

A Formalism for Expressing the Probability Density Functions of Interrelated Quantities

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In this paper we address measurement problems involving several quantities that are interrelated by model equations. Available knowledge about some of these quantities is represented by probability density functions (PDFs), which are then propagated through the model in order to obtain the PDFs attributed to the quantities for which nothing is initially known. A formalism for analyzing such models is presented. It comprises the concept of a „base parameterization“, which is used in conjunction with the change-of-variables theorem. The calculation procedure that results from this formalism is described in very general terms. Guidance is given on how to employ it in practice by presenting both an elementary example and a much more involved one.

Keywords: Probability density functions, change of variables, parameterizations, Bayesian statistics.

1. INTRODUCTION

IN A PREVIOUS PAPER [1] we presented the main elements of a Bayesian procedure for assigning state of knowledge probability density functions (PDFs) to metrological quantities having essentially unique true values. In accordance with the prevalent view advocated in well-known international documents [2], [3], the mean and standard deviation of any such PDF are, respectively, taken as the best estimate and associated standard uncertainty of the quantity to which the distribution pertains, and the area under the PDF over a given interval is regarded as the probability of finding the true value of the quantity within that interval, given the available information.

For some of the quantities appearing in the model of measurement this information may be in the form of measurement data, for others some type of knowledge may be at hand (e.g., that their true values are known to be contained within prescribed intervals) and for still others there may be no information at all. The assignment of PDFs to those quantities about which something is known follows in general from tools such as Bayes' theorem [3, subclause 6.2] and the „Principle of Maximum Entropy“ [3, subclause 6.3], but expert's judgment is also needed, e.g., to identify discordant observations [4]. These PDFs are then propagated through the measurement model that links the corresponding quantities with those for which there is no knowledge. In this way, the PDFs for the latter quantities are obtained.

The procedure explained in [1] relies on the use of Dirac delta functions for effecting the propagation of probability distributions analytically [3, subclause 5.2]. Though the delta function is a very powerful concept, the rules for its manipulation may not be familiar to some metrologists. For this reason, in this paper we employ an alternative but entirely equivalent treatment based on the more widely known change-of-variables theorem [5]-[7]. To this end we provide a formal definition of the concept of „parameterization“, which is common in Bayesian statistics

[8],[9] but which in metrology has hitherto been used rather intuitively [10]. Two examples illustrate the application of the formalism.

2. STATEMENT OF THE PROBLEM

Consider a set of quantities $\mathbf{X} = \{X_1, \dots, X_m\}$ interrelated through a consistent system of equations of the form

$$F_i(\mathbf{X}_i) = 0, \quad i=1, \dots, n < m, \quad (1)$$

where the \mathbf{X}_i are subsets of \mathbf{X} , none of which is disjoint with all others, such that their union is equal to \mathbf{X} . It is assumed that none of the quantities is perfectly known and that their true values are unique. The goal is to obtain the PDF for the quantities of interest (the measurands) taking into account the existing information I about some of the quantities in the system (1), which is hereafter symbolized by the letter M , for „model“.

3. ANALYSIS

To analyze this problem it is useful to start from the concept of parameterization. In the present context, a parameterization is defined as a set $\mathbf{X}_p = \{X_{p1}, \dots, X_{pl}\}$, where $l = m - n$, such that the model (1) allows all quantities in the complement of the parameterization to be expressed as explicit or implicit functions of some or all of the quantities it contains. There can be no more than $m!/(n! \times l!)$ parameterizations. For example, in the model $X_1 = \sqrt{X_2}$, $X_3 = \ln X_4$, $X_5 = X_1 X_3$, the set $\{X_1, X_3\}$ is a parameterization but the set $\{X_1, X_2\}$ is not, because it is not possible to express X_3, X_4 and X_5 as functions of X_1 and X_2 .

Three situations arise depending on the number of quantities to which the information I refers. The first occurs when there exists no parameterization for which information on all its quantities is provided. It is then not possible to obtain the PDF for at least one of the quantities about which there is no knowledge. The proof is simple. Suppose that the

available information refers to less than l quantities and that it is precise, so that these quantities become known constants. The model (1) then turns into a „regular” under-determined system of equations, from which no unique values of all unknowns can be found. This is true *a fortiori* if the information is imprecise (i.e., if for less than l quantities only probability distributions rather than their exact values are given).

