating the density: e.g., we can use seismic data [5], or we can use gravity measurement. Each of the techniques for estimating ρ has its own advantages and limitations. For example:

- seismic measurements often lead to a more accurate value of ρ than gravity measurements, but
- seismic measurements mostly provide information about the areas above the Moho surface.

It is desirable to combine ("fuse") the models obtained from different types of measurements into a single model that would combine the advantages of all of these models.

To properly combine several models into a single one, it is important to know the accuracy of different models; see, e.g., [10, 14].

In geophysics, the model's accuracy usually depends on the depth: the deeper the layer that we want to estimate, the less accurate our estimate. The accuracy may also depend on other parameters. We want to find out, for each model and for each value of the corresponding parameter (such as depth), how accurate is this model.

How can we describe model accuracy. We cannot determine the actual value of the approximation error. Indeed, if we knew the value of the approximation error, we would be able to correct for this known error and thus, get a more accurate estimate. What we can, in principle, determine is:

- the bounds on approximation error, and
- how frequently different values within these bounds may occur.

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In other words, what we can, in principle, estimate, is the probability distribution describing different possible values of the approximation error.

Traditional methods of estimating accuracy cannot be directly used in geophysics. The problem of estimating approximation accuracy is ubiquitous in measurement practice. The most widely used method of estimating the accuracy of a given measuring technique is available when we have a "standard" measuring instrument or technique which is several times more accurate than the technique whose accuracy we are estimating; see, e.g., [10]. Since the "standard" measuring technique is much more accurate than the one we testing, the result of using this "standard" measuring instrument is practically equal to the actual value of the measured quantity. Thus, the model inaccuracy can be well approximated by the difference between the measurement results obtained by the two techniques.

In geophysics, however, seismic (and other) methods are state-of-the-art, no method leads to more accurate determination of the densities. As a result, this "calibration" method cannot be directly applied to estimating approximation errors in the geophysical problems.

Another accuracy estimation technique is applicable when we have several independent measuring instruments of the same type. In this case, the random inaccuracies corresponding to different instruments are independent and thus, when we average a large number of such measurement results, we get a very accurate approximation to the actual value. So, by comparing the measurement results obtained by each technique with this average, we can get a very good understanding of each model's accuracy [10].

In geophysics, however, we only have one model coming from the application of each technique, so we cannot directly use this method either.

Estimating accuracy of different models: towards a precise formulation of the problem. Let $v_{1,k}$, $v_{2,k}$, ... are the estimates of the same quantity v_k in different models. For example, in geophysical applications, v_k is the density at a certain depth, measured at different geographical locations k.

In the ideal cases, all models are exact, i.e., $v_{ik} = v_k$ for i and k. In this case, there is no difference between estimates produced by different models: $v_{ik} - v_{jk} = 0$ for all i, j, and k. In reality, models are approximate, so, in general, the estimates corresponding to different models $i \neq j$ are different: $v_{ik} - v_{jk} \neq 0$.

For each pair of models (i, j), we can view the corresponding differences $v_{ik} - v_{jk}$ as a sample of a random variable $\Delta v_{ij} = v_i - v_j$ that describes the difference between the two models' estimates v_i and v_j at the given depth.

It is reasonable to assume that inaccuracies $\Delta v_i \stackrel{\text{def}}{=} v_i - v$ corresponding to different models i are independent. Our objective is to reconstruct the probability distributions for model inaccuracies Δv_i based on the observed distributions of the differences $\Delta v_{ij} = v_i - v_j = \Delta v_i - \Delta v_j$.

What is known: Gaussian case. The above problem has been largely solved in the case when all the inaccuracies are assumed to be normally distributed; see, e.g., [7, 13].

Indeed, a normal distribution is uniquely characterized by its mean and its standard deviation σ. Of course, if we only know the differences, we cannot detect the systematic bias, we can only hope to determine the random component of the model inaccuracies. If we limit ourselves to random components, all the means become 0, and all we need to determine is the standard deviation σ_i of each approximation error Δv_i.

