Computing Population Variance and Entropy under Interval Uncertainty: Linear-Time Algorithms

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Abstract

In statistical analysis of measurement results, it is often necessary to compute the range $[\underline{V}, \overline{V}]$ of the population variance $V = \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - E)^2$ (where $E = \frac{1}{n} \cdot \sum_{i=1}^{n} x_i$) when we only know the intervals $[\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$ of possible values of the x_i. While $\underline{V}$ can be computed efficiently, the problem of computing $\overline{V}$ is, in general, NP-hard. In our previous paper, we showed that in a practically important case, we can use constraints techniques to compute $\overline{V}$ in time $O(n \cdot \log(n))$. In this paper, we provide new algorithms that compute $\underline{V}$ and, for the above case, $\overline{V}$ in linear time $O(n)$.

Similar linear-time algorithms are described for computing the range of the entropy $S = -\sum_{i=1}^{n} p_i \cdot \log(p_i)$ when we only know the intervals $\mathbf{p}_i = [\underline{p}_i, \overline{p}_i]$ of possible values of probabilities p_i.

1 Computing Population Variance under Interval Uncertainty: Formulation of the Problem

Once we have n measurement results $x_1, \ldots, x_n$, the traditional statistical analysis starts with computing the standard statistics such as population mean $E = \frac{1}{n} \cdot \sum_{i=1}^{n} x_i$ and population variance $V = M - E^2$, where $M \stackrel{\text{def}}{=} \frac{1}{n} \cdot \sum_{i=1}^{n} x_i^2$;

see, e.g., [12]. In many real-life situations, due to measurement uncertainty, instead of the actual values x_i of the measured quantity, we only have intervals $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$ of possible values of x_i [7, 12]. Usually, the interval $\mathbf{x}_i$ has the form $[\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$, where $\widetilde{x}_i$ is the measurement result, and Δ_i is the known upper bound on the absolute value of the measurement error $\Delta x_i \stackrel{\text{def}}{=} \widetilde{x}_i - x_i$.

Different values $x_i \in \mathbf{x}_i$ lead, in general, to different values of E and V. It is therefore desirable to compute the ranges $\mathbf{E} = [\underline{E}, \overline{E}]$ and $\mathbf{V} = [\underline{V}, \overline{V}]$ of possible values of E and V when $x_i \in \mathbf{x}_i$. Since the population mean E is a monotonic function of its n variables $x_1, \ldots, x_n$, its range can be easily computed as $\mathbf{E} = \left[\frac{1}{n} \cdot \sum_{i=1}^{n} \underline{x}_i, \frac{1}{n} \cdot \sum_{i=1}^{n} \overline{x}_i\right]$. For the variance V, there exist an algorithm that computes the lower bound $\underline{V}$ in time $O(n \cdot \log(n))$, but computing the exact upper bound $\overline{V}$ is, in general, NP-hard; see, e.g., [5, 11].

In [3], we described a $O(n \cdot \log(n))$ algorithm for computing $\overline{V}$ in a practically reasonable case when no "narrowed interval" $[x_i^-, x_i^+]$, where $x^- \stackrel{\text{def}}{=} \widetilde{x}_i - \frac{\Delta_i}{n}$ and $x_i^+ \stackrel{\text{def}}{=} \widetilde{x}_i + \frac{\Delta_i}{n}$, is a proper subinterval of the interior of another narrowed interval, i.e., when $|\widetilde{x}_i - \widetilde{x}_j| \geq \frac{|\Delta_i - \Delta_j|}{n}$ for all $i \neq j$.

In this paper, we describe two new linear-time algorithms:

- a linear-time algorithm that computes $\underline{V}$ for all possible intervals, and
- a linear-time algorithm that computes $\overline{V}$ for intervals that satisfy the above subset property.

2 Linear-Time Algorithm for Computing $\overline{V}$

Algorithm. Our new algorithm is based on the known fact that we can compute the median of a set of n elements in linear time (see, e.g., [2]); our use of median is similar to the one from [1, 6]. Let us first describe the algorithm itself; in the following subsections, we provide a justification for this algorithm.

For simplicity, let us first consider the case when all the intervals are non-degenerate, i.e., when $\Delta_i > 0$ for all i.

The proposed algorithm is iterative. At each iteration of this algorithm, we have three sets:

- the set I^- of all the indices i from 1 to n for which we already know that for the optimal vector x, we have $x_i = \underline{x}_i$;
- the set I^+ of all the indices j for which we already know that for the optimal vector x, we have $x_j = \overline{x}_j$;
- the set $I = \{1, \ldots, n\} - I^- - I^+$ of the indices i for which we are still undecided.

In the beginning, $I^- = I^+ = \emptyset$ and $I = \{1, \ldots, n\}$. At each iteration, we also update the values of two auxiliary quantities $E^- \stackrel{\text{def}}{=} \sum\limits_{i \in I^-} \underline{x}_i$ and $E^+ \stackrel{\text{def}}{=} \sum\limits_{j \in I^+} \overline{x}_j$. In principle, we could compute these values by computing these sums, but to speed up computations, on each iteration, we update these two auxiliary values in a way that is faster than re-computing the corresponding two sums. Initially, since $I^- = I^+ = \emptyset$, we take $E^- = E^+ = 0$.

