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Uncertainty inherent in empirical fitting of distributions to experimental data

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Abstract. Treatment of experimental data often entails fitting frequency functions, in order to draw inferences on the population underlying the sample at hand, and/or identify plausible mechanistic models. Several families of functions are currently resorted to, providing a broad range of forms; an overview is given in the light of historical developments, and some issues in identification and fitting procedure are considered. But for the case of fairly large, well behaved data sets, empirical identification of underlying distribution among a number of plausible candidates may turn out to be somehow arbitrary, entailing a substantial uncertainty component. A pragmatic approach to estimation of an approximate confidence region is proposed, based upon identification of a representative subset of distributions marginally compatible at a given level with the data at hand. A comprehensive confidence region is defined by the envelope of the subset of distributions considered, and indications are given to allow first order estimation of uncertainty component inherent in empirical distribution fitting.

Keywords: Uncertainty; fitting distribution; empirical distribution; confidence region

1 Introduction

In experimental research established theoretical models and/or accumulated experience may be lacking, implying that inferences concerning underlying phenomena must be drawn mainly in terms of the data base at hand. When theoretical distributions fail to fit data properly, owing to their inherent lack of flexibility, empirical distributions capable of accommodating a comprehensive range of forms are conveniently resorted to. Identification of distributions underlying data may be a critical step in the treatment of experimental values, e.g. when dealing with unusual observations. A set of times recorded between observations of neutrinos from a supernova [1] exhibits an upper extreme value, which might well be deemed an outlier according to several established criteria [2,3]. That value however does not appear exceptional at all – the lower extreme might then appear questionable, see Figure 1 – if log times are considered, a sensible option for such data, and in other instances as well.

When fitting distributions to experimental data, uncertainty pertaining to estimates of parameters owing to sampling variation is routinely taken into account; if data are well behaved, sample size is large and fairly conservative levels are considered, a confidence zone may be mapped readily in terms of basic order statistics [4,5]. Otherwise, realistic evaluation of uncertainty concerning inferences may call for closer scrutiny, taking explicitly into account an often overlooked uncertainty component, inherent in selecting – on less than cogent evidence – out of a set of plausible candidates a distribution, and then assuming it to be the one underlying data at hand without further ado. Usually, the smaller the sample size the more comfortably data sit on the friendly rump of normal distribution, allowing straightforward, easy treatment. Those data however may just as well be also fitted by several other distributions, which might be assumed as describing the underlying population. While these distributions may all approximate data rather closely, and fall within a narrow confidence band within the range of experimental data, beyond that range no such agreement may be expected, if only since neither bounded nor unbounded frequency functions may be ruled out in the light of available evidence. Tail regions are however crucial when such instances as estimation of life of critical components and systems, or evaluation of "safe" thresholds of exposure to life threatening agents are concerned, where underestimation of uncertainty may entail catastrophic effects.

Some basic questions must be then squarely addressed, namely how to find out how much either tail may wag and still be deemed consistent at a given level with the data set at hand, and how to define a confidence region taking into account such tail wagging. A straightforward solution is proposed, based upon identifying, out of a comprehensive family of empirical distributions, a representative subset of forms and related parameters, marginally compatible at a given level with the sample at hand. The envelope of such a subset of frequency functions is then deemed to represent a confidence region, providing information relevant to evaluation of Type A uncertainty [6,7]. The concept

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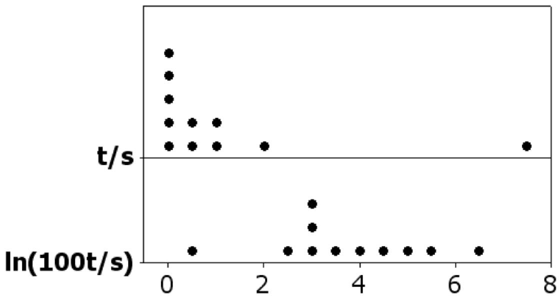

Fig. 1. Dotplot of elapsed times (in seconds) and their logarithms; in the first case the upper extreme may be tagged as outlier, in the second possibly the lower one.

proposed fits within the framework of a seldom challenged hypothesis, namely that should a distribution appear to fit well enough a sample, inferences on parent population may be drawn from that distribution [8]. Given a representative set of distributions, all of which may be legitimately assumed as underlying the sample at hand at a given confidence level, it makes sense to submit that the set of those distributions – instead of a single one somehow arbitrarily selected – should be taken into account for a realistic evaluation of uncertainty of inferences drawn in terms of that sample.