The second situation is frequently encountered in metrological practice. It occurs when there is information on just the l quantities of a certain parameterization $\mathbf{X}_b = \{X_{b1}, \dots, X_{bl}\}$, henceforth called the *base parameterization*, such that their joint PDF, denoted by $f_b(\xi_b | I)$, is either given or can be constructed by duly processing the available information (as explained, e.g., in section 3 of [1]). Here, the symbol ξ_b designates the set of variables that represent the possible values of the quantities \mathbf{X}_b . In this case, the PDF for the quantities in any other parameterization \mathbf{X}_p can be obtained from the change-of-variables theorem

$$f_p(\xi_p | I, M) = |J_{pb}| \times f_b[\mathbf{G}_b(\xi_p) | I], \quad (2)$$

where the l functions \mathbf{G}_b are defined by

$$X_{bk} = G_{bk}(\mathbf{X}_p), \quad k=1, \dots, l \quad (3)$$

and

$$J_{pb} = \left| \frac{\partial \mathbf{G}_b(\xi_p)}{\partial \xi_p} \right| \quad (4)$$

is the determinant of the Jacobian matrix of the transformation. The symbols standing for „given I ” and „given I and M ” in the arguments of the PDFs have been added for clarity; they may be dropped in practice, as in section 5 below. The functions \mathbf{G}_b (which need not be explicit) are obtained from the model (1); they are assumed to be differentiable at least once within the domains of interest of the quantities in the base parameterization. Equation (2) needs to be modified if the mapping $\mathbf{X}_b = \mathbf{G}_b(\mathbf{X}_p)$ is not one-to-one in all quantities, but this brings about only a formal complication that is of no interest to our exposition. Note that the intersection of \mathbf{X}_b and \mathbf{X}_p may or may not be empty.

In this second situation the l quantities forming the base parameterization are frequently called *input* quantities. Similarly, the n quantities completely unknown originally are called *output* quantities, some or all of which may be the measurands. Their joint PDF may be obtained by including the output quantities in the above-mentioned parameterization \mathbf{X}_p . Provided the latter also contains quantities that are not measurands, subsequent integration of the PDF $f_p(\xi_p | I, M)$ over these quantities is required.

Finally, in the third situation information exists on more than l quantities. It is easily seen that in this case one can use the change-of-variables theorem with different choices of \mathbf{X}_b , leading to different PDFs $f_p(\xi_p | I, M)$ for any fixed parameterization \mathbf{X}_p . This means that there is more than enough information. Either some of it must be discarded in order to keep just a single base parameterization (and consequently, a single PDF for any parameterization \mathbf{X}_p) or

some compromise must be reached if all information is to be retained. (The same may happen in case information is provided on all quantities of a set of size l that is not a parameterization. For example, in the model $X_1 = \sqrt{X_2}$, $X_3 = \ln X_4$, $X_5 = X_1 X_3$, providing information on both X_1 and X_2 would be more than enough with respect to these two quantities, but still not sufficient to establish the PDFs for X_3 , X_4 and X_5 . So this would, in fact, represent a situation of the first type.) The case of more than enough information is of interest in metrology, but it will not be addressed in the examples below.

4. ONE OUTPUT QUANTITY

The GUM [2] and its Supplement 1 [3] address explicit measurement models of the form

$$X_m = F(\mathbf{X}_b), \quad (5)$$

where the single measurand X_m is initially completely unknown and the information I pertains only to the input quantities in the base parameterization $\mathbf{X}_b = \{X_1, \dots, X_{m-1}\}$. These models are easily handled with the present formalism. Indeed, by setting, e.g., $\mathbf{X}_p = \{X_1, \dots, X_{m-2}, X_m\}$, (5) may be (partially) inverted according to

$$X_i = G_i(X_i), \quad i = 1, \dots, m-2, \quad (6)$$

$$X_{m-1} = G_{m-1}(X_1, \dots, X_{m-2}, X_m). \quad (7)$$

Then (2) yields

$$f_p(\xi_p | I, M) = \left| \frac{\partial \mathbf{G}_{m-1}}{\partial \xi_m} \right| \times f_b(\xi_1, \dots, \xi_{m-2}, \mathbf{G}_{m-1} | I). \quad (8)$$

Similar equations are obtained by choosing other parameterizations \mathbf{X}_p that contain X_m .

