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An Improved Framework for Uncertainty Analysis: Accounting for Unsuspected Errors

Alexander I. Shlyakhter[1,2]

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I use an analogy with the history of physical measurements, population and energy projections, and analyze the trends in several data sets to quantify the overconfidence of the experts in the reliability of their uncertainty estimates. Data sets include (i) time trends in the sequential measurements of the same physical quantity; (ii) national population projections; and (iii) projections for the U.S., energy sector. Probabilities of large deviations for the true values are parametrized by an exponential distribution with the slope determined by the data. Statistics of past errors can be used in probabilistic risk assessment to hedge against unsuspected uncertainties and to include the possibility of human error into the framework of uncertainty analysis. By means of a sample Monte Carlo simulation of cancer risk caused by ingestion of benzene in soil, I demonstrate how the upper 95th percentiles of risk are changed when unsuspected uncertainties are included. I recommend to inflate the estimated uncertainties by default safety factors determined from the relevant historical data sets.

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KEY WORDS: Uncertainty analysis; physical measurements; population projections; energy projections; Monte Carlo simulations.

1. INTRODUCTION

Probabilistic analysis of uncertainty and variability is receiving growing acceptance as a vital part of risk assessment.(1) However, such analysis is often plagued with its own uncertainties that have profound effect on the tails of the probability distributions. In particular, the commonly used 95% bounds for normal and lognormal distributions of exposure variables are very sensitive to the underestimation of the true uncertainty. The history of natural sciences offers many examples of overconfidence of the experts in the reliability of their uncertainty estimates.(2,3) The goal of this paper is to show how a systematic analysis of the trends in historical data sets of measurements and projections can be used to quantify the effects of unsuspected uncertainties in current models. I analyze several data sets derived from three different fields: nuclear physics, energy, and population projections. It appears that empirical probability distributions of the normalized deviations of the measured quantities from the true values do not follow the usually implied normal distribution. These distributions are better described by an exponential distribution with one additional parameter, *u*. To illustrate how the statistics of past errors can be used in the development of improved safety factors for current uncertainty estimates, I consider Monte Carlo simulation of cancer risk caused by ingestion of benzene in soil.

2. OVERCONFIDENCE IN PHYSICAL MEASUREMENTS

If the uncertainty in a measurement is dominated by random errors, then by the central limit theorem (CLT), the distribution of the arithmetic mean, *A*, of many observations around the true value, *a*, is asymptotically normal with standard deviation Δ. In this dis-

[1] Department of Physics and Center for Global Environmental Change, Harvard University, Cambridge, Massachusetts 02138, and Harvard Center for Risk Analysis, 718 Huntington Ave., Boston, Massachusetts 02115.
[2] To whom correspondence should be addressed at Department of Physics, Harvard University, Cambridge, Massachusetts 02138.

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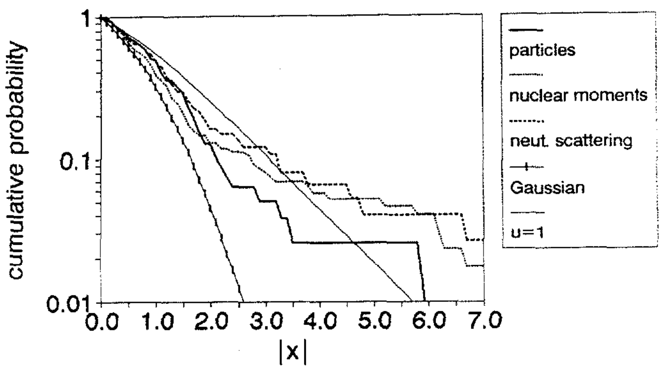

Fig. 1. Probability of unexpected results in physical measurements. The plots depict the cumulative probability, $S(x) = \int_x^\infty p(t)dt$, that new measurements (a) will be at least $|x|$ standard deviations (Δ) away from the old results (A); $x = (a - A)/\Delta$ as defined in the text. The cumulative probability distributions of $|x|$ are shown for the three data sets: particle data from the LBL data file,[12] magnetic moments[13] of excited nuclear states, and neutron scattering lengths.[14] Also plotted is a cumulative normal distribution, erfc($x/\sqrt{2}$), and compound exponential distribution with parameter $u = 1$ from Fig. 5.