At each iteration, we do the following:

- first, we compute the median m of the set I (median in terms of sorting by $\widetilde{x}_i$);
- then, by analyzing the elements of the undecided set I one by one, we divide them into two subsets $P^- = \{i : \widetilde{x}_i \le \widetilde{x}_m\}$ and $P^+ = \{j : \widetilde{x}_j > \widetilde{x}_m\}$;
- we compute $e^- = E^- + \sum\limits_{i \in P^-} \underline{x}_i$ and $e^+ = E^+ + \sum\limits_{j \in P^+} \overline{x}_j$;
- if $n \cdot x_m^- < e^- + e^+$, then we replace I^- with $I^- \cup P^-$, E^- with e^-, and I with P^+;
- if $n \cdot x_m^- > e^- + e^+$, then we replace I^+ with $I^+ \cup P^+$, E^+ with e^+, and I with P^-;
- if $n \cdot x_m^- = e^- + e^+$, then we replace I^- with $I^- \cup P^-$, I^+ with $I^+ \cup P^+$, and I with $\emptyset$.

At each iteration, the set of undecided indices is divided in half. Iterations continue until all indices are decided, after which we return, as $\overline{V}$, the value of the population variance for the vector x for which $x_i = \underline{x}_i$ for $i \in I^-$ and $x_j = \overline{x}_j$ for $j \in I^+$.

Comment. If some intervals $\mathbf{x}_i$ are degenerate, i.e., $\mathbf{x}_i = [x_i, x_i]$, then we need the following modifications to the above algorithm:

- first, as the initial set I, we take the set of all indices corresponding to non-degenerate intervals;
- second, we pre-compute the sum e of all the exactly known values x_i (corresponding to degenerate intervals);
- third, on each iteration, instead of comparing the product $n \cdot x_m^-$ with the sum $e^- + e^+$, we compare the product with the sum $e^- + e^+ + e$;
- finally, when computing the population variance that will be returned in $\underline{V}$, we must include the degenerate values x_i as well.

Proof that the new algorithm for computing $\overline{V}$ requires linear time. At each iteration, computing median requires linear time, and all other operations with I require time t linear in the number of elements $|I|$ of I: $t \le C \cdot |I|$ for some C. We start with the set I of size n; on the next iteration, we have a set of size $n/2$, then $n/4$, etc. Thus, the overall computation time is $\le C \cdot (n + n/2 + n/4 + \ldots) \le C \cdot 2n$, i.e., linear in n.

Proof that under the subset property, the new algorithm always computes $\overline{V}$. Similarly to [11], one can easily show that since no two narrowed intervals are proper subsets of one another, they can be linearly ordered in lexicographic order. In this order, we have $x_1^- \le x_2^- \le \ldots \le x_n^-$, $x_1^+ \le x_2^+ \le \ldots \le x_n^+$, and, thus, the averages $\widetilde{x}_i = (x_i^- + x_i^+)/2$ are also sorted: $\widetilde{x}_1 \le \widetilde{x}_2 \le \ldots \le \widetilde{x}_n$.

In [3], we have shown that in this sorting, the value $\overline{V}$ is attained at one of the vectors $x^{(k)} = (\underline{x}_1, \ldots, \underline{x}_k, \overline{x}_{k+1}, \ldots, \overline{x}_n)$, i.e., that $V = V(x^{(k)})$ for some k.

In [3], we also analyzed the change in $V(x^{(k)})$ when we replace $x^{(k)}$ with $x^{(k-1)}$, i.e., when we replace $\underline{x}_k$ with $\overline{x}_k = \underline{x}_k + 2\Delta_k$; we have shown that $V_{k-1} - V_k = \dfrac{4\Delta_k}{n} \cdot (x_k^- - E_k)$, where $E_k \stackrel{\text{def}}{=} E(x^{(k)})$.

Hence, $V_{k-1} < V_k$ if and only if $x_k^- < E_k$. Multiplying both sides of this inequality by n, we get an equivalent inequality $x_k^- < n \cdot E_k$, where $n \cdot E_k = \sum\limits_{i=1}^{k} \underline{x}_i + \sum\limits_{j=k+1}^{n} \overline{x}_j$. Similarly, $V_{k-1} > V_k$ if and only if $x_k^- > E_k$, and $V_{k-1} = V_k$ if and only if $x_k^- = E_k$.

When we go from k to $k+1$, we replace the larger value $\overline{x}_{k+1}$ in the sum $n \cdot E_k$ by a smaller value $\underline{x}_k$. Thus, the sequence $n \cdot E_k$ is strictly decreasing with k, while x_k^- is (maybe non-strictly) increasing with k.So, once we have $n \cdot x_k^- < E_k$, i.e., $V_{k-1} < V_k$, these inequalities will hold for smaller k as well. Similarly, once we have $n \cdot x_k^- > E_k$, i.e., $V_{k-1} > V_k$, these inequalities will hold for larger k as well.