2 Empirical distributions

The notion of statistical regularity, described by laws governing apparent chaos, gained broad acceptance by the middle of the nineteenth century, along with a widely shared belief that normal distribution was the universal law of most if not all phenomena [9]. Examples such as measurements of 5738 Scottish soldiers were deemed to prove that deviations from normality might be due only to inadequacy of samples, errors and chance disturbances, if not outright fraud [10, 11]. It became however apparent that some samples did not lend themselves to description in terms of normal distribution, even to a first approximation, as skewed data sets started begging for appropriate models. Some absurdities implied by abusive use of normal distribution were exposed by Galton [12], who proposed a first solution in terms of lognormal transformation, and prompted McAlister [13] to provide the basic mathematical developments required. However lognormal distribution, although more adaptable than normal and indeed often worthy of wider use [14], just as gamma, exponential and other theoretical distribution, proves unable to accommodate a sizable number of data sets, only a fraction of which may be fitted by slightly more flexible models such as e.g. beta distribution [15]. Towards the end of the nineteenth century, research in biometry stimulated development of families of empirical distributions, capable of fitting a broad range of unimodal data sets by covering a comprehensive range of combinations of parameters related to the first four moments. A general solution, prompted by the search of models for size of crab bodies [16], was first provided and further on thoroughly

Table 1. Correspondence between some Pearson's distributions and several theoretical ones.

Pearson's type	Theoretical distribution
I	Beta (limit uniform), Normal
II	Beta (symmetric), Normal
III	Chi-squared, Exponential, Gamma, Normal
IV	Cauchy, Normal
V	Inverse Chi-squared, Inverse Gamma, Normal
VI	Beta prime, Fisher's F, Lognormal, Normal
VII	Student's t

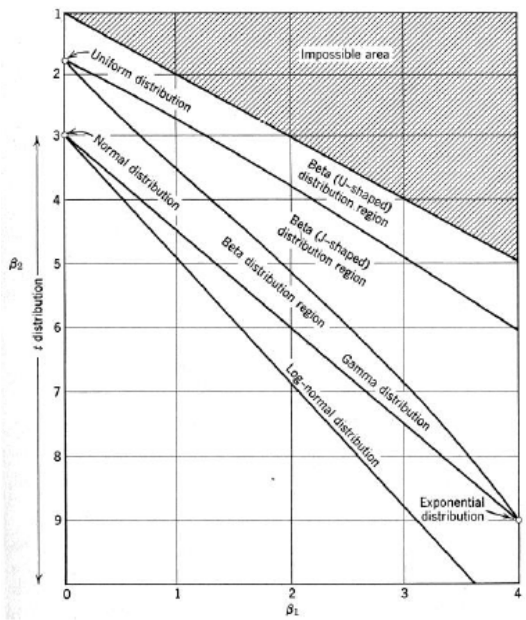

Fig. 2. Regions on $\beta_1 - \beta_2$ plane pertaining to some theoretical distributions [22].

developed by Pearson [17, 18]. The basic concept apparently originated from considerations on the derivative of log normal density, and a recurrence relation for the probability mass function of hypergeometric distribution [19]. In every family of the dozen odd making up Pearson's system, the density $f(x)$ may be generated as a solution of the differential equation.

$$\frac{df(x)}{dx} = \frac{(x - \varphi_3) f(x)}{\varphi_0 + \varphi_1 x + \varphi_2 x^2}. \quad (1)$$

By proper selection of the four parameters $\varphi_0 - \varphi_3$ a broad range of forms is obtained, see Table 1, covering normal (limit of type I through VI) and other theoretical distributions [20].

Pearson's distributions first provided a comprehensive coverage of the skewness – kurtosis plane [21, 22], where a plot of sample parameters suggests tentatively which type(s) may cater for a given case, Figure 2.

While the laborious fitting procedure by the method of moments, made somewhat easier by ad hoc routines and tables [23], still finds some applications [24], Pearson's distributions are nowadays seldom resorted to, owing to later introduction of more user friendly families.