tribution, the range $A \pm 1.96\Delta$ has a 95% probability of including a.[4] The presence of systematic errors, however, violates the assumptions necessary for use of the CLT. If much of the uncertainty comes from systematic errors, the usual justification for the normal distribution does not apply. Despite this fact, the normal distribution is often a reasonable approximation for small deviations and remains implicit when researchers report measured values and their corresponding uncertainties.

A clear message from the history of physical measurements is that unsuspected systematic errors are quite common, and new measurements are often far from the previous values. The long record of measurements of elementary particle properties has prompted several early studies of the temporal evolution of errors.[5–7] Shlyakhter *et al.*[8–11] expanded these original studies by following trends in several data sets. Here I present the results of the analysis of masses and lifetimes of elementary particles,[12] magnetic moments,[13] of the excited nuclear states, and neutron scattering lengths.[14]

All data sets were first converted into a standard format. Each measurement that produced an experimental value, A, and an estimate of uncertainty, Δ, together with the date of publication (or incorporation into an electronic data bank) formed a separate line (record). For each quantity, the earliest measurement was paired with the most recent one. I defined the early value as A_{old} and the recent value as A_{new} (assuming that A_{new} is a good surrogate for the true value a) with the corresponding uncertainties Δ_{old} and Δ_{new}. I also define the normalized deviation $x=(A_{new} - A_{old})/\Delta_{old}$. For example, the recommended value for the electron mass in the year 1961 was $A_{old} \pm \Delta_{old}$ = (0.510976 ± 0.000007) MeV/c^2, while in 1990 it was $A_{new} \pm \Delta_{new}$ = (0.51099906 ± 0.00000015) MeV/c^2 (1 MeV/c^2 = $1.782676 \cdot 10^{-30}$ kg). Therefore the old mean value was x=3.3 times its estimated standard error away from the presently accepted value.

To limit the effects of "noise" in the data on the final results, two selection criteria were applied. First, the standard error of the recent measurement, Δ_{new}, had to be much smaller than the old error, Δ_{old}, so that the value A_{new} is close to the true value a: $\Delta_{old}/\Delta_{new} \geq r$; the value r=4.0 was used. Second, only those measurements were considered for which the deviation from the true value was not too large: $|x| < m$; m=10 was used. This ensured that no major mistake occurred in the old measurement. The selection procedure considerably reduced the number of records remaining in each data set; the distribution of errors in the remaining data was stable with respect to variations in the values of the parameters r and m.

All the data satisfying the selection criteria were analyzed. There were 79 pairs of old and new measurements in elementary particle data, 185 pairs for nuclear moments, and 76 pairs for neutron scattering. For each pair of measurements of a given quantity the normalized deviation $x=(A_{new}-A_{old})/\Delta_{old}$ was calculated and the empirical probabilities of $|x|$ were derived. As Fig. 1 shows, normal distribution underestimates the probability of large deviations; instead of the predicted 5% there is a 15 to 30% chance of $|x| > 2$ for the empirical probability distributions. These distributions also suggest that there is a 5% chance of $|x|>4$, while the normal distribution predicts the value $6.8 \cdot 10^{-5}$, about 700 times less. A better fit to the data at large values of $|x|$ is obtained with a compound exponential distribution, described below, which is close to a straight line on the semilogarithmic graph of the cumulative probability, $S(x)$, *vs* the number of standard deviations, $|x|$.

