Computing Best-Possible Bounds for the Distribution of a Sum of Several Variables is NP-Hard

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Abstract

In many real-life situations, we know the probability distribution of two random variables x_1 and x_2, but we have no information about the correlation between x_1 and x_2; what are the possible probability distributions for the sum x_1+x_2? This question was originally raised by A. N. Kolmogorov. Algorithms exist that provide best-possible bounds for the distribution of $x_1 + x_2$; these algorithms have been implemented as a part of the efficient software for handling probabilistic uncertainty. A natural question is: what if we have several ($n > 2$) variables with known distribution, we have no information about their correlation, and we are interested in possible probability distribution for the sum $y = x_1 + \ldots + x_n$? Known formulas for the case $n = 2$ can be (and have been) extended to this case. However, as we prove in this paper, not only are these formulas not best-possible anymore, but in general, computing the best-possible bounds for arbitrary n is an NP-hard (computationally intractable) problem.

Real-life problem: error estimation for indirect measurements. In many real-life situations, we are interested in the value of a physical quantity y that is difficult or impossible to measure directly. Examples of such quantities are the distance to a star and the amount of oil in a given well. Since we cannot measure y directly, a natural idea is to measure y *indirectly*. Specifically, we find some easier-to-measure quantities $x_1, \ldots, x_n$ which are related to y by a known relation $y = f(x_1, \ldots, x_n)$; this relation may be a simple functional transformation, or complex algorithm (e.g., for the amount of oil, numerical solution to an inverse problem). Then, to estimate y, we first measure the

values of the quantities $x_1, \ldots, x_n$, and then we use the results $\widetilde{x}_1, \ldots, \widetilde{x}_n$ of these measurements to to compute an estimate $\widetilde{y}$ for y as $\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n)$.

Computing an estimate for y based on the results of direct measurements is called *data processing*; data processing is the main reason why computers were invented in the first place, and data processing is still one of the main uses of computers as number crunching devices.

Measurement are never 100% accurate, so in reality, the actual value x_i of i-th measured quantity can differ from the measurement result $\widetilde{x}_i$. Because of these *measurement errors* $\Delta x_i \stackrel{\text{def}}{=} \widetilde{x}_i - x_i$, the result $\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n)$ of data processing is, in general, different from the actual value $y = f(x_1, \ldots, x_n)$ of the desired quantity y; see, e.g., [13].

It is desirable to describe the error $\Delta y \stackrel{\text{def}}{=} \widetilde{y} - y$ of the result of data processing. To do that, we must have some information about the errors of direct measurements. In the ideal case, if each measuring instrument has been thoroughly analyzed and calibrated, we know the exact probability distribution for each random variable Δx_i. As a result, after i-th measurement, we know the probability distribution of actual values x_i. This probability distribution can be described, e.g., by the corresponding cumulative distribution function (cdf) $F_i(t) \stackrel{\text{def}}{=} \text{Prob}(x_i < t)$.

It is worth mentioning that in most practical cases, the distribution functions $F_i(t)$ are not Gaussian [10, 11].

Based on n known cdfs $F_1(t), \ldots, F_n(t)$ and on a known function $y = f(x_1, \ldots, x_n)$, we must determine the distribution (cdf) $F(t)$ for $y = f(x_1, \ldots, x_n)$.

When measurement errors of individual x_i are possibly correlated, this problem becomes difficult. When all the measurement errors are independent, i.e., if x_i are independent random variables, then we can, e.g., use Monte-Carlo simulations and/or analytical formulas to come up with the desired distribution for y. In many practical situations, however, we know that the measurement errors of different measuring instruments are not independent, because they contain components that come from the same outside error source (e.g., from the power grid).

Ideally, we should find out how exactly the variables x_i are correlated, i.e., we should get the joint probability distribution of the corresponding n variables. Unfortunately, this is very difficult: to get a distribution of a single variable with "k bins" accuracy, it is sufficient to divide the real line into k bins; however, to describe a joint distribution of n variables with the same accuracy, we need k^n bins. For large n, the number k^n becomes larger than the number of particles in the Universe (see, e.g., [7, 12]), so this is not practically possible.

As a result, for n variables, we face the following problem: we know the distributions $F_i(t)$ for n variables $x_1, \ldots, x_n$, we know the function $y = f(x_1, \ldots, x_n)$, but we do not have any information about the correlation between x_i. In such

situation, there may be many different joint distributions for $x_1, \ldots, x_n$, and for these different joint distributions, we may get different distributions $F(t)$ for y. What we would like to find, in this situation, is the range $[\underline{F}(t), \overline{F}(t)]$ of possible values of $F(t)$ for each t. In other words, we would like to find the best-possible bounds for a distribution of a function $y = f(x_1, \ldots, x_n)$ of several random variables $x_1, \ldots, x_n$. Let us formulate this problem in precise mathematical terms.