Since the approximation errors Δv_i are independent and normally distributed, each (observed) difference $v_i - v_j = \Delta v_i - \Delta v_j$ is also normally distributed, with 0 mean and variance $\sigma_{ij}^2 = \sigma_i^2 + \sigma_j^2$.

In the simplest case, when we only have two models, the only information that we can extract from the observations $v_1 - v_2$ is the sum $\sigma_{12}^2 = \sigma_1^2 + \sigma_2^2$ of these models' variances. Of course, when we only know the sum of the two numbers, we cannot uniquely reconstruct both of these numbers. So, in this case, it is not possible to estimate the accuracy of different models.

However, once we have at least three different models, the situation changes: for each three of these models, by observing the variances of the differences $v_1 - v_2$, $v_2 - v_3$, and $v_2 - v_3$, we can determine the three sums $\sigma_{12}^2 = \sigma_1^2 + \sigma_2^2$, $\sigma_{23}^2 = \sigma_1^2 + \sigma_3^2$, and $\sigma_{13}^2 = \sigma_1^2 + \sigma_3^2$. Once we know the values of these three sums, we can uniquely determine all three values σ_i^2. For example, one can easily check that we can determine σ_1^2 as

$$\sigma_1^2 = \frac{\sigma_{12}^2 + \sigma_{13}^2 - \sigma_{23}^2}{2} = \frac{(\sigma_1^2 + \sigma_2^2) + (\sigma_1^2 + \sigma_3^2) - (\sigma_2^2 + \sigma_3^2)}{2}.$$

Problem: distributions are often non-Gaussian. In measurement practice, Gaussian distributions occur in only about 60% of the cases; see, e.g., [6, 9]. In all other cases, the distribution of the approximation error

is different from Gaussian; see, e.g., [1]. To cover such cases, it is therefore desirable to extend the above model estimation techniques to the non-Gaussian case. This is the problem that we analyze in this paper.

2 Analysis of the Problem

We also need correlation. At first glance, all we need to do is to find, for each quantity v (e.g., for densities at a given depth) and for each model i, the probability distribution of the corresponding approximation error $\Delta v_i = v_i - v$. This would indeed be sufficient if the approximation errors corresponding to different quantities v were independent.

In practice, the approximation errors Δv_i and Δw_i corresponding to different quantities v and w (corresponding, e.g., to different depths) are usually correlated, since they are largely caused by the same global inaccuracies. In the geophysical example, this correlation is especially strong if the variables v and w correspond to nearby depths. As a result, to properly describe model accuracy:

- we need to know not only the probability distributions for each approximation error Δv_i or Δw_i,
- we also need to know, for each model i, the joint probability distribution of the pair $(\Delta v_i, \Delta w_i)$.

It is convenient to use characteristic functions. We want to reconstruct the probability distribution of each approximation error $(\Delta v_i, \Delta w_i)$ based on the known probability distributions for the differences

$$(v_i - v_j, w_i - w_j) = (\Delta v_i - \Delta v_j, \Delta w_i - \Delta w_j).$$

The usual way to represent a 2-D probability distribution of a random variable $(\Delta v_i, \Delta w_i)$ is by describing its probability density function (pdf) $\rho_i(\Delta v_i, \Delta w_i)$. However, in terms of the pdfs, the relation between the distributions of two independent random variables and the distribution $\rho_{ij}(v, w)$ for their difference is rather complicated:

$$\rho_{ij}(v, w) = \int \rho_i(\Delta v_i, \Delta w_i) \cdot \rho_j(v + \Delta v_i, w + \Delta w_i)\, d\Delta v_i\, d\Delta w_i.$$

This relation can be described in a much simpler way if, for each random variable, instead of the pdf, we use its *characteristic function*

$$\chi_i(\omega_v, \omega_w) \stackrel{\text{def}}{=} E[\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_i + \omega_w \cdot \Delta w_i))],$$

where $\mathrm{i} \stackrel{\text{def}}{=} \sqrt{-1}$, i.e.,

$$\rho_i(\omega_v, \omega_w) = \int \rho_i(\Delta v_i, \Delta w_i) \cdot \exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_i + \omega_w \cdot \Delta w_i))\, d\Delta v_i\, d\Delta w_i.$$

From the mathematical viewpoint, the characteristic function is the Fourier transform of the pdf, and efficient algorithms are known both for computing the Fourier transform and for reconstructing a function from its Fourier transform (this reconstruction is known as the *inverse Fourier transform*); see, e.g., [2, 4, 8, 15].