Environmental measurements are rarely repeated with the same samples, and it is hard to estimate how widespread the unaccounted errors are in routinely collected data. An opportunity to address this issue is provided by the data on the excess uranium in the soil around the former Feed Materials Production Center at Fernald, Ohio, which had been a key uranium metals fabrication facility for the U.S. defense projects until it was closed in 1989.[15] The measurements were repeated at the request of the legal counsel to establish their credibility for litigation purposes. About 200 pairs of measurements of the radioactivity of three uranium isotopes (^{234}U, ^{235}U, and ^{238}U) in the same samples have been

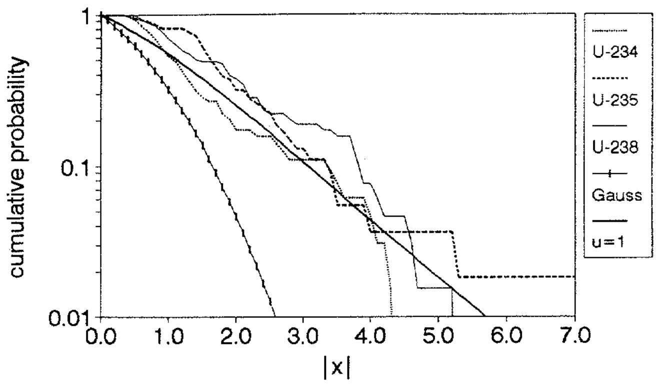

Fig. 2. Distribution of errors in measurement of excess uranium in soil. Presentation is similar to that in Fig. 1. The cumulative probability distributions of $|x|$ are shown for the three uranium isotopes: ^{234}U, ^{235}U, and ^{238}U.

provided by K. A. Stevenson (U.S. DOE Environmental Measurements Laboratory).

The distribution of deviations between the original and new measurements, normalized by the reported standard error of the old measurement, is shown in Fig. 2. The distribution is similar to the distribution of errors in the measurements in nuclear physics shown in Fig. 1. This similarity suggests that the pattern of overconfidence may be similar in a wide variety of measurements.

4. OVERCONFIDENCE: LESSONS FROM ENERGY AND POPULATION PROJECTIONS

Uncertainty in future forecasts is defined less formally than uncertainty in physical measurements. Uncertainty in the projections is usually presented in the form of "reference," "lower," and "upper" estimates (R, L, and U respectively). I assume that the range of parameter variation presented by a forecaster represents a subjective judgment about the probability that the true value $T \in [L, U]$. Generally, lower and upper bounds present what is believed to be an "envelope" most likely to bracket the true value and include the majority of possible outcomes.

One can estimate the standard deviation Δ of an equivalent normal distribution, as shown below, and then draw the empirical probability distributions of the deviations of the old projections from the true values normalized by Δ. Experts may not necessarily imply the normally distributed errors, nevertheless, the users of the results tend to base their decisions on the assumption of a normal or triangular distribution. Note that bounded distributions (such as triangular) assign zero probability to the outliers. Historical data presented below, however, suggest that deviations exceeding the expected uncertainty range are not uncommon. Using a normal (unbounded) distribution as a frame of reference *underestimates* true overconfidence.

The standard deviation of the equivalent normal distribution is calculated as follows:

(a) Specify the subjective probability α that the true value will lie between the low (L) and the high (U) estimates. I assume $\alpha=68\%$; larger values of α increase the discrepancy between the Gaussian model and the data.

(b) Draw an equivalent normal distribution that would have a specified cumulative probability α between L and U. For $\alpha = 68\%$ the standard deviation of the equivalent normal distribution is $(U - L)/2$, so that $x=2 \cdot (T\text{-}R)/(U\text{-}L)$. Therefore this choice of α corresponds to the usual practice of splitting the uncertainty range in half and using it as a surrogate of standard deviation.

(c) If the reference value (R) is not in the middle of the (L, U) interval, use two separate normal distributions truncated at zero: "left half" for the (L, R) interval and "right half" for the (R, U) interval, each with $\alpha/2$ as the cumulative probability.

Shlyakhter and Kammen[8,9,16] used this algorithm in their analysis of the United Nations population projections made in 1973[17] for the year 1985. The data subsequently obtained in 1985 can serve as the set of "exact" values, *a*. The population database includes projections for 164 nations, each with a population exceeding 100,000, presented in the form of "high," "medium," and "low" estimates for each nation. Data for 114 nations satisfying the criteria $|x| < 10$ were included in the study. Although the population estimates came from an authoritative source, there is a considerable number of very large deviations from the projected values (Fig. 3).