A. Example

As an example, suppose the model is

$$X_3 = \frac{X_2}{X_1} \quad (9)$$

and let the base parameterization be $\mathbf{X}_b = \{X_1, X_2\}$. We then have, with $\mathbf{X}_p = \{X_1, X_3\}$,

$$f_{1,3}(\xi_1, \xi_3 | I, M) = |\xi_1| f_{1,2}(\xi_1, \xi_1 \xi_3 | I) \quad (10)$$

or, with $\mathbf{X}_p = \{X_2, X_3\}$,

$$f_{2,3}(\xi_2, \xi_3 | I, M) = \left| \frac{\xi_2}{\xi_3^2} \right| f_{1,2} \left(\frac{\xi_2}{\xi_3}, \xi_2 | I \right). \quad (11)$$

The PDF for the measurand X_3 can now be obtained by marginalizing either of these two equations. Seemingly different but mathematically identical expressions for $f_3(\xi_3 | I, M)$ are obtained.

Incidentally, it is easily shown that by integrating (10) and (11) with respect to ξ_3 one gets $f_1(\xi_1|I, M) = f_1(\xi_1|I)$ and $f_2(\xi_2|I, M) = f_2(\xi_2|I)$, meaning that the model does not increase the state of knowledge about those quantities belonging to the base parameterization.

B. Numerical illustration

To illustrate, suppose (as in [10]) that X_3 is the length of a gauge block at a reference temperature T_0 , that X_2 is its length at temperature T and that X_1 is equal to $1 + \alpha(T - T_0)$, where α is the linear thermal expansion coefficient. The information I consists of knowing that α is contained within an interval of width w centered at the value a , and that the mean of N direct measurements of X_2 is x_2 with standard deviation s_2 . For simplicity, assume that T is measured with negligible uncertainty, so that it becomes perfectly known.

Since the information about X_1 is independent from that about X_2 , the joint PDF for these two quantities is equal to the product of their individual PDFs, $f_1(\xi_1|I)$ and $f_2(\xi_2|I)$. The former is a rectangular distribution of width $w(T - T_0)$ centered at $1 + \alpha(T - T_0)$ [3, paragraph 6.4.2] while the latter may be taken as a t -distribution with location parameter x_2 , scale parameter s_2/\sqrt{N} and $N - 1$ degrees of freedom [3, paragraph 6.4.9]. Fig.1. shows the PDF for X_3 that results from the numerical integration of $f_{1,3}(\xi_1, \xi_3|I, M)$ over ξ_1 , or of $f_{2,3}(\xi_2, \xi_3|I, M)$ over ξ_2 , when $T - T_0 = 5$ K, $a = 12 \times 10^{-6}$ K $^{-1}$, $w = 10^{-6}$ K $^{-1}$, $N = 5$, $x_2 = 50.0030$ mm and $s_2 = 0.0016$ mm. The mean and standard deviation of this PDF are $x_3 = 50.0000$ mm and $u_3 = 0.0010$ mm, respectively.

It is worth mentioning that the recommendation in [3] about the use of a t -distribution follows from Bayes' theorem and the assumption that the data are generated in accordance with a Gaussian random process of unknown mean and variance. The latter then becomes a further quantity that does not enter into any parameterization because it does not appear in the measurement model. This is in contrast to the concept of parameterization as used in [10].