For the difference

$$(\Delta v_{ij}, \Delta w_{ij}) \stackrel{\text{def}}{=} (\Delta v_i - \Delta v_j, \Delta w_i - \Delta w_j),$$

the characteristic function has the form

$$\chi_{ij}(\omega_v, \omega_w) \stackrel{\text{def}}{=} E[\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_{ij} + \omega_w \cdot \Delta w_{ij})] = E[\exp(\mathrm{i} \cdot (\omega_v \cdot (\Delta v_i - \Delta v_j) + \omega_w \cdot (\Delta w_i - \Delta w_j))].$$

This expression can be equivalently reformulated as

$$\chi_{ij}(\omega_v, \omega_w) = E[\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_i + \omega_w \cdot \Delta w_i) - \mathrm{i} \cdot (\omega_v \cdot \Delta v_j + \omega_w \cdot \Delta w_j))].$$

Since the exponent of the sum is equal to the product of the exponents, we have

$$\chi_{ij}(\omega_v, \omega_w) = E[\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_i + \omega_w \cdot \Delta w_i)) \cdot \exp(-\mathrm{i} \cdot (\omega_v \cdot \Delta v_j + \omega_w \cdot \Delta w_j))].$$

Due to the fact that different approximation errors $(\Delta v_i, \Delta w_i)$ and $(\Delta v_j, \Delta w_j)$ are independent random variables, we can conclude that

$$\chi_{ij}(\omega_v, \omega_w) = E[\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_i + \omega_w \cdot \Delta w_i))] \cdot E[\exp(-\mathrm{i} \cdot (\omega_v \cdot \Delta v_j + \omega_w \cdot \Delta w_j))].$$

The first factor is simply a characteristic function of the i-th variable. The quantity $\exp(-\mathrm{i}\cdot(\omega_v\cdot\Delta v_j+\omega_w\cdot\Delta w_j))$ used in the second factor is a complex conjugate of the term used in the characteristic function:

$$\exp(-\mathrm{i} \cdot (\omega_v \cdot \Delta v_j + \omega_w \cdot \Delta w_j) = (\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_j + \omega_w \cdot \Delta w_j))^*,$$

where the conjugation operation z^** is defined in the usual way: for $z = a + b \cdot \mathrm{i}$, we have $z^* = a - b \cdot \mathrm{i}$. Thus, the expected value of the second factor is equal to the complex conjugate of the expected value of the term $\exp(\mathrm{i} \cdot (\omega_v \cdot \Delta v_j + \omega_w \cdot \Delta w_j))$, i.e., to the complex conjugate of the j-th characteristic function. So, we conclude that

$$\chi_{ij}(\omega_v, \omega_w) = \chi_i(\omega_v, \omega_w) \cdot \chi_j^*(\omega_v, \omega_w). \tag{1}$$

This relation is indeed much simpler than the above pdf-based formula.

How can we determine the characteristic functions $\chi_{ij}(\omega_v, \omega_w)$ based on the samples. To find the characteristic function, we must use the sample values $(v_{ik} - v_{jk}, w_{ik} - w_{jk})$ of the corresponding differences.