Once we have $n \cdot x_k^- = E_k$, i.e., $V_{k-1} = V_k$, then we will have $V_k > V_{k+1} > \ldots$ and $V_k = V_{k-1} > V_{k-2} > \ldots$, i.e., $V_k = V_{k-1}$ will be the largest value of V.

In other words, the sequence V_k first increases ($V_{k-1} < V_k$) and then starts decreasing ($V_{k-1} > V_k$), with one or two top values.

For each m, if $V_{m-1} < V_m$ (i.e., if $n \cdot x_m^- < E_m$), this means that the value $k_{\max}$ corresponding to the maximum of V is $\le m$; hence for all the indices $\le m$, we already know that in the optimal vector x, $x_i = \underline{x}_i$. Thus, these indices can be added to the set I^-.

If $V_m > V_{m-1}$ (i.e., if $n \cdot x_m^- > E_m$), this means that the value $k_{\max}$ corresponding to the maximum of V is $> m$; hence for all the indices $> m$, we already know that in the optimal vector x, $x_i = \overline{x}_i$. Thus, these indices can be added to the set I^+.

Finally, if $V_m = V_{m-1}$ (i.e., if $n \cdot x_m^- = E_m$), then this m is where maximum is attained.

The algorithm has been justified.

3 Linear-Time Algorithm for Computing $\underline{V}$

Algorithm. The proposed algorithm is iterative. At each iteration of this algorithm, we have three sets:

- the set I^- of all the endpoints $\underline{x}_i$ and $\overline{x}_j$ for which we already know that for the optimal vector x, we have, correspondingly, $x_i \neq \underline{x}_i$ (for $\underline{x}_i$) or $x_j = \overline{x}_j$ (for $\overline{x}_j$);
- the set I^+ of all the endpoints $\underline{x}_i$ and $\overline{x}_j$ for which we already know that for the optimal vector x, we have, correspondingly, $x_i = \underline{x}_i$ (for $\underline{x}_i$) or $x_j \neq \overline{x}_j$ (for $\overline{x}_j$);
- the set I of the endpoints $\underline{x}_i$ and $\overline{x}_j$ for which we have not yet decided whether these endpoints appear in the optimal vector x.

In the beginning, $I^- = I^+ = \emptyset$ and I is the set of all $2n$ endpoints. At each iteration, we also update the values $N^- = \#(I^-)$, $N^+ = \#(I^+)$, $E^- = \sum\limits_{\overline{x}_j \in I^-} \overline{x}_j$, and $E^+ = \sum\limits_{\underline{x}_i \in I^+} \underline{x}_i$. Initially, $N^- = N^+ = E^- = E^+ = 0$.

At each iteration, we do the following:

- first, we compute the median m of the set I;
- then, by analyzing the elements of the undecided set I one by one, we divide them into two subsets

$$P^- = \{x \in I : x \leq m\}; \quad P^+ = \{x \in I : x > m\};$$

  we also compute $m^+ = \min\{x : x \in P^+\}$;
- we compute $e^- = E^- + \sum\limits_{\overline{x}_j \in P^-} \overline{x}_j$, $e^+ = E^+ + \sum\limits_{\underline{x}_i \in P^+} \underline{x}_i$,

$$n^- = N^- + \#\{\overline{x}_j \in P^-\}, \quad n^+ = N^+ + \#\{\underline{x}_i \in P^+\},$$

  and $r = \dfrac{e^- + e^+}{n^- + n^+}$;
- if $r < m$, then we replace I^- with $I^- \cup P^-$, E^- with e^-, I with P^+, and N^- with n^-;
- if $r > m^+$, then we replace I^+ with $I^+ \cup P^+$, E^+ with e^+, I with P^-, and N^+ with n^+;

- if $m \le r \le m^+$, then we replace I^- with $I^- \cup P^-$, I^+ with $I^+ \cup P^+$, I with $\emptyset$, E^- with e^-, E^+ with e^+, N^- with n^-, and N^+ with n^+.

At each iteration, the set of undecided indices is divided in half. Iterations continue until all indices are decided, after which we return, as $\underline{V}$, the value of the population variance for the vector x for which:

- $x_j = \overline{x}_j$ for indices j for which $\overline{x}_j \in I^-$,
- $x_i = \underline{x}_i$ for indices i for which $\underline{x}_i \in I^+$, and
- $x_i = r$ for all other indices i.

Proof that the new algorithm for computing $\underline{V}$ requires linear time. At each iteration, computing median requires linear time, and all other operations with I require time t linear in the number of elements $|I|$ of I. We start with the set I of size n; on the next iteration, we have a set of size $n/2$, then $n/4$, etc. Thus, the overall computation time is $\le C \cdot (n + n/2 + n/4 + \ldots) \le C \cdot 2n$, i.e., linear in n.