Formulation of the problem in mathematical terms. We know n cdfs $F_1(t), \ldots, F_n(t)$, and we know a function $y = f(x_1, \ldots, x_n)$ from R^n to R. Based on this information, we would like to compute the range $[\underline{F}(t), \overline{F}(t)]$, where:

- $\underline{F}(t)$ is the infimum of possible values $F(t) = \mathrm{Prob}(f(x_1, \ldots, x_n) < t)$ over all joint distributions of $(x_1, \ldots, x_n)$ for which the marginal distributions coincide with the given cdfs $F_i(t)$, and
- $\overline{F}(t)$ is the supremum of possible values $F(t)$ over all such joint distributions.

What is known: case of $n = 2$ variables. In spite of the clear practical importance of this problem, no general solution was known until the early 1980s, when G. D. Makarov, a student of A. N. Kolmogorov, provided the exact formulas for $\underline{F}(t)$ and $\overline{F}(t)$ for the simplest case when $n = 2$ and $f(x_1, x_2) = x_1 + x_2$ [9]. These formulas were later simplified, in [4], into the following form:

$$\underline{F}(t) = \max_{t_1, t_2 : t_1 + t_2 = t} \max(F_1(t_1) + F_2(t_2) - 1, 0); \tag{1}$$

$$\overline{F}(t) = \min_{t_1, t_2 : t_1 + t_2 = t} \min(F_1(t_1) + F_2(t_2), 1). \tag{2}$$

The fact that these formulas do provide lower and upper bounds for $F(t)$ is reasonably easy to understand. Indeed, it is well known that for any two events A and B, the probability $P(A \vee B)$ cannot exceed $P(A) + P(B)$. Since $A \,\&\, B$ is equivalent to $\neg(\neg A \vee \neg B)$, we conclude that

$$1 - P(A \,\&\, B) = P(\neg A \vee \neg B) \le P(\neg A) + P(\neg B) = (1 - P(A)) + (1 - P(B)),$$

hence $P(A \,\&\, B) \ge P(A) + P(B) - 1$. Since the probability is always non-negative, we conclude that $P(A \,\&\, B) \ge \max(P(A) + P(B) - 1, 0)$.

For every t_1 and t_2 for which $t_1 + t_2 = t$, the inequalities $x_1 < t_1$ and $x_2 < t_2$ imply that $y \stackrel{\mathrm{def}}{=} x_1 + x_2 < t_1 + t_2$. Thus, the probability $F(t)$ that $y < t$ cannot be smaller than the probability $\mathrm{Prob}((x_1 < t_1) \,\&\, (x_2 < t_2))$. Due to the above inequality, this probability, in turn, cannot be smaller than

$$\max(\mathrm{Prob}(x_1 < t_1) + \mathrm{Prob}(x_2 < t_2) - 1, 0) = \max(F_1(t_1) + F_2(t_2) - 1, 0),$$

so $F(t) \geq \max(F_1(t_1) + F_2(t_2) - 1, 0)$. Since $F(t)$ is larger than or equal to this expression for all t_1 and t_2 for which $t_1 + t_2 = 1$, it must be also larger than or equal to the largest of these expressions – which is exactly the above lower bound $\underline{F}(t)$.

The proof that teh expression (2) is the upper bound is similar. The non-trivial part of the result (1), (2) is proving that these bounds are indeed the best possible.

Further developments: brief overview. The seminal paper [16] extended the above formulas to the situations with more complex functions $f(x_1, x_2)$ and/or situations in which we have some information about the correlation between x_1 and x_2. The formulas proposed in [16] formed the basis for an efficient software system for handling probabilistic uncertainty [1]; for a theoretical foundation of the corresponding formulas, see, e.g., [3, 14].

Similar formulas have also been analyzed, clarified, implemented, and tested in [8].

Case of $n > 2$ variables: what is known. For the sum of $n > 2$ random variables $x_1, \ldots, x_n$, similar arguments lead to similar formulas. Specifically, it is known that for any two sequence of events $A_1, \ldots, A_n$, the probability $P(A_1 \vee \ldots \vee A_n)$ cannot exceed $P(A_1) + \ldots + P(A_n)$. Since $A_1 \,\&\, \ldots \,\&\, A_n$ is equivalent to $\neg((\neg A_1) \vee \ldots \vee (\neg A_n))$, we conclude that

$$1 - P(A_1 \,\&\, \ldots \,\&\, A_n) = P((\neg A_1) \vee \ldots \vee (\neg A_n)) \leq$$

$$P(\neg A_1) + \ldots + P(\neg A_n) = (1 - P(A_1)) + \ldots + (1 - P(A_n)),$$

hence $P(A_1 \,\&\, \ldots \,\&\, A_n) \geq P(A_1) + \ldots + P(A_n) - (n-1)$. Since the probability is always non-negative, we conclude that

$$P(A_1 \,\&\, \ldots \,\&\, A_n) \geq \max(P(A_1) + \ldots + P(A_n) - (n-1), 0).$$

