Confidence curves are used in uncertainty validation to assess how large uncertainties ($u_E$) are associated with large errors ($E$). An oracle curve is commonly used as reference to estimate the quality of the tested datasets. The oracle is a perfect, deterministic, error predictor, such as $|E| = \pm u_E$, which corresponds to a very unlikely error distribution in a probabilistic framework and is unable to inform us on the calibration of $u_E$. I propose here to replace the oracle by a probabilistic reference curve, deriving from the more realistic scenario where errors should be random draws from a distribution with standard deviation $u_E$. The probabilistic curve and its confidence interval enable a direct test of the quality of a confidence curve. Paired with the probabilistic reference, a confidence curve can be used to check the calibration and tightness of predictive uncertainties.

>>> WARNING: This is a work in progress.
>>> All comments and suggestions are welcomed.
I. INTRODUCTION

Uncertainty quantification (UQ) is becoming a major issue for chemical machine learning (ML), notably for the prediction of molecular and material properties. As a corollary, UQ validation plays an essential role to assess the calibration of various UQ methods, and validation methods should be chosen according to the nature of UQ metrics. UQ metrics quantify properties of the prediction errors, and one can distinguish those targeting the amplitude of errors from those targeting the dispersion of errors, typically through their variance or quantiles.

Amplitude metrics have been used a lot in computer vision, but appear also in the physico-chemical context. The validation of amplitude metrics is mostly based on ranking-based methods, either correlation coefficients between the metric and absolute errors, or so-called confidence curves. To assess the quality of confidence curves, a best case scenario curve, the oracle, is usually plotted as reference. The distance between a confidence curve and the oracle is estimated by statistics such as the Area Under the Confidence-Oracle error (AUCO). As the oracle implies a perfect ranking between the amplitude metric and the absolute errors, it corresponds to a correlation coefficient equal to 1. A property of these ranking-based statistics is that they do not depend on the scale of the amplitude metric. As such, they cannot be used to estimate the calibration of the metric.

Dispersion metrics are based on a probabilistic model of errors as defined in metrology, and their validation should account for this specificity. Typical validation methods compare the variance of errors to the mean-squared prediction uncertainty or compare the coverage of error prediction intervals to their target probability. The main difference with the amplitude metrics is that there is not a symmetric relation between errors and uncertainty: large errors are expected to be associated to large uncertainties, but small errors can be associated to either small or large uncertainties.

In this context, the use of ranking-based validation methods has limited interest. For instance, sets of probabilistically valid errors and uncertainties reach very modest correlation coefficients, around 0.5, and one should not expect them to reach much larger values. Similarly, the use of the oracle as a reference for confidence curves does not make much sense. Still, ranking-based methods benefit of some popularity in the chemistry ML-UQ community. For instance, Scalia et al. used the oracle and the associated distance metrics (AUCO) to compare variance-based prediction uncertainties, and Korolev et al. used it to compare variance-based uncertainties and their new amplitude-based $\Delta$-metric.
One solution to this conflict would be to avoid the use of confidence curves in the variance-based UQ framework. However, there are two features of confidence curves that make them stand out from the other methods used in calibration validation: (1) they provide a unique and easy validation method for uncertainty metrics in active learning\textsuperscript{11}; and (2) they do not depend on a binning scheme which might introduce some design problems in other validation methods (e.g., reliability diagrams)\textsuperscript{4}.

In this article, I focus on the variance-based UQ framework and I propose to switch from the oracle to a probabilistic reference, and show that the resulting method, when carefully designed, can be used as a validation tool for the calibration and tightness of variance-based uncertainties. The next section (Sect. II) introduces the concepts and numerical methods and presents the options to design a reliable probabilistic reference. Sect. III presents the application of the confidence curves to a selection of datasets from the physico-chemical ML-UQ literature. These results are discussed in Sect. IV.