Proof that the new algorithm always computes $\underline{V}$. In [5], we proved that if we sort all $2n$ endpoints into a sequence $x_{(1)} \le x_{(2)} \le \ldots \le x_{(2n)}$, then for some $k = k_{\min}$, the minimum $\underline{V}$ is attained for the vector x for which:

- for all indices j for which $\overline{x}_j \le x_{(k)}$, we have $x_j = \overline{x}_j$;
- for all indices i for which $\underline{x}_i \ge x_{(k+1)}$, we have $x_i = \underline{x}_i$;
- for all other indices, we have $x_i = r_k \stackrel{\text{def}}{=} \dfrac{E_k}{N_k}$, where

$$E_k = \sum_{j:\overline{x}_j \le x_{(k)}} \overline{x}_j + \sum_{i:\underline{x}_i \ge x_{(k+1)}} \underline{x}_i;$$

$$N_k = \#\{j : \overline{x}_j \le x_{(k)}\} + \#\{i : \underline{x}_i \ge x_{(k+1)}\}.$$

It has also been proven that for the optimal k, we have $r_k \in [x_{(k)}, x_{(k+1)}]$.

In general, the condition $x_{(k)} \le r_k = \dfrac{E_k}{N_k}$ is equivalent to

$$N_k \cdot x_{(k)} \le E_k = \sum_{j:\overline{x}_j \le x_{(k)}} \overline{x}_j + \sum_{i:\underline{x}_i \ge x_{(k+1)}} \underline{x}_i.$$

Subtracting $x_{(k)}$ from each of N_k terms in the right-hand side (RHS), and moving the sum of the resulting non-positive differences into the left-hand side (LHS), we conclude that

$$\sum_{j:\overline{x}_j \le x_{(k)}} (x_{(k)} - \overline{x}_j) \le \sum_{i:\underline{x}_i \ge x_{(k+1)}} (\underline{x}_i - x_{(k)}). \qquad (1)$$

When we increase k, we get, in general, more terms in the LHS and fewer in the RHS, so LHS (non-strictly) increases, while the RHS non-strictly decreases. So, if the inequality (1) holds for some k, it holds for all smaller values of k as well. Thus, this inequality holds for all k until a certain value k_0.

Similarly, the condition $x_{(k+1)} \geq r_k = \dfrac{E_k}{N_k}$ is equivalent to

$$N_k \cdot r_{k+1} \geq \sum_{j:\overline{x}_j \leq x_{(k)}} \overline{x}_j + \sum_{i:\underline{x}_i \geq x_{(k+1)}} \underline{x}_i.$$

Subtracting $x_{(k+1)}$ from each of N_k terms in RHS, and moving the sum of the resulting non-positive differences into LHS, we conclude that

$$\sum_{j:\overline{x}_j \leq x_{(k)}} (x_{(k+1)} - \overline{x}_j) \geq \sum_{i:\underline{x}_i \geq x_{(k+1)}} (\underline{x}_i - x_{(k+1)}). \tag{2}$$

When we increase k, the LHS (non-strictly) increases, while the RHS non-strictly decreases. So, if the inequality (2) holds for some k, it holds for all larger values of k as well. Thus, this inequality holds for all k after a certain value l_0.

So, both conditions (1) and (2) are satisfied (which is equivalent to the condition $r_k \in [x_{(k)}, x_{(k+1)}]$) either for a single value $k_{\min}$, or for several sequential values $l_0, l_0 + 1, \ldots, k_0$. Let us show that if this condition is satisfied for several sequential values, this simply means that the same minimum $\underline{V}$ is attained for all these values. For that, it is sufficient to show that if both conditions (1) and (2) holds for k and for $k + 1$, then the variance V has the same value for both k and $k + 1$. Indeed, since (1) is true for $k + 1$, we have

$$\sum_{j:\overline{x}_j \leq x_{(k+1)}} (x_{(k+1)} - \overline{x}_j) \leq \sum_{i:\underline{x}_i \geq x_{(k+2)}} (\underline{x}_i - x_{(k+1)}).$$

The LHS of this new inequality is smaller than or equal to the LHS of the inequality (2), and its RHS is larger than or equal to the RHS of the inequality (2). Thus, the only way for both inequalities to hold is when both sides are equal, i.e., when replacing $x_{(k)}$ with $x_{(k+1)}$ and replacing $x_{(k+1)}$ with $x_{(k+2)}$ does not change which endpoints are in I^- and which are in I^+ – and thus, does not change the corresponding value of the variance.

So:

- for $k < k_{\min}$, we have $r_k > x_{(k+1)}$,
- for $k > k_{\min}$, we have $r_k < x_{(k)}$, and
- for $k = k_{\min}$ (or, to be more precise, for $l_0 \leq k \leq k_0$), we have $x_{(k)} \leq r_k \leq x_{(k+1)}$.