Now, for every tuple $(t_1, \ldots, t_n)$ for which $t_1 + \ldots + t_n = t$, the inequalities $x_1 < t_1, \ldots, x_2 < t_2$ imply that $y \stackrel{\text{def}}{=} x_1 + \ldots + x_n < t_1 + \ldots + t_n$. Thus, the probability $F(t)$ that $y < t$ cannot be smaller than the probability

$$\text{Prob}((x_1 < t_1) \,\&\, \ldots \,\&\, (x_n < t_n)).$$

Due to the above inequality, this probability, in turn, cannot be smaller than

$$\max(\text{Prob}(x_1 < t_1) + \ldots + \text{Prob}(x_n < t_n) - (n-1), 0) =$$

$$\max(F_1(t_1) + \ldots + F_n(t_n) - (n-1), 0),$$

so $F(t) \geq \max(F_1(t_1) + \ldots + F_n(t_n) - (n-1), 0)$. Since $F(t)$ is larger than or equal to this expression for all tuples $(t_1, \ldots, t_n)$ for which $t_1 + \ldots + t_n = 1$,

it must be also larger than or equal to the largest of these expressions – hence $F(t) \geq F^-(t)$, where

$$F^-(t) \stackrel{\text{def}}{=} \max_{t_1,\ldots,t_n : t_1+\ldots+t_n=t} \max(F_1(t_1) + \ldots + F_n(t_n) - (n-1), 0). \quad (3)$$

Similarly, we can conclude that $F(t) \leq F^+(t)$, where

$$F^+(t) \stackrel{\text{def}}{=} \min_{t_1,\ldots,t_n : t_1+\ldots+t_n=t} \min(F_1(t_1) + \ldots + F_n(t_n), 1). \quad (4)$$

Are these bounds best possible? For $n = 2$, as we have mentioned, the bounds (1)–(2) are the best possible. A natural question is: are the corresponding bounds (3)–(4) best possible for $n > 2$ as well?

The paper [15] implicitly formulates a hypothesis that these bounds are indeed the best possible. In this paper, we show that these bounds are not the best possible, and that, moreover, computing the best-possible bounds for a general n is an NP-hard (computationally intractable) problem.

Example when the bounds (3)–(4) are not the best possible. We will consider the simplest possible example when $n = 3$ and all 3 distributions are uniform distributions on the interval $[0,1]$, i.e., $F_i(x) = 0$ for $x \leq 0$, $F_i(x) = x$ for $0 \leq x \leq 1$, and $F_i(x) = 1$ for $x \geq 1$.

In this case, once $t_i \in [0,1]$, we have $F_1(t_1) + F_2(t_2) + F_3(t_3) = t_1 + t_2 + t_3$. Therefore, once $t_1 + t_2 + t_3 = t$, we have $F_1(t_1) + F_2(t_2) + F_3(t_3) = t_1 + t_2 + t_3 = t$ hence $\min(F_1(t_1) + F_2(t_2) + F_3(t_3), 1) = \min(t, 1)$. Therefore, the minimum in the formula (4) is the minimum of identical values, hence $F^+(t) = \min(t, 1)$. In particular, for $t = 1$, we have $F^+(1) = \min(1, 1) = 1$.

So, for an arbitrary joint distribution of 3 random variables x_1, x_2, x_3 for which each marginal distribution is uniform on $[0,1]$, for the cdf $F(t)$ of the sum $y = x_1 + x_2 + x_3$, we have $F(1) \leq F^+(1) = 1$.

Let us now show that this bound $F(1) \leq F^+(1) = 1$ cannot be the best possible, i.e., that we cannot have $F(1) = 1$. Indeed, if $F(1) = 1$, this means that with probability 1, we have $y < 1$. Thus, the expected value $E[y]$ of y cannot exceed 1: $E[y] \leq 1$. On the other hand, since $y = x_1 + x_2 + x_3$, we have $E[y] = E[x_1] + E[x_2] + E[x_3] = 3 \cdot 0.5 = 1.5$ – a contradiction with the fact that $E[y] = 1$.