II. CONFIDENCE CURVE, ORACLE AND PROBABILISTIC REFERENCE

Let us consider a validation dataset composed of paired errors and uncertainties $V = \{E, u_E\} = \{E_i, u_{E_i}\}_{i=1}^M$ to be tested for calibration. In a recent article,\textsuperscript{11} I reviewed the main variance-based UQ validation methods. These are built on a probabilistic model

$$E_i \sim D(0, u_{E_i})$$

linking errors to uncertainties, where $D(\mu, \sigma)$ is a probability density function with mean $\mu$ and standard deviation $\sigma$. This model states that errors should be unbiased ($\mu = 0$) and that uncertainties describe their dispersion, according to the metrological standard.\textsuperscript{20}

The calibration of $u_E$ is based on testing that it correctly describes the dispersion of $E$.\textsuperscript{10,11} One can for instance test that

$$\text{Var}(E) \simeq <u_E^2>$$

where the average is taken over the dataset $V$, and which is valid only if errors are unbiased. However, this formula does not take into account the pairing between errors and uncertainties, and a better test can be written as

$$\text{Var}(Z = E/u_E) \simeq 1$$

The satisfaction of these tests validates the average calibration, which is a minimum requisite, but does not guarantee the reliability of individual uncertainties. To achieve this, one can split $V$
into subsets by binning $u_E$ and, within each subset, test Eq. 2, leading to reliability diagrams$^{22}$, or test Eq. 3, leading to the Local Z-Variance analysis (LZV)$^{10,11}$.

In the following, I will refer to average calibration as calibration and to small-scale calibration as tightness.$^{11}$ An ideal UQ method, i.e., a UQ method which provides reliable individual uncertainties, should satisfy both calibration and tightness.$^{11}$

A. Confidence curve

A confidence curve (CC) is established by estimating an error statistic $S$ on subsets of $V$ pruned from the points with uncertainties larger than a threshold.$^4$ It is also called a sparsification error curve in computer vision.$^{4,15}$ Technically, it is a ranking-based method, as (1) it is insensitive to the scale of the uncertainties, and (2) the relative ordering of the errors and uncertainties plays a determinant role.

If one defines the threshold $u_k$ as the largest uncertainty after removing the $k \%$ largest uncertainties from $u_E$ ($k \in \{0, 1, \ldots, 99\}$), a confidence statistic is defined by

$$c_S(k; E, u_E) = S(E | u_E < u_k)$$

and its normalized version by

$$\tilde{c}_S(k; E, u_E) = c_S(k; E, u_E)/S(E)$$

where $S$ is an error statistic – typically the Mean Absolute Error (MAE) or Root Mean Squared Error (RMSE) – and $S(E | u_E < u_k)$ denotes that only those errors $E_i$ paired with uncertainties $u_E_i$ smaller than $u_k$ are selected to compute $S$. A confidence curve is obtained by plotting $c_S$ or $\tilde{c}_S$ against $k$. Both normalized and non-normalized CCs are used in the literature.

A continuously decreasing CC reveals a desirable association between the larger errors and the larger uncertainties, an essential feature for active learning or to detect unreliable predictions.

B. Reference curves

As already mentioned, only the order of $u_E$ values is used in a CC, and any change of scale of $u_E$ leaves $c_s$ unchanged. Without a proper reference, $c_S$ cannot inform us on calibration or tightness. One should note also that the normalized version, $\tilde{c}_S$, is also insensitive to scale changes of $E$, which excludes it for any calibration validation application, whichever the chosen reference, unless it is complemented by another calibration test.
1. Oracle

An oracle curve can be generated from the validation dataset $V$ by reordering $u_E$ to match the order of absolute errors. This can be expressed as

$$O(k; E) = c_s(k; E, |E|)$$

with a similar expression for the normalized version.

It is evident from the above equation that the oracle is independent of $u_E$ and therefore useless for calibration testing. Recast in the probabilistic framework introduced above, the oracle would correspond to a very implausible error distribution $D$, such that $E_i = \pm u_{E_i}$.