Hence:

- if $r_k < x_{(k)}$, then we cannot have $k < k_{\min}$ and $k = k_{\min}$, hence $k > k_{\min}$;
- if $r_k > x_{(k+1)}$, then we cannot have $k > k_{\min}$ and $k = k_{\min}$, hence $k < k_{\min}$;
- if $x_{(k)} \le r_k \le x_{(k+1)}$, then we cannot have $k < k_{\min}$ and $k > k_{\min}$, hence $k = k_{\min}$.

Thus, the above algorithm finds the correct value of $k_{\min}$ and thence, the correct value of $\underline{V}$.

4 Computing Entropy under Interval Uncertainty: Formulation of the Problem

For a probability distribution with probabilities $p_1, \ldots, p_n$, $\sum p_i = 1$, the amount of uncertainty can be described by Shannon's entropy

$$S = -\sum_{i=1}^{n} p_i \cdot \log(p_i).$$

In practice, we sometimes only know the intervals $\mathbf{p}_i = [\underline{p}_i, \overline{p}_i]$ of possible values of p_i. Different values $p_i \in \mathbf{p}_i$ lead to different S; it is therefore desirable to find the range $[\underline{S}, \overline{S}]$ of the entropy S [8].

Since the function S is concave, computation of $\overline{S}$ is feasible [9, 13]; however, computing $\underline{S}$ is NP-hard [14]. For the case when no interval $[\underline{p}_i, \overline{p}_i]$ is a proper subset of the interior of another interval $\mathbf{p}_j$, we have proposed, in [14], an $O(n \cdot \log(n))$ algorithm for computing $\underline{S}$.

In this paper, we describe two new linear-time algorithms:

- a linear-time algorithm that computes $\overline{S}$ for all possible intervals, and
- a linear-time algorithm that computes $\underline{S}$ for intervals that satisfy the above subset property.

5 Linear-Time Algorithm for Computing $\underline{S}$

Algorithm. The proposed algorithm is iterative. At each iteration of this algorithm, we have three sets:

- the set I^- of all the indices i from 1 to n for we already know that for the optimal vector p, we have $p_i = \underline{p}_i$;
- the set I^+ of all the indices j for which we already know that for the optimal vector p, we have $p_j = \overline{p}_j$;

- the set $I = \{1, \ldots, n\} - I^- - I^+$ of the indices i for which we are still undecided.

In the beginning, $I^- = I^+ = \emptyset$ and $I = \{1, \ldots, n\}$. At each iteration, we also update the values $p^- = \sum\limits_{i \in I^-} \underline{p}_i$ and $p^+ = \sum\limits_{j \in I^+} \overline{p}_j$. Initially, $p^- = p^+ = 0$.

At each iteration, we do the following:

- first, we compute the median m of the set I (median in terms of sorting by $\widetilde{p}_i$);
- then, by analyzing the elements of the undecided set I one by one, we divide them into two subsets $P^- = \{i : \widetilde{p}_i \le \widetilde{p}_m\}$ and $P^+ = \{j : \widetilde{p}_j > \widetilde{p}_m\}$;
- we compute $e^- = E^- + \sum\limits_{i \in P^-} \underline{p}_i$ and $e^+ = E^+ + \sum\limits_{i \in P^+} \overline{p}_i$;
- if $e^- + e^+ > 1$, then we replace I^- with $I^- \cup P^-$, E^- with e^-, and I with P^+;
- if $e^- + e^+ + 2\Delta_m < 1$, then we replace I^+ with $I^+ \cup P^+$, E^+ with e^+, and I with P^-;
- finally, if $e^- + e^+ \le 1 \le e^- + e^+ + 2\Delta_m$, then we replace I^- with $I^- \cup (P^- - \{m\})$, I^+ with $I^+ \cup P^+$, I with $\{m\}$, E^- with $e^- - \underline{p}_m$, and E^+ with e^+.

At each iteration, the set of undecided indices is divided in half. Iterations continue until we have only one undecided index $I = \{k\}$, after which we return, as $\underline{S}$, the value of the entropy for the vector p for which $p_i = \underline{p}_i$ for $i \in I^-$, $x_j = \overline{p}_j$ for $j \in I^+$, and $p_k = 1 - e^- - e^+$ for the remaining value k.

Comment. If some intervals $\mathbf{p}_i$ are degenerate, i.e., $\mathbf{p}_i = [p_i, p_i]$, then we need the following modifications to the above algorithm:

- first, as the initial set I, we take the set of all indices corresponding to non-degenerate intervals;
- second, we pre-compute the sum e of all the exactly known values p_i (corresponding to degenerate intervals);
- third, on each iteration, instead of comparing 1 with the sum $e^- + e^+$, we compare 1 with the sum $e^- + e^+ + e$.

Proof that the new algorithm requires linear time. Similarly to the population variance case, at each iteration, we require time t linear in the number of elements $|I|$ of I: $t \le C \cdot |I|$ for some C. We start with the set I of size n; on the next iteration, we have a set of size $n/2$, then $n/4$, etc. Thus, the overall computation time is $\le C \cdot (n + n/2 + n/4 + \ldots) \le C \cdot 2n$, i.e., linear in n.