A similar analysis was conducted[18] for the history of recent projections for the U.S. energy sector.[19] Figure 4 shows the cumulative probability distributions of $|x|$ for the projections made for 1990 in 1983, 1985, and 1987, together with the Gaussian and exponential distributions. The three empirical distributions are strikingly similar. Although the absolute error in projections made in 1987 for 1990 is somewhat smaller than that made in 1983 for 1990 because of the shorter time interval, the estimated uncertainty is also smaller, so that the probability of the deviations from the true values normalized by Δ are roughly the same as for the other 2 years. One

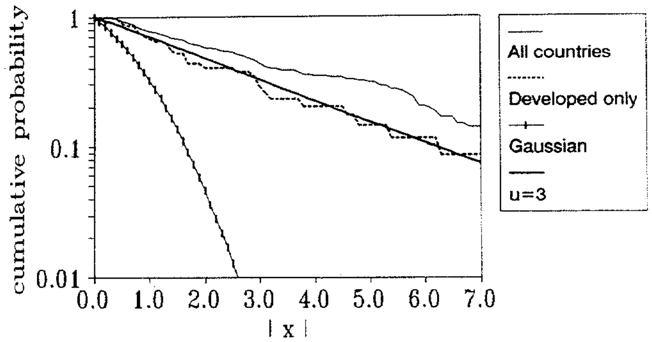

Fig. 3. Population projections. The plots depict the cumulative probability, $S(x) = \int_x^\infty p(t)dt$, that true values (T) will be at least $|x|$ standard deviations (Δ) away from the reference value of old projections (R). The population database is described in the text. The cumulative probability distributions of $|x|$ are shown for the total dataset of 114 countries (solid line) and for a subset of 37 industrialized countries. Also shown are the normal distribution and the compound distribution with $u = 3$ from Fig. 5.

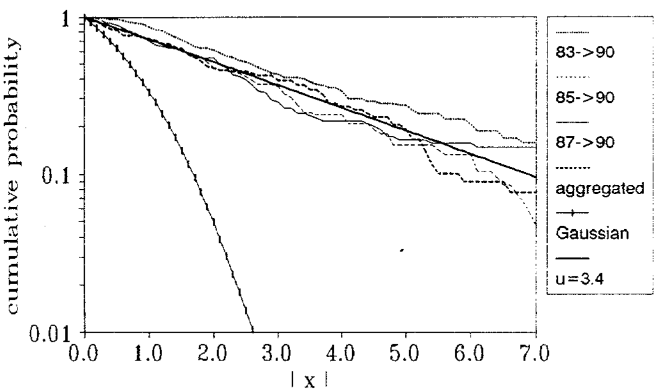

Fig. 4. Annual Energy Outlook projections. The presentation is as in Fig. 3: Projections from 1983 to 1990, 1985 to 1990, and 1987 to 1990, aggregated sectors of economy for all three forecast years; normal distribution and exponential distribution with $u = 3.4$.

would expect that energy projections for aggregated sectors of the economy would be more reliable that projections for individual sectors. However, this is not the case (Fig. 4, heavy dashed line). As shown in Figs. 3 and 4 (heavy solid line), the empirical distributions for both energy and population projections fit the exponential curves very well.

5. PARAMETRIZATION OF THE OBSERVED DISTRIBUTIONS

The nature of uncertainties considered above is very diverse: from genuine measurement errors in physics to subjective estimates of uncertainty in population and energy forecasts. However, the data sets analyzed in the previous sections share one common feature: Long tails in the distributions of the normalized deviations from the true values are grossly underestimated by the normal distribution and are better described by the exponential functions.