2. Probabilistic reference

Using Eq. 1, a probabilistic reference curve $P$ can be generated by sampling pseudo-errors $\tilde{E}_i$ for each uncertainty $u_{E_i}$ and calculating a CC for $\{\tilde{E}, u_E\}$, i.e.,

$$P(k; u_E) = \left\langle c_S(k; \tilde{E}, u_E) \right\rangle_{\tilde{E}}$$

where a Monte Carlo average is taken over samples of

$$\tilde{E}_i \sim D(0, u_{E_i})$$

The sampling is repeated a number of times sufficient to have a stable mean and confidence band (at the 95% level).

In contrast to the oracle, which depends exclusively on the errors, the probabilistic reference depends on $u_E$ and a choice of distribution $D$. It does not depend on the actual errors $E$. Comparison of the data CC to $P$ enables to test if $E$ and $u_E$ are correctly linked by the probabilistic model, Eq. 1, i.e. to test if the uncertainties quantify correctly the dispersion of the errors.

Examples. A comparison of both reference curves for synthetic datasets is shown in Fig. 1. The statistic $S$ is the RMSE. The probabilistic reference and its 95% confidence band have been obtained from samples of 500 realizations.

SYNT01 is a dataset generated using Eq. 1 and a normal distribution ($M = 1000$). Its CC is conform to the probabilistic reference, confirming the validity of the uncertainties to describe the dispersion of the errors. It is impossible to get such information by using the oracle curve as a reference. The oracle curves decrease to zero because the smallest errors (even though they
Figure 1. Examples of RMSE-based confidence curves for two synthetic datasets: (a) SYNT01 is a dataset where the errors are conform to the probabilistic model Eq. 1; (b) SYNT02 is a dataset of errors sampled from a probabilistic model with constant uncertainty.

might originate randomly from large uncertainties) are associated by the oracle to the smallest uncertainties. Note that the confidence band of the probabilistic reference widens notably for large $k$ values, as the size of the remaining set in this area might get small. In this case, the last bin ($k = 99$) contains only $M/100 = 10$ pairs.

The SYNT02 dataset [Fig. 1(b)] uses the same uncertainties as SYNT01 (it has therefore the same probabilistic reference), but the errors are now generated from a normal distribution with a constant standard deviation. The absence of link between errors and uncertainties is clearly revealed by the non-decreasing confidence curve.

Effect of the generative distribution and error statistic. The probabilistic reference $P$ depends on the choice of a generative distribution $D$ and of an error statistic $S$ (which should be the same as for the CC itself). I show here how these two factors might interfere and how to minimize the dependence of $P$ on $D$.

A default choice for $D$ would be the normal distribution which is often assumed in ML-UQ calibration studies. However, the error budget is very often dominated by model errors, which have no reason to be normally distributed. In consequence, I consider four other candidate distributions covering a wide range of kurtosis values: Uniform ($\kappa = 1.8$), Exponential power distribution with $p = 4$ (Normp4; $\kappa = 2.2$), Laplace ($\kappa = 6.0$), and Student’s-t with four degrees
of freedom (T4; \( \kappa = \infty \)).

The corresponding probabilistic reference curves for the SYNT01 dataset are reported in Fig. 2, for \( c_S \) and \( \tilde{c}_S \) and two S statistics (MAE and RMSE). In all cases, except for the non-normalized CC using the MAE, the reference curves are overlapping. As the pseudo-errors are generated by a distribution with prescribed standard deviation, the RMSE-based reference curves are not sensitive to the choice of \( D \). This is not the case for the MAE-based reference curves (note that the Laplace and T4 curves are overlapping). However, this difference is fully compensated by normalization. It appears thus that for non-normalized CCs, it is better to use the RMSE and benefit from the insensitivity of the corresponding probabilistic reference on \( D \).

Let us now consider the confidence bands of the probabilistic reference due to the choice of \( D \), given the RMSE statistic [Fig. 3 and Fig. 1(a)]. One can see a notable effect of \( D \) on the width of the confidence band: distributions with higher kurtosis values lead to wider confidence bands. This has to be kept in mind, but it can be considered as a secondary order effect that can be discussed when a CC lies close to the reference. In absence of specific information about the generative distribution \( D \), the normal provides thus a balanced default choice.