Among a system of several other frequency functions, Burr Type XII, a right-skewed continuous probability distribution – used in econometrics, insurance and related fields [25, 26] – is defined in terms of parameters c and k by its cdf

$$F(x) = 1 - \frac{1}{(1 + x^c)^k}, x \geqslant 0 \tag{2}$$

where c and k are nonnegative real numbers. The pdf

$$f(x) = \frac{ckx^{c-1}}{(1 + x^c)^{k+1}}, x \geqslant 0 \tag{3}$$

is unimodal, inverse J-shaped if $c = 1$, less skewed if $c > 1$. Coverage of $\beta_1 - \beta_2$ plane is limited to a fairly narrow wedge (apex normal) bounded by gamma and lognormal distributions [27].

The introduction of a method such that the transformed variables follow a normal distribution, originally defined as the method of translation [28], paved the way towards major advances; a widely used family of distributions was developed along those lines [29]. Johnson's empirical distributions are based upon a transformation having the general form.

$$z = \gamma + \eta k_i(x; \lambda, \varepsilon) \tag{4}$$

where z is a standard normal variable, γ and η are shape parameters, λ is a scale parameter, ε is a location parameter, and k is an arbitrary function. The latter may take three alternate forms, leading to as many Johnson's families, namely S_U (unbounded)

$$k_1(x; \lambda, \varepsilon) = \ln\left[\frac{x - \varepsilon}{\lambda + \varepsilon - x}\right] \tag{5}$$

S_B (bounded on ε, $\varepsilon + \lambda$)

$$k_2(x; \lambda, \varepsilon) = \sinh^{-1}\left[\frac{\mathrm{x} - \varepsilon}{\lambda}\right] \tag{6}$$

and S_L (log-normal)

$$k_3(x; \lambda, \varepsilon) = \ln\left[\frac{\mathrm{x} - \varepsilon}{\lambda}\right]. \tag{7}$$

Advantages of Johnson's system for simulation input modeling over beta, normal and triangular distributions were discussed by DeBrota et al. [30]. Correspondences shown in Table 2 between some theoretical, Pearson's and Johnson's distributions, underline how introduction of the latter brought about remarkable simplifications.

Fitting a Johnson distribution to data involves selecting a proper family, and obtaining estimates of the four parameters $\gamma, \eta, \varepsilon, \lambda$, assessed as a rule in terms of sample estimates of mean μ, standard error σ, skewness β_1 and kurtosis β_2. Lacking closed-form expressions for parameter estimates, good approximations may be obtained

Table 2. Correspondence between theoretical, Pearson's and Johnson's distributions.

Johnson's type	Pearson's type	Theoretical distribution
S_B	I, II, VII, VIII, IX, XII	Beta, Chi-squared, Exponential, Gamma, Lognormal, Normal, Uniform
S_L	III, VII, X	Lognormal, Normal
S_U	IV, V, VI, VII, XI	Fisher's F, Lognormal, Normal, Student's t

using iterative procedures [31], made substantially easier by dedicated software packages [32, 33]. Direct approaches based on symmetry considerations were also developed [34], aimed at overcoming some of the difficulties due to the large variance of estimates of third and fourth order moments, and their substantial bias particularly for small samples [35, 36]. Three typical methods are used, namely based upon selected percentile points, evaluation of moments, and maximum likelihood, mentioned in order of ease of application. But for the first one, fitting may entail numerical difficulties, liable sometimes to prevent convergence.

Since a Johnson S_B variate ranges between ε and $\varepsilon + \lambda$, when both end points are known only estimation of γ and η is required, readily performed in terms of selected percentile points. Equating two percentiles from the sample at hand – obtained by ranking and interpolation as required – with those corresponding for normal distribution lead to equations in terms of α 100th and $(1 - \alpha)$ 100th percentiles of sample and of standard normal distribution respectively, which may be solved in a straightforward way. When only the lower bound ε is known, an additional equation is obtained by matching data median with that of standard normal distribution, that is zero. Fitting is somehow more laborious when neither end points are known, a less common occurrence in practice.