Proof that under the subset property, the new algorithm always computes $\underline{S}$. Due to the subset property, we can sort the intervals in lexicographic order, in which case their lower endpoints $\underline{p}_i$, their upper endpoints $\overline{p}_i$, and their midpoints $\widetilde{p}_i$ are also sorted: $\underline{p}_i \le \underline{p}_{i+1}$, $\overline{p}_i \le \overline{p}_{i+1}$, and $\widetilde{p}_i \le \widetilde{p}_{i+1}$. Let us thus assume that the intervals are thus sorted.

Let us now show that it is sufficient to consider monotonic optimal tuples $p_1, \ldots, p_n$, for which $p_i \le p_{i+1}$ for all i. Indeed, if $p_i > p_{i+1}$, then, since $p_i \le \overline{p}_i \le \overline{p}_{i+1}$ and $p_i > p_{i+1} \ge \underline{p}_{i+1}$, we have $p_i \in [\underline{p}_{i+1}, \overline{p}_{i+1}]$ and similarly $p_{i+1} \in [\underline{p}_i, \overline{p}_i]$. Thus, we can swap the values p_i and p_{i+1} without changing the value of S. We can repeat this swap as many times as necessary until we get a monotonic tuple that has the exact same value $S = \underline{S}$.

Let us now show that in the optimal tuple, at most one p_i can be inside the corresponding interval. Indeed, if we have two values p_j and p_k strictly inside their intervals, then for an arbitrary small Δ, replacing p_j with $p_j - \Delta$ and p_k with $p_k + \Delta = p + \Delta$ should not increase the resulting entropy. This is only possible when the derivative of the resulting expression w.r.t. Δ is 0, i.e., when $p_j = p_k$.

Now, for $p_j - \Delta = p - \Delta$ and $p_k + \Delta = p + \Delta$, the function S should have a minimum at $\Delta = 0$ and thus, its second derivative relative to Δ should be non-negative. However, an explicit computation shows that this derivative is negative. Thus, our assumption is false, and at most one p_j can be inside the corresponding interval.

Since the values $\underline{p}_i$ are sorted by i, and the values $\overline{p}_j$ are sorted by j, we can now conclude that:

- if $p_j = \underline{p}_j$ and $p_m > \underline{p}_m$, then $p_j \le p_m$; and
- if $p_m = \overline{p}_m$ and $p_j < \overline{p}_j$, then $p_m \ge p_j$.

Thus, each value $p_j = \underline{p}_j$ precedes all the values $p_m = \overline{p}_m$, and the only value p_i which is strictly inside the corresponding interval lies in between these values. Thus, in a monotonic optimal tuple $p_1, \ldots, p_n$, the first elements are equal to $\underline{p}_j$, then we may have one element which is strictly inside its interval, and then we have values $p_m = \overline{p}_m$.

For the resulting vector $p = (\underline{p}_1, \ldots, \underline{p}_{k-1}, p_k, \overline{p}_{k+1}, \ldots, \overline{p}_n)$, with $\underline{p}_k \le p_k \le \overline{p}_k$, the condition $\sum\limits_{i=1}^{n} p_i = 1$ implies that $\Sigma_k \le 1 \le \Sigma_{k-1}$, where $\Sigma_k \stackrel{\text{def}}{=} \sum\limits_{i=1}^{k} \underline{p}_i + \sum\limits_{j=k+1}^{n} \overline{p}_j$. When we go from Σ_k to Σ_{k+1}, we replace a larger value $\overline{p}_{k+1}$ with a smaller value $\underline{p}_{k+1}$, hence $\Sigma_k > \Sigma_{k+1}$. Thus, there has to be exactly one $k_{\max}$ for which $\Sigma_k \le 1 \le \Sigma_{k-1}$.

So, if we have $\Sigma_m > 1$, this means that the value $k_{\max}$ corresponding to the minimum of S is $> m$; hence for all the indices $\le m$, we already know that in the optimal vector p, $p_i = \underline{p}_i$. Thus, these indices can be added to the set I^-.

If Σ_{m-1} $(= \Sigma_m + 2\Delta_m) < 1$, this means that the value $k_{\min}$ corresponding to the minimum of S is $< m$; hence for all the indices $\geq m$, we already know that in the optimal vector p, $p_j = \overline{p}_j$. Thus, these indices can be added to the set I^+.

Finally, if $\Sigma_m \leq 1 \leq \Sigma_{m-1}$, then this m is where the minimum of S is attained.

The algorithm has been justified.

Comment: a similar linear-time algorithm can be used to compute the expected value under interval uncertainty. In addition to computing the range for entropy, it is often useful to compute the range $[\underline{a}, \overline{a}]$ of the expected value $a = \sum a_i \cdot p_i$ of a known variable $(a_1, \ldots, a_n)$ under the constraints $p_i \in [\underline{p}_i, \overline{p}_i]$ and $\sum\limits_{i=1}^{n} p_i = 1$. For this problem, linear-time algorithms are known; see, e.g., [1, 6]. Let us show that this problem can be also solved by a simple modification of the above algorithm.