One possibility is to used these sample values to estimate the corresponding pdf $\rho_{ij}(v, w)$, and then use Fourier Transform to compute the characteristic function. Another possibility is to use the fact that, due to the Large Numbers Theorem (see, e.g., [14]), for each quantity, its mean is approximately equal to the average over sample values. So, we can estimate the characteristic function as

$$\chi_{ij}(\omega_v, \omega_w) = \frac{1}{K} \cdot \sum_{k=1}^{K} \exp(\mathrm{i} \cdot (\omega_x \cdot (v_{ik} - v_{jk}) + \omega_w \cdot (w_{ik} - w_{jk}))),$$

where K is the number of pairs in the available sample.

Analysis of the problem. Let us consider three different models. For these models, we know, for each pair $\omega = (\omega_v, \omega_w)$, the values of the characteristic functions $\chi_{12}(\omega_v, \omega_w)$, $\chi_{23}(\omega_v, \omega_w)$, and $\chi_{13}(\omega_v, \omega_w)$. We want to use this information to estimate the characteristic functions $\chi_1(\omega_v, \omega_w)$, $\chi_2(\omega_v, \omega_w)$, and $\chi_3(\omega_v, \omega_w)$ that describe the desired distributions $\rho_i(\Delta v_i, \Delta w_i)$ of the approximation errors. For this estimation, we can use the following equalities:

$$\chi_{12}(\omega_v, \omega_w) = \chi_1(\omega_v, \omega_w) \cdot \chi_2^*(\omega_v, \omega_w), \tag{2}$$

$$\chi_{13}(\omega_v, \omega_w) = \chi_1(\omega_v, \omega_w) \cdot \chi_3^*(\omega_v, \omega_w), \tag{3}$$

and

$$\chi_{23}(\omega_v, \omega_w) = \chi_2(\omega_v, \omega_w) \cdot \chi_3^*(\omega_v, \omega_w). \tag{4}$$

Based on the known functions $\chi_{ij}(\omega_v, \omega_w)$, we want to reconstruct the functions $\chi_1(\omega_v, \omega_w)$, $\chi_2(\omega_v, \omega_w)$, and $\chi_3(\omega_v, \omega_w)$.

Without losing generality, let us consider the problem of determining the first characteristic function $\chi_1(\omega_v, \omega_w)$. Let us see what we can deduce about $\chi_1(\omega_v, \omega_w)$ based the available information. For this, we need to eliminate the additional variables $\chi_2(\omega_v, \omega_w)$ and $\chi_3(\omega_v, \omega_w)$ from the above system of equations (2)–(4). From the first equation (2), we can express $\chi_2(\omega_v, \omega_w)$ as

$$\chi_2(\omega_v, \omega_w) = \frac{\chi_{12}(\omega_v, \omega_w)}{\chi_1(\omega_v, \omega_w)}.$$

Similarly, from the second equation (3), we can express $\chi_3(\omega_v, \omega_w)$ as

$$\chi_3(\omega_v, \omega_w) = \frac{\chi_{13}(\omega_v, \omega_w)}{\chi_1(\omega_v, \omega_w)}.$$

Substituting the resulting expressions for $\chi_2(\omega_v, \omega_w)$ and $\chi_3(\omega_v, \omega_w)$ into the third equation (4), we conclude that

$$\chi_{23}(\omega_v, \omega_w) = \frac{\chi_{12}(\omega_v, \omega_w)}{\chi_1(\omega_v, \omega_w)} \cdot \frac{\chi_{13}^*(\omega_v, \omega_w)}{\chi_1^*(\omega_v, \omega_w)} = \frac{\chi_{12}(\omega_v, \omega_w) \cdot \chi_{13}^*(\omega_v, \omega_w)}{\chi_1(\omega_v, \omega_w) \cdot \chi_1^*(\omega_v, \omega_w)}.$$

Thus, for $|\chi_1(\omega_v,\omega_w)|^2 = \chi_1(\omega_v,\omega_w)\cdot\chi_1^*(\omega_v,\omega_w)$, we get

$$|\chi_1(\omega_v,\omega_w)|^2 = \frac{\chi_{12}(\omega_v,\omega_w)\cdot\chi_{13}^*(\omega_v,\omega_w)}{\chi_{23}(\omega_v,\omega_w)}. \tag{5}$$

So, by using the observed values, we can find the *absolute value* $|\chi_1(\omega_v,\omega_w)|$ of the desired characteristic function.