Introduction of Lambda symmetric distribution [37], and its later generalization to cover a wide range of forms, marked a further step towards providing handy empirical models. The Tukey-Lambda density function is computed numerically, lacking a closed form. Since its general form may be expressed in terms of the standard normal distribution, the Tukey-Lambda distribution is defined in terms of its quantile or percentile function as:

$$Q(x; \lambda) = \frac{x^\lambda - (1 - x)^\lambda}{\lambda}, \qquad 0 \leqslant x \leqslant 1. \tag{8}$$

The shape parameter λ may be identified exploiting e.g. the probability plot correlation coefficient plot, a graphical technique evaluating the capability of describing appropriately the data set at hand by families of distributions [38]. A number of theoretical distributions, namely Cauchy, logistic, normal, U-shaped and uniform, are obtained (exactly or approximately) when λ is taken, respectively, equal to -1, 0, 0.14, 0.5, 1. As with other probability distributions, empirical data fitting entails also introducing location and scale parameters [39, 40].

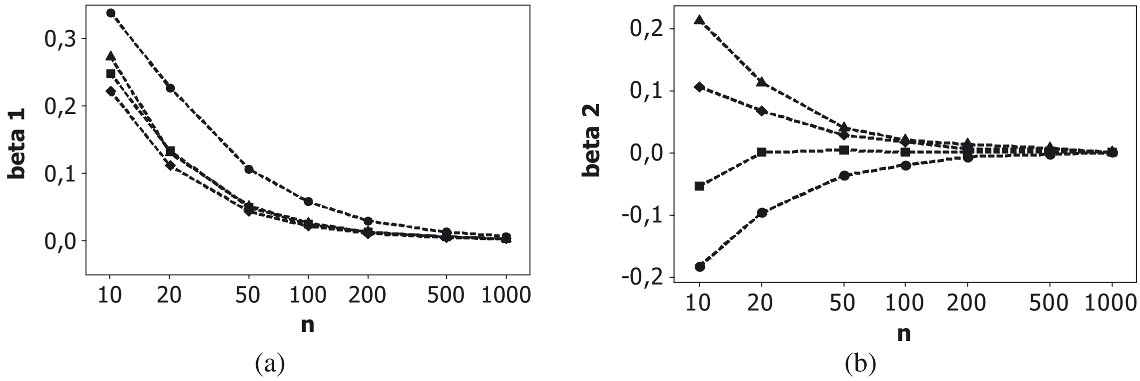

Fig. 3. Average bias in numerical estimates of β_1 (a) and β_2 (b) versus sample size n for standard normal (circles), triangular (squares), uniform (diamonds) and U-shaped (triangles) distribution.

Generalization of Tukey's Lambda distribution with three or four parameters provides a versatile algorithm for generating values of unimodal random variables [41, 42]. Multimodal distributions may be taken care of with the usual device of sampling from several unimodal distributions. The generalized lambda distribution (GLD) family is given in terms of its quantile or percentile function

$$Q(x) = Q(x; \lambda_1, \lambda_2, \lambda_3, \lambda_4) = \lambda_1 + \frac{x^{\lambda_3} - (1-x)^{\lambda_4}}{\lambda_2}, \qquad 0 \leqslant x \leqslant 1 \qquad (9)$$

where x is a uniform random variable. Skewness, peakedness and variance are determined by λ_3, λ_4 and λ_2, respectively, while the mean is shifted as required by λ_1; the latter is however equal to the expected value only in case of symmetry, $\lambda_3 = \lambda_4$. Some conditions must be however fulfilled by the set of parameters in order to specify a valid distribution, such as:

$$\frac{\lambda_2}{\lambda_3 x^{\lambda_3} + \lambda_4 (1-x)^{\lambda_4 - 1}} \geqslant 0 \ . \qquad (10)$$

Accordingly, GLD is valid only in some regions of the $\lambda_3 - \lambda_4$ plane. Applications cover quite a broad range, extending to process capability evaluation [43]. Dedicated software tools made short shrift of the laborious fitting chores typical only a generation ago [23]. Techniques for non-parametric estimation of functions such as kernel smoothing should be mentioned too, which may effectively deal also with multimodal data sets [44].

3 Management of uncertainty

Realistic evaluation of uncertainty pertaining to inferences drawn from a distribution, assumed to be underlying a set of experimental data, and identified in terms of that data set, should take into account the uncertainty component inherent to empirical identification of form, besides the errors in estimates of parameters routinely computed. Uncertainty pertaining to identification of form, largest when no information is available besides the data set at hand, may however whittle down or even vanish should substantial relevant information become available, theoretical and/or derived from accumulated experience.