C. Distance from the probabilistic reference

In the same spirit as the AUCO, the distance of the confidence curve from its probabilistic reference can be used as a calibration/tightness metric

\[
DFPR = \sum_{i=0}^{99} |c_S(i; E, u_E) - P(i; u_E)|
\]

For the validation of the DFPR, a threshold UP95 is estimated as the 95th quantile of the distribution of DFPR values generated by random sampling of the probabilistic model. If DFPR < UP95 one can conclude that the uncertainties and errors are in agreement with Eq. 1. Note that the value of UP95 depends on the choice of generative distribution \( D \) [Fig. 3], as is the case for the confidence bands of the probabilistic reference, and its use comes with the same caveats as for the confidence bands.

In order to avoid interpretation confusions, I do not define this metric for normalized confidence curves.
Figure 2. Impact of the probabilistic model distribution on the reference curve for non-normalized (a,c) and normalized (b,d) confidence curves and two statistics, MAE (a,b) and RMSD (c,d)

III. APPLICATIONS

In a recent article, Palmer et al.\textsuperscript{23} proposed a calibrated bootstrap method to improve UQ resulting from various ML methods. They provide as supplementary information 20 validation datasets with errors and uncertainties for uncalibrated and calibrated results. I do not consider here the synthetic ones, but focus on those based on physical data, i.e. the Diffusion\textsuperscript{24} ($M = 2040$) and Perovskite\textsuperscript{25} ($M = 3836$) datasets. I want to emphasize that it is not my intent here to evaluate the calibrated
Figure 3. Impact of the probabilistic model distribution on the confidence band of the reference curve for non-normalized confidence curves. For the Normal case, see Fig. 1(a).

bootstrap method, but only to show how the confidence curves can be used in replacement or as complement to a LZV analysis.

In Fig 4, I present the results of the LZV analysis and confidence curves for the Random Forest application to the Diffusion dataset (denoted Diffusion_RF). For the uncalibrated results [Figs 4(a,b)], one sees that average calibration is off (Var(Z) = 0.5), indicating an average overestimation of the uncertainties by a factor around $\sqrt{1/0.5} = \sqrt{2}$. The CC lies below the probabilistic reference, indicating overestimation of the uncertainties, in agreement with the LZV analysis. The
DFPR statistic (9.5) is largely above the UP95 limit (1.1).

The calibrated bootstrap results [Figs 4(c,d)] show that average calibration has been reached \( \text{Var}(Z) = 0.96 \), but at the cost of large local deviations for the smaller uncertainties. Both graphs indicate a good tightness for uncertainties above \( u_E \simeq 0.3 \) (about 50\% of the dataset) and present mirrored deviations below this value. The DFPR statistics (1.5) is still above UP95 (0.91), but much less than before calibration.

By comparing the confidence curves for uncalibrated and calibrated data, one sees that the confidence curve of the calibrated data does not get closer to the oracle. Moreover, the calibration curves are very similar, except for the smaller uncertainties, indicating that the calibration process preserves the ranks of the 60-70\% larger uncertainties. By contrast, the probabilistic reference is sensitive to calibration and lies much closer to the confidence curve of calibrated data.

Interestingly, the LZV curve for the uncalibrated data oscillates around a constant value, suggesting that a simple scaling of the uncertainties might provide a notable improvement. In this case, a simple \textit{a posteriori} calibration by division of the uncalibrated uncertainties by a factor \( \sqrt{2} \) provides calibrated (\( \text{Var}(Z) = 1 \)) and fairly tight uncertainties (not shown), with a DFPR value (0.77) smaller than UQ95 (0.83). However, this \textit{ad hoc} scaling would not be successful for the other datasets presented below.

The Diffusion_RF example is representative of the efficiency the calibrated bootstrap.\textsuperscript{23} In the following, I focus on the analysis of calibrated data.