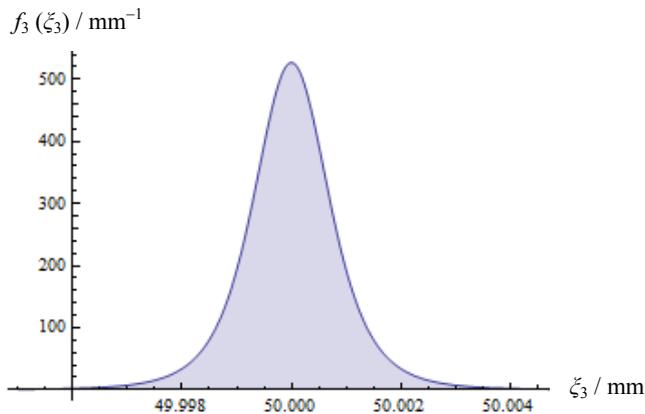


Fig.1. Probability density function for the length of a gauge block $X_3 = X_2/X_1$ given information about X_2 and X_1 .

5. EXAMPLE: MEASUREMENT OF FLOW RATE

An analytically more complicated example, but conceptually just as simple, is similar to the one considered in subsection 4.3 of [1]. The model consists of the Darcy-Weisbach and Colebrook-White equations, which are commonly used for determining pipe-flow resistance in fully developed, steady state and incompressible flow within a pipe running full, see e.g., [11]. Consider a straight segment of a circular pipe of length L and diameter D inside which a fluid moves with average (bulk) velocity V . The pressure drop between the two ends of the segment is given by

$$\Delta p = \lambda \frac{\rho V^2 L}{2D}, \quad (12)$$

where λ is the dimensionless Darcy-Weisbach friction factor and ρ is the density of the fluid. The friction factor depends on the flow regime and on the material of the pipe through its internal roughness ε . In case the Reynolds number $Re = VD\rho/\mu$ is greater than about 4000, where μ is the dynamic viscosity of the fluid, the flow is turbulent. One then obtains the friction factor from the (implicit) Colebrook-White equation

$$\frac{1}{\sqrt{\lambda}} = -2 \log_{10} \left(\frac{2.51}{Re \sqrt{\lambda}} + \frac{\varepsilon}{3.7D} \right). \quad (13)$$

Normally, these two equations are used for establishing the power needed by the prime mover to overcome the pressure loss in the design stage of a piping system. In this application, if the properties of the fluid are regarded as perfectly known, the base parameterization is the set $\{V, D, \varepsilon\}$ and the measurand is the pressure drop along a unit length of pipe. But if the system is already in place, the same equations provide a means for measuring the volumetric flow rate Q through the duct. Thus, the mass flow rate $\dot{m} = \rho Q$ can be obtained in an alternative manner to direct measurement, e.g., by a vortex mass flowmeter [12]. The volumetric flow rate is given by

$$Q = VA, \quad (14)$$

where $A = \pi D^2/4$ is the pipe's cross-section. In this situation the base parameterization is the set $\{L, D, \Delta p, \varepsilon\}$.

Table 1. Equivalence of symbols for the quantities in the flow rate example.

Quantity	New symbol
L	X_1
D	X_2
V	X_3
λ	X_4
Δp	X_5
ε	X_6
Q	X_7

Let us analyze this second scenario where, for simplicity, the symbols for the relevant quantities are redefined as shown in Table 1. The model then becomes

$$X_5 = a \frac{X_1 X_3^2 X_4}{X_2}, \quad (15)$$

$$\frac{1}{\sqrt{X_4}} = -2 \log_{10} \left(\frac{b}{X_2 X_3 \sqrt{X_4}} + \frac{X_6}{c X_2} \right), \quad (16)$$

and

$$X_7 = d X_2^2 X_3, \quad (17)$$

where $a = \rho/2$, $b = 2.51\mu/\rho$, $c = 3.7$ and $d = \pi/4$. (The fluid's properties are regarded as perfectly known.)

Let the base parameterization be $\mathbf{X}_b = \{X_1, X_2, X_3, X_6\}$. Several parameterizations can now be chosen, as long as they contain the measurand X_7 . For example, choosing $\mathbf{X}_p = \{X_1, X_2, X_4, X_7\}$ gives

$$f_{1,2,4,7}(\xi_1, \xi_2, \xi_4, \xi_7) = J \times f_{1,2,5,6}(\xi_1, \xi_2, G_5, G_6), \quad (18)$$

where

$$G_5 = \frac{a}{d^2} \frac{\xi_1 \xi_4 \xi_7^2}{\xi_2^5}, \quad (19)$$

$$G_6 = c \xi_2 \left(10^{-1/(2\sqrt{\xi_4})} - \frac{bd \xi_2}{\sqrt{\xi_4 \xi_7}} \right), \quad (20)$$