If the form of an empirical function, assumed to approximate the unknown distribution underlying a given data set, is tentatively identified in terms of the sample estimates of average, standard deviation, asymmetry and peakedness, a joint confidence region for these parameters in a four dimensional space (three in case of symmetry) may provide information on the relevant uncertainty. Individual confidence intervals are readily obtained for average, thanks to central limit theorem, and for standard deviation, albeit less accurately; numerical methods such as bootstrap may be resorted to for skewness and kurtosis, taking into account if need be corrections for bias, see Figures 3a and 3b [45, 46].

Treating to a first approximation parameters as independent, a prismatic joint confidence region is readily obtained, the coordinates of every vertex out of sixteen (eight in case of symmetry) corresponding to a limit distribution marginally compatible with data at hand at the level considered [8]. A more pleasing to the eye, convenient to handle ellipsoid shaped confidence region may also be identified, along the lines pertaining to estimation of a joint confidence zone for parameters in multiple regression analysis [47].

By suitably scaling and centering the confidence intervals for mean, standard deviation, skewness and kurtosis, the ellipsoid may be reduced to spherical form,

$$\mu^2 + \sigma^2 + \beta_1^2 + \beta_2^2 = 1 \qquad (11)$$

the corresponding prism being then reduced to a (hyper) cube; the third variable drops out in case of symmetry. An estimate of type A uncertainty covering both identification of form, and estimation of parameters of empirical distributions underlying the data set at hand (assumed to be the only source of relevant information), may be obtained in terms of the confidence zone identified as the envelope of the sixteen (eight in case of symmetry) limit distribution functions, conveniently selected among Johnson's family, each corresponding either to a vertex of the prism(s), or to twelve (six as above) points on

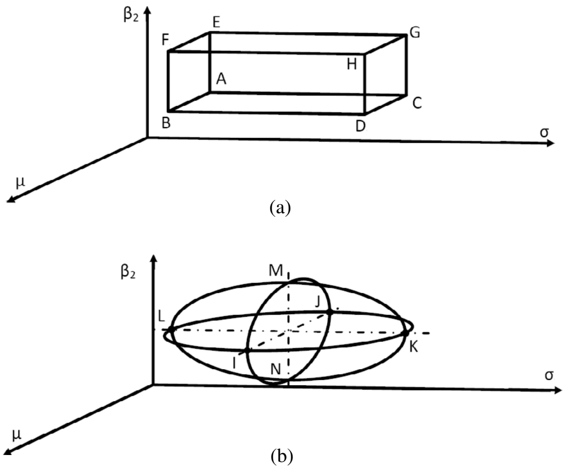

Fig. 4. Joint confidence regions in the $\mu - \sigma - \beta_2$ space for location, spread and peakedness of symmetrical distributions estimated from sample data, approximated by a prism (a) or an ellipsoid (b). Coordinates of points A to H in the former case, I to N in the latter, identify parameters of typical distributions marginally compatible with data at hand at given level.

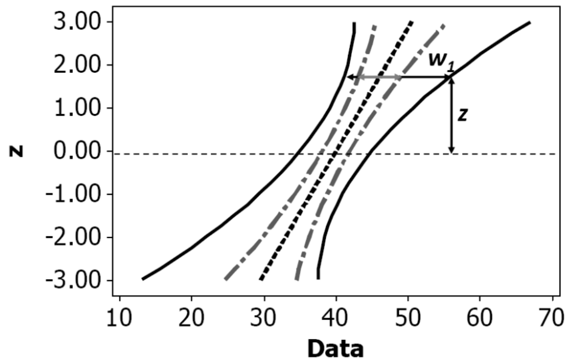

Fig. 5. Typical envelope of a set of Johnson distributions (continuous) and confidence band (chain dotted) pertaining to normal approximation (dashed). Ratio RA (function of z) is defined as the width of the comprehensive confidence interval w_1 (black) divided by the conventional one w_2 (gray).

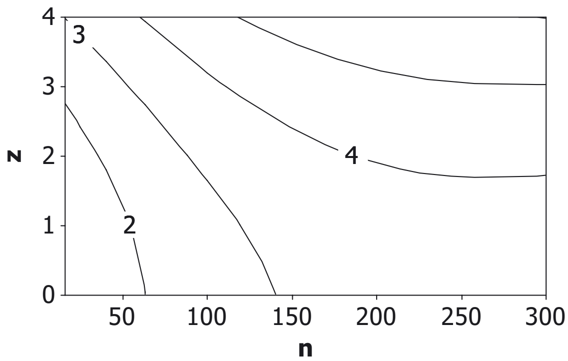

Fig. 6. Contour plot of ratio $RA = w_1/w_2$ versus normal variate z and sample size n.

ellipsoid's surface according to the model selected, see Figure 4 for a symmetrical case.