Bukhvostov[6] and Shlyakhter *et al.*[8,11,18] suggested simple heuristic arguments to describe how an exponential distribution of errors might arise. Let us assume that the estimate of the mean, A (which I have been calling A_{old}), is unbiased but that the estimate (Δ) of the true standard deviation, (Δ') is randomly biased with a distribution $f(t)$, where $t=\Delta'/\Delta$. Here Δ is the estimated standard deviation, which I have been calling Δ_{old}. In other words, I assume that the deviations normalized by Δ', $X'=(a-A)/\Delta'$, follow the standard normal distribution, while the deviations normalized by Δ, $x=(a-A)/\Delta$, follow a normal distribution with a randomly chosen standard deviation t:

$$p_t(x) = \frac{1}{\sqrt{2\pi}t} e^{-(x^2/2t^2)} \tag{1}$$

Integrating over all values of t gives a compound distribution:

$$p(x)=\frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{dt}{t} f(t) e^{-(x^2/2t^2)} \tag{2}$$

If $f(t)$ has a sharp peak near $t=1$, Eq. (2) reduces to the normal distribution. If $f(t)$ is broad, however, the result is different. For simplicity, let us assume that for large t, $f(t)$ follows the Gaussian distribution with the standard deviation u: $f(t) \sim \exp[-t^2/(2u^2)]$. The main contribution to the integral in Eq. (2) comes from the vicinity of the saddle point where the exponential term reaches a maximum (at $t^2 = u \cdot |x|$). It is straightforward to show that, for large values of x, the probability distribution $p(x)$ is not *Gaussian* but *exponential*: $p(x) \sim \exp(-|x|/u)$. To reflect the fact that experts are mostly overconfident ($\Delta' \geq \Delta$), I use a truncated normal form of $f(t)$:

$$f(t) = 0, \qquad t \leq 1$$
$$f(t) = \sqrt{\frac{2}{\pi}} \frac{1}{u} e^{-[(t-1)^2/2u^2]}, \qquad t>1 \tag{3}$$

Integrating Eq. (2) with $f(t)$ from Eq. (3) gives the cumulative probability $S(x)$ of deviations exceeding $|x|$:

$$S(x)=\sqrt{\frac{2}{\pi}} \cdot \frac{1}{u} \int_1^\infty e^{-[(t-1)^2/2u^2]} \operatorname{erfc}\left(\frac{|x|}{t\sqrt{2}}\right) dt \tag{4}$$

Here erfc(x) is the complementary error function.[20] The normal ($u = 0$) and the exponential distributions ($u > 1$) are members of a single-parameter family of curves

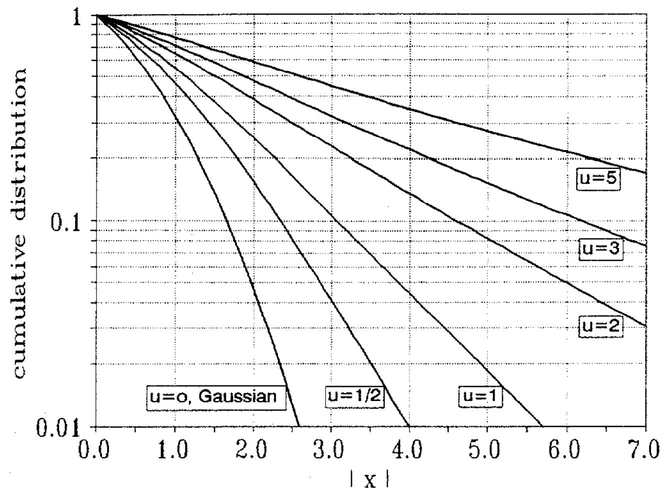

Fig. 5. One-parameter family of compound distributions. Parameter u is defined in Eq. (3); it is a measure of uncertainty in the standard deviation Δ. The values of u are indicated. The curves demonstrate the continuum of probability distributions, from Gaussian ($u = 0$) to exponential ($u > 1$). Note that the number of standard deviations for 95% confidence intervals is 1.96 for normal distribution and 3.8 for exponential distribution.

(Fig. 5). For quick estimates for $u \geq 1$, $X \geq 3$, one can use the approximation $e^{-|x|/(0.7u+0.6)}$. Uncertainty estimates can be improved by analyzing the record of prior projections and estimating the value of u. Data presented in Figs. 1–4 show that $u \sim 1$ for laboratory and environmental measurements and $u \sim 3$ for population and energy projections fit the empirical data best.