We can show that not only $F(1)$ cannot be equal to 1, it cannot be even close to 1: e.g., if $E(1) \geq 0.9$, this means that the probability that $y \geq 1$ is at most 0.1. So, with probability ≤ 1, we have $y \leq 1$, and with probability ≤ 0.1, we have $y = x_1 + x_2 + x_3 \leq 3 \cdot 1 = 3$. Thus, the expected value $E[y]$ of y cannot exceed $1 \cdot 1 + 0.1 \cdot 3 = 1.3$ – still a contradiction.

In this particular example, we can add additional inequalities on the cdf $F(t)$ caused by the fact that we know the value $E[y] = 1.5$ of the first moment [3]. We will show, however, that in general, the problem of computing the best-possible bounds on $F(t)$ is NP-hard.

Computing best-possible bounds for the distribution of a sum of several variables is NP-hard: a proof. To prove NP-hardness of the problem of computing the best-possible bounds for $F(t)$, we will reduce, to this problem, a known NP-problem, namely, the following *partition* problem [7, 12]: given n positive integers $s_1, \ldots, s_n$, check whether it is possible to find values $\varepsilon_i \in \{-1, 1\}$ for which $\varepsilon_1 \cdot s_1 + \ldots + \varepsilon_n \cdot s_n = 0$.

We will reduce each instance of this problem to the case when we have n random variables; for every i from 1 to n, i-th variable x_i is equal to $-s_i$ with probability 1/2 and to s_i with probability 1/2. For each of these variables, we have $E[x_i] = (1/2) \cdot (-s_i) + (1/2) \cdot s_i = 0$, hence for their sum $y \stackrel{\text{def}}{=} x_1 + \ldots + x_n$, we have $E[y] = E[x_1] + \ldots + E[x_n] = 0$.

Let us show that $\underline{F}(0) = 0$ if and only if the original instance of the partition problem has a solution. Indeed, if the original instance has a solution $(\varepsilon_1, \ldots, \varepsilon_n)$, then we can take the joint distribution in which $x = (x_1, \ldots, x_n)$ is equal to $(\varepsilon_1 \cdot s_1, \ldots, \varepsilon_n \cdot s_n)$ with probability 1/2 and to $(-\varepsilon_1 \cdot s_1, \ldots, -\varepsilon_n \cdot s_n)$ with probability 1/2. In this case, all n marginal distributions are as desired; on the other hand, the sum $y = x_1 + \ldots + x_n$ is equal to 0 with probability 1, hence $F(0) = \text{Prob}(y < 0) = 0$.

Vice versa, let us assume that $\underline{F}(0) = 0$. By definition of $\underline{F}(t)$, this means that for every $\delta > 0$, there exists a joint distribution for which $F(0) \le \delta$. Let us select some small $\varepsilon > 0$ (we will later determine which value to select), and let us select a distribution F that satisfies the above inequality for this δ. We will use reduction to a contradiction to prove that in this case, the original instance of the partition problem has a solution.

According to our choice of the random variables x_i, the only possible values of x_i are $\pm s_i$, i.e., the values $\varepsilon_i \cdot s_i$ for some $\varepsilon_i \in \{-1, 1\}$. So, if the original instance does not have a solution, then all possible values of $y = \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \varepsilon_i \cdot s_i$ are non-zero integers. Thus, if $y \ge 0$, we have $y \ge 1$.

The smallest possible value of y is $-S$, where $S \stackrel{\text{def}}{=} s_1 + \ldots + s_n$.

The expected value $E[y] = \sum_j p_j \cdot y_j$ of y can be represented as the sum $E = E^+ + E^-$ of two sub-sums E^+ and E^- corresponding to positive and negative y_j.

For the joint distribution F for which $F(0) = \text{Prob}(y < 0) \le \delta$, with probability $\le \delta$, we have values $\ge -S$, and with probability at least $1 - \delta$, we have values ≥ 1.

The overall probability of positive values is at least $1 - \delta$, and each positive value is at least 1, so $E^+ \ge (1 - \delta) \cdot 1 = 1 - \delta$. On the other hand, the probability of negative values is $\le \delta$, and each negative value is $\ge -S$, so $E^- \ge -\delta \cdot S$. Therefore, $E[y] = E^- + E^+ \ge (1 - \delta) - \delta \cdot S = 1 - (S + 1) \cdot \delta$; so, for $\delta < 1/(S+1)$, we have $E[y] > 0$ – a contradiction with $E[y] = 0$. This contradiction shows that our assumption was false, and the original instance of the partition problem

has a solution.

The reduction is proven, thus computing best-possible bounds for the distribution of a sum of several variables is indeed NP-hard.

Comment. The fact that problem turns out to be NP-hard is not very surprising: many other interval problems are NP-hard [7], as well as many problems related to combination of interval and probabilistic uncertainty [2, 5, 6].

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