Can we reconstruct a function from its absolute value? It is known that for functions of two or more variables, it is almost always possible to reconstruct a function from the absolute value of its Fourier transform – modulo a transformation that maps each function $\rho_i(\Delta v_i,\Delta w_i)$ to its mirror image $\rho_i'(\Delta v_i,\Delta w_i) = \rho_i(-\Delta v_i,-\Delta w_i)$ [11, 12, 13]. Thus, in almost all cases (in some reasonable sense), we can estimate the accuracy $\rho_i(\Delta v_i,\Delta w_i)$ of each model i.

How can we reconstruct a function from its absolute value? There are many methods for reconstructing a pdf from the absolute value of its Fourier transform. The most widely used method takes into account that we want to find a probability distribution $\rho_i(v,w)$ which has the given absolute value of the characteristic function $A_i(\omega_v,\omega_w) = |\chi_i(\omega_v,\omega_w)|$ for the difference; see, e.g., [11]. In precise terms, we want to find a function $\rho_i(v,w)$ which satisfies the following two conditions:

- the first condition is that $\rho_i(v,w)\ge 0$ for all v and w, and
- the second condition is that $|\chi_i(\omega_v,\omega_w)| = A_i(\omega_v,\omega_w)$, where $\chi_i(\omega_v,\omega_w)$ denotes the Fourier transform of the function $\rho_i(v,w)$.

One way to find the unknown function that satisfies two conditions is to use the method of successive projections. In this method, we start with an arbitrary function $\rho_i^{(0)}(v,w)$. On the k-th iteration, we start with the result $\rho_i^{(k-1)}(v,w)$ of the previous iteration, and we do the following:

- first, we project this function $\rho_i^{(k-1)}(v,w)$ onto the set of all functions which satisfy the first condition; to be more precise, among all the functions which satisfy the first condition, we find the function $\rho'(v,w)$ which is the closest to $\rho_i^{(k-1)}(v,w)$;
- then, we project the function $\rho'(v,w)$ onto the set of all functions which satisfy the second condition; to be more precise, among all the functions which satisfy the second condition, we find the function $\rho_i^{(k)}(v,w)$ which is the closest to $\rho'(z)$.

We continue this process until it converges.

As the distance between the two functions $f(v,w)$ and $g(v,w)$ – describing how close they are – it is reasonable to take the natural analog of the Euclidean distance: $d(f,g) \stackrel{\text{def}}{=} \sqrt{\int (f(v,w)-g(v,w))^2\,dv\,dw}$. One can check that for this distance function:

- the closest function in the first part of the iteration is the function $\rho'(v,w) = \max(0,\rho_i^{(k-1)}(v,w))$, and
- on the second part, the function whose Fourier transform is equal to

$$F_i^{(k)}(\omega_x,\omega_y) = \frac{A(\omega_x,\omega_y)}{|F'(\omega_x,\omega_y)|}\cdot F'(\omega_x,\omega_y).$$

Comment. Recently, more efficient methods have been proposed; see, e.g., [3].

We are now ready to present an algorithm. Thus, we arrive at the following algorithms for estimating model accuracy.

3 Resulting Algorithms for Estimating Model Accuracy

What is given. We have several models $i = 1, 2, 3, \ldots$ estimating the values of the same quantities – e.g., density values at different depths and at different spatial locations.

We divide all the quantities estimated by each model into groups, so that within each group, we expect approximately the same accuracy. For each group v, we denote the corresponding quantities by $v_1, \ldots, v_k, \ldots$, where $k = 1, \ldots, K$. In geophysics, k indicates geographical location of the corresponding 3-D point.

Let us denote the i-th model's estimate of the quantity v_i by v_{ik}.