It is known that the smallest possible value $\underline{a}$ of the linear form $\sum\limits_{i=1}^{n} a_i \cdot p_i$ under given constraints is equal to $-\overline{b}$, where $\overline{b}$ is the largest possible value of the form $\sum\limits_{i=1}^{n} b_i \cdot p_i$, with $b_i = -a_i$. Thus, it is sufficient to describe how to compute $\overline{a}$.

For that, we follow the above iterative algorithm while it computes I^- and I^+. We continue iterations until we have only one undecided index $I = \{k\}$, after which we return, as $\overline{a}$, the value of the linear function $\sum\limits_{i=1}^{n} a_i \cdot p_i$ for the vector p for which $p_i = \underline{p}_i$ for $i \in I^-$, $x_j = \overline{p}_j$ for $j \in I^+$, and $p_k = 1 - e^- - e^+$ for the remaining value k.

6 Linear-Time Algorithm for Computing $\overline{S}$

Algorithm. The proposed algorithm is iterative. At each iteration of this algorithm, we have three sets:

- the set I^- of all the endpoints $\underline{p}_i$ and $\overline{p}_j$ for which we already know that for the optimal vector p, we have, correspondingly, $p_i \neq \underline{p}_i$ (for $\underline{p}_i$) or $p_j = \overline{p}_j$ (for $\overline{p}_j$);
- the set I^+ of all the endpoints $\underline{p}_i$ and $\overline{p}_j$ for which we already know that for the optimal vector p, we have, correspondingly, $p_i = \underline{p}_i$ (for $\underline{p}_i$) or $p_j \neq \overline{p}_j$ (for $\overline{p}_j$);
- the set I of the endpoints $\underline{p}_i$ and $\overline{p}_j$ for which we have not yet decided whether these endpoints appear in the optimal vector p.

In the beginning, $I^- = I^+ = \emptyset$ and I is the set of all $2n$ endpoints. At each iteration, we also update the values $N^- = \#(I^-)$, $N^+ = \#(I^+)$, $E^- = \sum\limits_{\overline{p}_j \in I^-} \overline{p}_j$, and $E^+ = \sum\limits_{\underline{p}_i \in I^+} \underline{p}_i$. Initially, $N^- = N^+ = E^- = E^+ = 0$.

At each iteration, we do the following:

- first, we compute the median m of the set I;
- then, by analyzing the elements of the undecided set I one by one, we divide them into two subsets

  $$P^- = \{x \in I : x \le m\}; \quad P^+ = \{x \in I : x > m\};$$

  we also compute $m^+ = \min\{x : x \in P^+\}$;
- we compute $e^- = E^- + \sum\limits_{\overline{p}_j \in P^-} \overline{p}_j$, $e^+ = E^+ + \sum\limits_{\underline{p}_i \in P^+} \underline{p}_i$,

  $$n^- = N^- + \#\{\overline{p}_j \in P^-\}, \quad n^+ = N^+ + \#\{\underline{p}_i \in P^+\},$$

  and $r = \dfrac{1 - e^- - e^+}{1 - n^- - n^+}$;
- if $r < m$, then we replace I^- with $I^- \cup P^-$, E^- with e^-, I with P^+, and N^- with n^-;
- if $r > m^+$, then we replace I^+ with $I^+ \cup P^+$, E^+ with e^+, I with P^-, and N^+ with n^+;
- if $m \le r \le m^+$, then we replace I^- with $I^- \cup P^-$, I^+ with $I^+ \cup P^+$, I with $\emptyset$, E^- with e^-, E^+ with e^+, N^- with n^-, and N^+ with n^+.

At each iteration, the set of undecided indices is divided in half. Iterations continue until all indices are decided, after which we return, as $\overline{S}$, the value of the entropy for the vector p for which:

- $p_j = \overline{p}_j$ for indices j for which $\overline{p}_j \in I^-$,
- $p_i = \underline{p}_i$ for indices i for which $\underline{p}_i \in I^+$, and
- $p_i = r$ for all other indices i.

Proof that the new algorithm for computing $\overline{S}$ requires linear time is similar to the previous proofs.