An observation is in order whenever to a first approximation normal distribution appears consistent with the sample at hand, a rather frequent instance, as the relevant confidence interval for kurtosis then necessarily straddles the nominal value $\beta_2 = 3$. When Johnson's distributions are fitted, neither bounded nor unbounded may then be ruled out as legitimate models, as for that matter neither type II nor type IV Pearson's distributions would be. Hyperbolae limiting the confidence zone pertaining to form on a normal probability plot therefore have both a vertical asymptote. Such a feature is however ruled out for the bounds of the confidence zone for a normal distribution assumed underlying the sample, but for the trivial case of zero variance; it follows necessarily that uncertainty concerning identification of form must exceed at both tails that due to sampling variability of (normal) parameters. Similar considerations apply, *mutatis mutandis*, also when lognormal form is assumed. Hyperbolae approximating limits of a confidence zone on a normal probability plot for the subsets of Johnson's distributions are then readily traced. Vertical asymptotes are identified by S_B distributions corresponding to point N (Fig. 4b), the slope of the other asymptotes being identified by point K in the same figure, where points I and J mark off a confidence interval for the mean. Dedicated algorithms may also be exploited [48, 49].

Disregard of uncertainty pertaining to identification of form leads to unwarranted overestimation of accuracy, minor around average, and fast increasing towards either tail beyond sample range. Ratio RA, defined as the width of comprehensive confidence intervals divided by conventional ones $-w_1/w_2$, see Figure 5 – is plotted as a response surface versus normal variate z and sample size n in Figure 6. Ratio RA is seen initially to be affected mainly by n, up to a point only; a change of trend may then be noticed, owing both to closer fit around average of all distributions, and to more marked effect of finite bounds, leading to increasing influence of z. Unwarranted faith into normal distribution entails a substantial risk of severely underestimating uncertainty of inferences, particularly when as large as six sigma levels are considered, as not uncommon in current practice.

4 Discussion

A striking example of gross under-evaluation of uncertainty by a number of leading astronomers is shown by a series of fifteen measurements of the Astronomical Unit between 1895 and 1961, where each estimate falls outside the confidence limits reported for the preceding one – even by the same author [50]. Had uncertainty component related to identification of underlying distribution been also taken into account, besides scatter observed in replication, larger estimates of errors would have been obtained, leading to less conflict between subsequent observations. Taking e.g. confidence intervals four times as broad as the average of those reported, agreement between following estimates would have been obtained in one half of the instances, while a multiplier of the order of ten would have resolved almost all conflicts.

Some families of empirical distributions capable of describing a broad range of unimodal data sets (multimodal may be handled in terms of mixture models) are described, and fitting procedures reviewed. When a set of experimental data of small to moderate size makes up the bulk of the information available for inference, it makes sense to consider also the uncertainty component inherent in assuming – somehow arbitrarily – a given form as that of the underlying distribution, out of a number of legitimate candidates. Type A uncertainty, pertaining to estimates of parameters owing to sampling variation only, may in fact be dwarfed by uncertainty concerning identification of form, particularly when inferences extending well beyond the range of the data set at hand are aimed at.

5 Conclusion

Unless size of data set is fairly large, empirical identification of form of underlying distribution is tentative at best; while data do not contradict the model proposed, they also don't contradict almost any other model you'd like to name, as Box once famously said [51]. The inherent uncertainty component may be readily estimated following the pragmatic approach proposed, rough estimates being provided by Figure 6 in case of symmetry. As a rule of thumb, take confidence intervals one half to an order of magnitude broader than those due only to sampling variation of parameters, in order to account also for uncertainty of form. The approach proposed leads to fairly broad estimates of uncertainty, exceeding definitely those derived singling out without further ado a given distribution as the correct one. Expert knowledge, established theoretical foundations, and additional specific information may bridge the gap, admittedly estimated to a first approximation only with the procedure proposed. As an excuse for such a shortcoming let us recall a classic aphorism, namely better to have an approximate answer to the right question than an exact answer to the wrong one [52].

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