For the Diffusion_LR (Line Ridge regression) set [Fig. 5(a,b)], calibration is not perfect (the confidence bar around the average \( \text{Var}(Z) \) value does not overlap the unity), and one observes notable deviations of the LZV values for the larger uncertainties (above \( u_E = 0.5 \)), albeit these deviations do no exceed a factor two. This is translated by a confidence curve lying above the probabilistic reference in the first 20-30 percent, after which the curve falls back onto the reference. Here again, one cannot conclude to a perfect calibration. The DFPR statistic leads to reject tightness.

The Diffusion_GPR_Bayesian (Gaussian Process) case [Fig. 5(c,d)] presents a somewhat pathological case, where the uncertainties cover a small range. In addition to a sub-optimal calibration (\( \text{Var}(Z) = 0.89 \)), the LZV analysis reveals tightness problems at both extremities of the \( u_E \) range. The confidence curve confirms the residual overestimation of uncertainties (it lies below the reference until \( k \simeq 80\% \)). Moreover, the initial 10\% of the confidence curve are flat and it starts an erratic non-decreasing trajectory above \( k \simeq 65\% \). Clearly, these uncertainties are not
Figure 4. LZV analysis (a,c) and confidence curves (b,d) for uncalibrated (a,b) and calibrated (c,d) uncertainties from the Diffusion_RF dataset of Palmer et al.\textsuperscript{23}. Threshold uncertainties $u_k$ for $k = 20$, 40, 60 and 80 have been added to the confidence plots to facilitate the comparison with LZV plots.

Let us now consider the Perovskite_GPR_Bayesian case [Fig. 6(a-c)] for which the confidence curve [Fig. 6(c)] presents a sharp drop to 0 before $k = 100\%$. In contrast, the smaller uncertainties appear to be well calibrated in a standard LZV analysis with 20 bins [Fig. 6(a)]. Using a higher resolution for the LZV analysis (30 bins) reveals the problem: a $z$-scores variance of nearly 0 is observed for uncertainties around $u_E = 0.01$. Inspection of the dataset shows that these uncer-
Figure 5. Validation of calibrated uncertainties for the LR and GPR_Bayesian ML methods applied to the Diffusion dataset of Palmer et al.\textsuperscript{23}.

tainties are associated with a set of errors of tiny amplitude ($|E| \leq 10^{-8}$). This “nugget” does not appear in the original analysis by Palmer et al.\textsuperscript{23} who checked calibration by a reliability diagram with 15 bins. It probably deserves further inquiry, as one might wonder about its leverage in the calibration process. Nevertheless, both the LZV analysis and confidence curves conclude to an absence of tightness, despite the correct average calibration.

It is notable here that, as it does not depend on a binning strategy, the confidence curve is more likely to reveal abnormal features of the dataset that would be averaged out in a LZV analysis (or
IV. DISCUSSION

The most direct diagnostic feature of a confidence curve is that it has to be continuously decreasing to reveal a proper association between the errors and a UQ metric. This enables to use a UQ metric as a proxy to detect the risk of large errors. To be able to use confidence curves for UQ datasets comparisons or for calibration inquiries, one needs a reference curve. I discuss below the main points relevant to the choice of a reference curve, the design of a meaningful confidence curve analysis, and the compared advantages of confidence curves versus other calibration validation methods.

The oracle is irrelevant to assess the calibration of variance-based UQ metrics. I have shown above that the often used oracle is not relevant to evaluate confidence curves for variance-based UQ metrics (typically the uncertainty as the standard deviation of an uncertain variable) for two main reasons: (1) it corresponds to an unsuitable distribution of errors; and (2) it does not depend on the scale of the UQ metric. Therefore, I strongly recommend against its use in the variance-based UQ framework. Similarly, it should not be used to compare the performances of amplitude-based and variance-based UQ metrics.