Our objective. Our objective is, for every model i_0 and for every pair of groups (v, w), to estimate the pdf $\rho_{i_0}(\Delta v_{i_0}, \Delta w_{i_0})$ that describes the probability distribution of the corresponding 2-D approximation error $(\Delta v_{i_0 k}, \Delta w_{i_0 k}) = (v_{i_0 k} - v_k, w_{i_0 k} - w_k)$.

Algorithm: Step 0. Let us assume that we are given a model i_0 and a a pair of groups (v, w). To find the desired distribution, we need to select two more models, j_0 and k_0.

Algorithm: Step 1. For each of the three pairs of models (i, j) from the triple (i_0, j_0, k_0), we use the corresponding sample values $(v_{ik} - v_{jk}, w_{ik} - w_{jk})$, $k = 1, \ldots, K$, to estimate the characteristic function $\chi_{ij}(\omega_v, \omega_w)$ of this distribution. This can be done in two possible way:

- One possibility is to use the available sample values to to estimate the corresponding pdf $\rho_{ij}(v, w)$ [14], and then use Fourier Transform to compute the characteristic function.
- Another possibility is directly estimate the characteristic function as

$$\chi_{ij}(\omega_v, \omega_w) = \frac{1}{K} \cdot \sum_{k=1}^{K} \exp(\mathrm{i} \cdot (\omega_x \cdot (v_{ik} - v_{jk}) + \omega_w \cdot (w_{ik} - w_{jk}))).$$

Algorithm: Step 2. On this step, we estimate the absolute value $A_{i_0}(\omega_v, \omega_w) = |\chi_{i_0}(\omega_v, \omega_w)|$ of the desired characteristic function by using formula (5), i.e., as

$$A_{i_0} = \sqrt{\frac{\chi_{i_0 j_0}(\omega_v, \omega_w) \cdot \chi^*_{i_0 k_0}(\omega_v, \omega_w)}{\chi_{j_0 k_0}(\omega_v, \omega_w)}}.$$

Algorithm: Step 3. On this step, we use the known absolute value $A_{i_0}(\omega_v, \omega_w)$ to reconstruct the desired pdf $\rho_{i_0}(\Delta v_{i_0}, \Delta w_{i_0})$.

One way to do it is by using the above-described iterative procedure. Namely, we start with an arbitrary function $\rho^{(0)}_{i_0}(\Delta v_{i_0}, \Delta w_{i_0})$. On the k-th iteration, we start with the function $\rho^{(k-1)}_{i_0}(\Delta v_{i_0}, \Delta w_{i_0})$ obtained on the previous iteration, and we do the following:

- first, we compute $\rho'(\Delta v_{i_0}, \Delta w_{i_0}) = \max(0, \rho^{(k-1)}_{i_0}(\Delta v_{i_0}, \Delta w_{i_0}))$;
- then, we apply Fourier transform to $\rho'(\Delta v_{i_0}, \Delta w_{i_0})$ and get $F'(\omega_v, \omega_w)$;
- after that, we compute $F^{(k)}_{i_0}(\omega_v, \omega_w) = \dfrac{A_{i_0}(\omega_v, \omega_w)}{|F'(\omega_v, \omega_w)|} \cdot F'(\omega_v, \omega_w)$;
- finally, as the next approximation $\rho^{(k)}_{i_0}(\Delta v_{i_0}, \Delta w_{i_0})$, we take the result of applying the inverse Fourier transform to $F^{(k)}_{i_0}(\omega_v, \omega_w)$.

We continue this process until it converges.

Comment. Alternatively, we can use one of the algorithms described in [3].

Conclusion. In almost all cases (in some reasonable sense), we get either the pdf $\rho_{i_0}(\Delta v_{i_0}, \Delta w_{i_0})$ of the desired distribution, or its mirror image function $\rho'_{i_0}(\Delta v_{i_0}, \Delta w_{i_0}) = \rho_{i_0}(-\Delta v_{i_0}, -\Delta w_{i_0})$.

Acknowledgments

This work was supported in part by the National Science Foundation grants HRD-0734825 and HRD-1242122 (Cyber-ShARE Center of Excellence).

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