Proof that the new algorithm always computes $\overline{S}$. It is known [8, 9, 14] that if we sort all $2n$ endpoints into a sequence $p_{(1)} \le p_{(2)} \le \ldots \le p_{(2n)}$, then for some $k = k_{\max}$, the maximum $\overline{S}$ is attained for the vector p for which:

- for all indices j for which $\overline{p}_j \le p_{(k)}$, we have $p_j = \overline{p}_j$;
- for all indices i for which $\underline{p}_i \ge x_{(k+1)}$, we have $p_i = \underline{p}_i$;
- for all other indices, we have $p_i = \text{const}$; since $\sum\limits_{i=1}^{n} p_i = 1$, we conclude that this constant is equal to $r_k \stackrel{\text{def}}{=} \dfrac{1 - E_k}{n - N_k}$, where

$$E_k = \sum_{j:\overline{p}_j \le p_{(k)}} \overline{p}_j + \sum_{i:\underline{p}_i \ge p_{(k+1)}} \underline{p}_i;$$

$$N_k = \#\{j : \overline{p}_j \le p_{(k)}\} + \#\{i : \underline{p}_i \ge p_{(k+1)}\}.$$

It can also be proven that for the optimal k, we have $r_k \in [p_{(k)}, p_{(k+1)}]$. These facts can proven, e.g., by the same analysis (adding Δp to one value p_j and subtracting Δp from another value p_k) as in our above analysis of $\underline{S}$.

Let us first prove that if $r_k = \dfrac{1 - E_k}{n - N_k} \le p_{(k+1)}$, then the similar inequality $r_{k+1} = \dfrac{1 - E_{k+1}}{n - N_{k+1}} \le p_{(k+2)}$ holds for the next value k. Indeed, the given inequality $\dfrac{1 - E_k}{n - N_k} \le p_{(k+1)}$ is equivalent to $1 - E_k \le (n - N_k) \cdot p_{(k+1)}$.

The only difference between the sums $E_k = \sum\limits_{j:\overline{p}_j \le p_{(k)}} \overline{p}_j + \sum\limits_{i:\underline{p}_i \ge p_{(k+1)}} \underline{p}_i$ and $E_{k+1} = \sum\limits_{j:\overline{p}_j \le p_{(k+1)}} \overline{p}_j + \sum\limits_{i:\underline{p}_i \ge p_{(k+2)}} \underline{p}_i$ is that:

- some terms equal to $p^{(k+1)}$ may be added (if there are j for which $\overline{p}_j = p_{(k+1)}$), and
- some other terms equal to to $p^{(k+1)}$ may be subtracted (if there are i for which $\underline{p}_i = p_{(k+1)}$).

In general, $E_{k+1} = E_k + c_k \cdot p_{(k+1)}$ for some integer c_k (positive, negative, or zero), and $N_{k+1} = N_k + c_k$. Subtracting $c_k \cdot p_{(k+1)}$ from both sides of the given inequality $1 - E_k \le (n - N_k) \cdot p_{(k+1)}$, we conclude that $1 - E_{k+1} \le (n - N_{k+1}) \cdot p_{(k+1)}$, i.e., that $r_{k+1} = \dfrac{1 - E_{k+1}}{n - N_{k+1}} \le p_{(k+1)}$. Since the sequence $p_{(k)}$ is sorted, we thus conclude that $p_{(k+1)} \le p_{(k+2)}$ and hence $r_{k+1} \le p_{(k+2)}$.

So, if the inequality $r_k \le p_{(k+1)}$ holds for some k, it holds for all larger values of k as well. Thus, this inequality holds for all k after a certain value l_0.

Similarly, we can prove that if the inequality $r_k \geq p_{(k)}$ holds for some k, then it holds for $k-1$ as well – since the only difference between E_k and E_{k-1} consists of adding and/or subtracting some values $p_{(k)}$. So, if the inequality $r_k \geq p_{(k)}$ holds for some k, it holds for all smaller values of k as well. Thus, this inequality holds for all k until a certain value k_0.

Similarly to the proof about $\underline{V}$, we can prove that if there are several values $k = l_0, l_0 + 1, \ldots, k_0$ for which both inequalities hold $p_{(k)} \leq r_k \leq p_{(k+1)}$, then for these k, the entropy has exactly the same value.

So:

- for $k < k_{\max}$, we have $r_k > p_{(k+1)}$,
- for $k > k_{\max}$, we have $r_k < p_{(k)}$, and
- for $k = k_{\max}$ (or, to be more precise, for $l_0 \leq k \leq k_0$), we have $p_{(k)} \leq r_k \leq p_{(k+1)}$.

Hence:

- if $r_k < p_{(k)}$, then we cannot have $k < k_{\max}$ and $k = k_{\max}$, hence $k > k_{\max}$;
- if $r_k > p_{(k+1)}$, then we cannot have $k > k_{\max}$ and $k = k_{\max}$, hence $k < k_{\max}$;
- if $p_{(k)} \leq r_k \leq p_{(k+1)}$, then we cannot have $k < k_{\min}$ and $k > k_{\min}$, hence $k = k_{\max}$.

Thus, the above algorithm finds the correct value of $k_{\max}$ and thence, the correct value of $\overline{S}$.

7 Open Questions

Can similar linear-time algorithms be proposed for computing the endpoints of the intervals for the quantities $E - \alpha \cdot \sqrt{V}$ and $E + \alpha \cdot \sqrt{V}$ – which are important in detecting outliers [4, 10]? for computing other statistical characteristics – like moments or covariance?

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