The probabilistic reference enables to assess tightness (and sometimes calibration) of uncertainties. By design, the probabilistic reference curve enables to test if $|E|$ and $u_E$ are in a correct probabilistic association. If a non-normalized confidence curve lies within the probabilistic reference band, one gets similar confirmation of calibration and tightness to what would be obtained from a reliability diagram or LZV analysis. For instance, a reference curve lying above the data
confidence curve means that the uncertainties are over-estimated, one can safely reject the calibration of the dataset. Moreover, notable excursions of the confidence curve out of the probabilistic reference band indicate a lack of tightness. It is not always possible to conclude about calibration. For instances, in cases where the confidence curve lies around the probabilistic reference but wanders out of the confidence band, one gets no direct information about calibration. In such cases, a complementary calibration test, such as $\text{Var}(Z)$ is necessary.

When using a probabilistic reference, the best choice of statistic is the RMSE. In order to validate calibration and tightness, the best configuration is a non-normalized RMSE-based confidence curve. For the reference, a normal generative distribution is a good default choice, unless additional information is available. The reference curves based on the MAE statistic are dependent on the chosen generative distribution, which makes them less suitable, unless when using normalized confidence curves.

The normalized confidence curves are less informative than the non-normalized ones. The non-normalized statistic $c_S$ is easier to interpret than $\tilde{c}_S$ and provides a richer diagnostic. The normalized version is invariant by any monotonous transformation of the uncertainties and scaling of the errors. Therefore, it cannot provide information about calibration. If one uses a normalized CC, it is always necessary to test average calibration, for instance by checking that $\text{Var}(Z) \simeq 1$. Conditional to a positive calibration test, the normalized confidence curve can help to appreciate the tightness of uncertainties.

Comparison to other validation methods. Except for clear cut cases where a confidence curve does not cross the probabilistic reference band, it does not provide unambiguous information about average calibration, nor does it provide a quantitative estimation. The proposed DFPR statistic does not escape to this ambiguity and is interesting to confirm tightness. If tightness is rejected, it cannot inform us about calibration. In this respect, the $\text{Var}(Z)$ statistic is a useful/necessary complement. The LZV analysis provides similar diagnostics about tightness as the confidence curve, with the added value of a quantitative estimation. Moreover, the LZV analysis can be performed against any quantity besides $u_E$, such as the predicted values, which might provide better indices to locate and solve tightness defaults. On the other hand, the applications above show that an advantage of the confidence curve over the LZV and reliability diagrams is that it is independent of a binning strategy. My recommendation would thus be to use in priority the confidence curve analysis including a DFPR statistic, and if the diagnostic is not clear cut (either a clear absence of calibration or a positive tightness diagnostic), to use a LZV analysis for more
quantitative information.

V. CONCLUSION

This study has shown that the oracle reference is unsuitable to evaluate confidence curves for variance-based UQ metrics, and should be confined to the analysis of amplitude-based ones. I introduced a probabilistic reference which presents the added value to enable calibration/tightness diagnostic, going much beyond the capacities of the purely ranking-based oracle. A good setup for a CC analysis has been shown to be: a normal generative distribution $D$ to estimate the samples necessary to the reference, and the RMSE statistic to estimate non-normalized confidence curves of the data and reference. Even if it has sometimes to be complemented by more quantitative methods, the CC analysis is a very interesting method to address UQ calibration/tightness validation.

CODE AND DATA AVAILABILITY

The code and data to reproduce the results of this article are available at https://github.com/ppernot/2022_Confidence/releases/tag/v1.0 and at Zenodo (https://doi.org/10.5281/zenodo.6793828). The R,26 ErrViewLib package implements the plotCC and plotLZV functions used in the present study, under version ErrViewLib-v1.6 (https://github.com/ppernot/ErrViewLib/releases/tag/v1.6), also available at Zenodo (https://doi.org/10.5281/zenodo.7445577). The UncVal graphical interface to explore the main UQ validation methods provided by ErrViewLib is also freely available (https://github.com/ppernot/UncVal).

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Confidence curves are also called a *sparsification error curve* in computer vision.4,15

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