and

$$J = \left| \frac{\partial G_5}{\partial \xi_4} \frac{\partial G_6}{\partial \xi_7} - \frac{\partial G_5}{\partial \xi_7} \frac{\partial G_6}{\partial \xi_4} \right| = \frac{ac \ln 10}{2d^2} \frac{\xi_1 \xi_7}{\xi_2^4 \sqrt{\xi_4}} 10^{-1/(2\sqrt{\xi_4})}. \quad (21)$$

A. Available information

Suppose estimates x_2 for the diameter and x_6 for the roughness of a pipe are available, with associated standard uncertainties u_2 and u_6 , respectively. Inside the pipe flows a liquid whose density and viscosity are known with negligible uncertainty. The pressure drop along a straight part of the duct is measured, giving the estimate x_5 with standard uncertainty u_5 . Finally, the distance x_1 between the pressure gauges is also measured with standard uncertainty u_1 . All these estimates are obtained independently of one another. According to the „Principle of Maximum Entropy“, it is then reasonable to assign univariate Gaussian PDFs to X_1 , X_2 , X_5 and X_6 . We restrict the calculation to the case where the ratios x_i/u_i are reasonably large, say greater than three. This enables us to formally extend the support of all four quantities to the whole real line [13]. We then have

$$f_{1,2,4,7}(\xi_1, \xi_2, \xi_4, \xi_7) = J \times f_1(\xi_1) f_2(\xi_2) f_5(G_5) f_6(G_6), \quad (22)$$

where

$$f_i(\xi_i) = \frac{1}{\sqrt{2\pi}u_i} \exp\left(-\frac{1}{2} \frac{(\xi_i - x_i)^2}{u_i^2}\right), \quad i = 1, 2, \quad (23)$$

$$f_i(G_i) = \frac{1}{\sqrt{2\pi}u_i} \exp\left(-\frac{1}{2} \frac{(G_i - x_i)^2}{u_i^2}\right), \quad i = 5, 6 \quad (24)$$

and where J , G_5 and G_6 are as above.

In these circumstances, integration over ξ_1 can be performed analytically. The result is

$$f_{2,4,7}(\xi_2, \xi_4, \xi_7) = H \times K \times f_2(\xi_2) f_6(G_6), \quad (25)$$

where

$$H = \frac{ac \ln 10}{2d^2} \times \frac{\xi_7 10^{-1/(2\sqrt{\xi_4})}}{\xi_2^4 \sqrt{\xi_4}}, \quad (26)$$

$$K = \exp\left(-\frac{1}{2} \frac{(k x_1 - x_5)^2}{k^2 u_1^2 + u_5^2}\right) \times \frac{u_5^2 x_1 + k u_1^2 x_5}{\sqrt{2\pi(k^2 u_1^2 + u_5^2)^{3/2}}}, \quad (27)$$

and

$$k = \frac{a}{d^2} \frac{\xi_4 \xi_7^2}{\xi_2^5}. \quad (28)$$

However, the integrations over ξ_2 and ξ_4 to obtain the marginal PDF $f_7(\xi_7)$ for the measurand X_7 have to be carried out numerically. If desired, the PDF $f_4(\xi_4)$ for the friction factor X_4 can be obtained likewise.

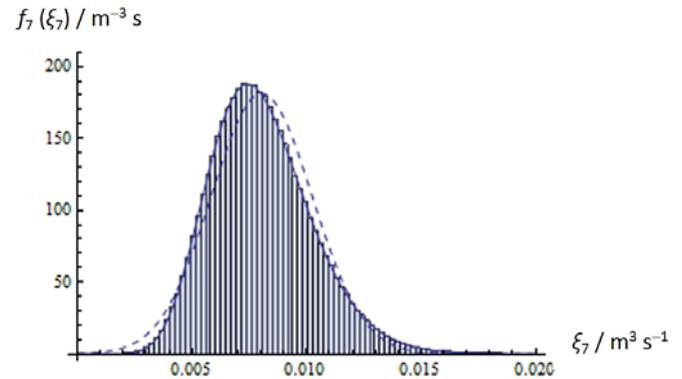


Fig.2. The solid line is the PDF for the volumetric flow rate X_7 of water in a pipe. The histogram is its numerical approximation computed by Monte Carlo integration. The dashed line is a Gaussian PDF with the same mean and standard deviation.