Parametrization with the one-parameter family of compound exponential distributions described above is not the only one possible. Another one-parameter fit is provided by a fractal model of errors described by Levy stable distribution.[11] A goodness-of-fit analysis of the data sets presented in Fig. 1[21] suggests that an inflated Gaussian distribution with the standard deviation, σ, as a free parameter describes the combined data very poorly and can be excluded. Exponential parametrization for the distribution of the absolute deviations $| x |$ with u as a free parameter produces a much better fit. This fit can be further improved with two independent exponential distributions if negative and positive errors are analyzed separately; this takes into account the asymmetry of the probability distributions. A good fit was also obtained with a sum of the inflated Gaussian distribution and a constant background term. Increasing the number of free parameters improves the quality of the fit to the data, however, it also makes it harder to describe the distribution of errors with a single formula. Safety factors for uncertainty estimates should depend only on the general form of the distribution of errors and for estimating these factors a simple one-parameter exponential parametrization is sufficient.

6. EXAMPLE: MONTE CARLO SIMULATIONS OF CANCER RISKS

To illustrate how the statistics of past errors can be used in the development of improved safety factors for risk estimates let us consider the Incremental Lifetime Cancer Risk (ILCR) for children due to benzene ingestion with soil.[22] One can write a model for ILCR in the form

$$\text{ILCR} = \frac{C_s \cdot \text{SingR} \cdot \text{RBA} \cdot \text{DpW} \cdot \text{WpY} \cdot \text{YpL} \cdot \text{CF}}{\text{BW} \cdot \text{DinY} \cdot \text{YinL}} \cdot \text{CPF} \tag{5}$$

Here C_s is the benzene concentration in soil (mg/kg) described by a lognormal distribution with $\mu=0.84$, $\sigma=0.77$; SingR is the soil ingestion rate (mg/day) described by the lognormal distribution with $\mu=3.44$, $\sigma=0.80$; RBA=1 is the relative bioavailability; DpW=1 day/week is the number of exposure days per week; WpY=20 weeks/year is the number of exposure weeks per year; YpL=10 years/life is the number of exposure years per life; CF= 10^{-6} kg/mg is the conversion factor; and BW is the body weight (kg). It is described by the normal distribution with the mean value $m=47.0$ and the standard deviation $s=8.3$; DinY=7 (days/week) · 52 (weeks/year) is the total number of days per year; YinL=70 years is the total number of years per lifetime; and CPF is the cancer potency factor (kg·day/mg) described by the lognormal distribution with $\mu= -4.33$, $\sigma=0.67$).

To simplify the discussion, let us assume that the probability distribution of body weights is well known. Assume that uncertainty in the values of $\sigma=\ln(\text{GSD})$ in the lognormal distributions of cancer potency factor, benzene concentration in soil, and soil ingestion rate can be characterized by a single u value applicable to the combined uncertainty of ILCR. Here I assume that the underestimation of uncertainty in measurements and projections also apply to the exposure variables described by lognormal distribution. I define x as $x=[\ln(a) - \ln(A)]/\ln(\text{GSD})$, and generate the distributions for x and t using Eq. (1) and Eq. (3) respectively. Figure 6 shows the results of 1000 Monte Carlo simulation trials of Eq. (5) for different u values. For comparison, the ILCR obtained by multiplying the upper 95th percentiles for the distributions of benzene concentration, soil ingestion,