B. Results

As an illustration, suppose the fluid is water at 22 °C, for which $\rho = 998 \text{ kg/m}^3$ and $\mu = 959 \times 10^{-6} \text{ Pa s}$, flowing inside a pipe of diameter $x_2 = 10 \text{ cm}$ and roughness $x_6 = 150 \mu\text{m}$. The pressure drop over the distance $x_1 = 10 \text{ m}$ is found to be $x_5 = 1180 \text{ Pa}$. Assume that the associated standard uncertainties are equal to one tenth of the corresponding estimates. The PDF $f_7(\xi_7)$ is depicted by the solid line in Fig.2. Its mean is $x_7 = 0.0080 \text{ m}^3/\text{s}$ and its standard deviation is $u_7 = 0.0022 \text{ m}^3/\text{s}$. Its skewness reflects the strong nonlinearity of the model (15)-(17). For comparison, the dashed line in Fig.2. shows a Gaussian PDF with the same mean and standard deviation.

The estimate x_7 allows calculating the velocity as $x_3 = 4 x_7 / (\pi x_2^2) = 1.02$ m/s, giving a Reynolds number greater than 10^5 . Therefore, the flow is fully turbulent, so the use of (16) is justified.

C. Integration by Monte Carlo

The Monte Carlo integration method proposed in Supplements 1 and 2 to the GUM [3],[14] can also be employed for finding a numerical approximation to $f_7(\xi_7)$. This method is entirely equivalent to applying the change-of-variables theorem. It is to be preferred, however, in instances that are too difficult to be addressed by analytical or numerical integration, e.g., if the number of variables is too large. In the present case the Monte Carlo method proceeds by sampling values ξ_1, ξ_2, ξ_3 and ξ_6 from the corresponding PDFs. The values

$$\xi_4 = \left[-2 \log_{10} \left(\frac{b \sqrt{a \xi_1}}{\xi_2 \sqrt{\xi_2 \xi_5}} + \frac{\xi_6}{c \xi_2} \right) \right]^{-2}, \quad (29)$$

$$\xi_3 = \left(\frac{\xi_2 \xi_5}{a \xi_1 \xi_4} \right)^{1/2}, \quad (30)$$

and

$$\xi_7 = d \xi_2^2 \xi_3 \quad (31)$$

are then computed and the process is repeated a large number of times. The relative frequency of the ξ_7 values obtained after one million repetitions is shown by the histogram in Fig.2., confirming that it is an excellent numerical approximation to the PDF $f_7(\xi_7)$.

One advantage of the Monte Carlo method is that the numerical approximations to the PDFs for X_3 and X_4 are immediately available as a by-product. They allow computing the means, standard deviations and correlation coefficients shown in Table 2.

Table 2. Means, standard deviations and (dimensionless) correlation coefficients computed by Monte Carlo integration.

Quantity	Symbol	Mean	Standard deviation	Correlation coefficients		
				X_3	X_4	X_7
Velocity / m s ⁻¹	X_3	1.01	0.10	1.0	-0.71	0.83
Friction factor	X_4	0.023 71	0.000 88	-0.71	1.0	-0.84
Flow rate / m ³ s ⁻¹	X_7	0.008	0.002 2	0.83	-0.84	1.0

5. CONCLUSION

A formalism for expressing the PDFs for interrelated quantities has been presented in general terms. The aim has been to identify clearly the different situations that may arise and to provide guidance by way of examples on how to employ the technique in practice. It relies on the concept of „base parameterization“, defined as a set of quantities constituting a parameterization for which information is provided so that its joint PDF can be constructed. The size of this set is equal to the total number of quantities minus the number of equations through which they are related. If information on a greater number of quantities exists, the problem cannot be solved uniquely. In case there is information on fewer quantities, one remains ignorant about at least one of the quantities that were initially completely unknown.

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