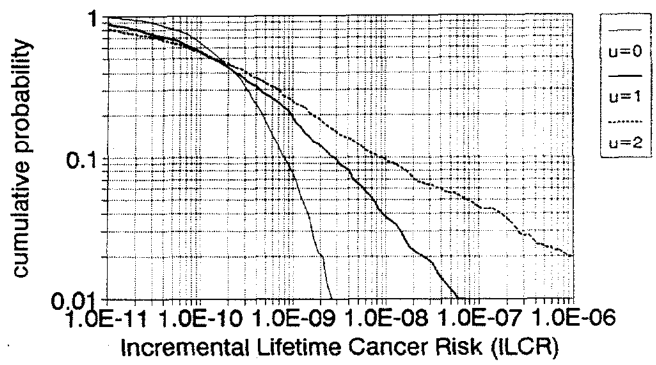

Fig. 6. Monte Carlo simulation of the incremental lifetime cancer risk (ILCR) for children caused by ingestion of benzene in soil (data from Ref. 22). The plot depicts cumulative probability that ILCR exceeds given value. Multiplying the upper 95th percentiles for the distributions of benzene concentration, soil ingestion, and cancer potency factor and the lower 5th percentile for body weight gives ILCR = $8.8 \cdot 10^{-9}$, which is close to the ILCR value for $u = 1$.

and cancer potency factor and the lower 5th percentile for body weight is $8.8 \cdot 10^{-9}$. Interestingly, in this case multiplying the 95th percentile upper limits gives about the same result as using the exponential curve with $u=1$. However, this is coincidental, and in other cases multiplying the upper limits may not be conservative. The value $u=1$ is typical for physical measurements but higher values of u will be necessary if unaccounted uncertainties in the lifetime exposure estimates are similar to those in energy and population projections.

7. DISCUSSION OF THE RESULTS

Statistical analysis of the distributions of the actual errors in natural and social sciences can provide valuable information about the credibility of the uncertainty estimates in the models used in risk assessment. Unsuspected uncertainties are probably widespread in the environmental health risk assessments. For example, Hattis and Burmaster[23] mention several sources of potential bias in the measurements of the emissions of dioxins and dibenzofurans from solid waste incinerators.

Data sets for the analysis of errors can be derived, for example, from time trends in sequential measurements of the same physical quantity (for models used in natural sciences) or comparison of energy and population projections with actual values that become available later (for models of social parameters). For all data sets analyzed so far, distributions of deviations from the true values show the same pattern: Long tails that do not follow a normal distribution but can be pragmatically parametrized by an exponential distribution, with the slope determined by the data.

The additional component of uncertainty derived from such analyses can be viewed as a safety factor accounting for overconfidence of the experts. It therefore incorporates the possibility of human error into the framework of uncertainty analysis. The observed similarities might indicate the existence of some common human thought processes that are responsible for the observed pattern of overconfidence.[11] Although data on past misunderstanding of a given situation cannot prevent our current misunderstanding of a significantly different situation, statistical analysis of the frequency of past underestimates of uncertainty can provide useful clues for the choice of appropriate safety factors.

One can hedge against unsuspected uncertainties by multiplying the reported uncertainty range by a default safety factor. The proposed procedure is as follows. First, find a data set of old measurements (prior projections) with uncertainty estimates together with more recent results. Calculate $x = (a - A)/\Delta$ for each estimate and plot the cumulative probability. Second, estimate u by comparing this empirical cumulative probability distribution with the compound distribution curves shown in Fig. 5. Finally, use the derived u value to expand the confidence intervals appropriately.

Real life is not quite that simple because only partially relevant historical databases are usually available. One has to select a value of u based on a data set that most closely resembles the data in question. From our previous analysis, trends in physical constants give $u \approx 1$, and energy and population projections give $u \geq 3$. More historical data sets, particularly from environmental studies, should be analyzed. In some situations, particularly when variability is dominant and well-known, the derived u values will be small, indicating that unsuspected uncertainties are not important. As more and more data are available, it will be easier to find relevant data sets for each particular problem and to get defensible estimates of the unsuspected uncertainties.

A legitimate concern about the use of the default safety factors is that they ignore the specifics of particular studies. Therefore these factors should be clearly specified and applied only *after* the uncertainty has been determined by a standard method, so that the operation may be easily reversed.[4] It is important to develop ways of incorporating data on past overconfidence, particularly in studies where elicitation of expert opinions is involved. In many situations it would be preferable if the experts themselves—not the decision makers—could include safety factors appropriate for different confidence levels into their uncertainty estimates.

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