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Abstract

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1 Introduction

Machine Learning (ML) models that can not only estimate single targets accurately, but that are capable of estimating distributional information as well as uncertainty are becoming exceedendly important [Hüllermeier and Waegeman, 2021; Gawlikowski et al., 2023]. The reason therefore is, that most modern ML techniques are mostly black box models that have little intuitive reason behind their predictions but often act on abstract latent representations, especially in the case of Artificial Neural Networks (NN). With a strong focus on regression tasks, in this work we aim to develop a novel understanding of uncertainty estimating methods, where in particular we show that we can combine ideas from multiple different task-types. We show that Conditional Density Estimation (CDE), Conformal Prediction (CP) and Quantile Regression (QR) are fundamentally the same task since they all require to model parts of the conditional probability density function (PDF). Moreover, we develop a novel way to perceive the maximum log likelihood (MLL) objective function, where we show that it is equivalent to the objective function of CP, as we define it. This allows us to split the MLL objective into a constrainted optimization problem, where we intuitively minimize the size of the peaks (we make them as narrow as possible) with the constraint that we maintain calibration. Finally, we aim to introduce a novel way of perceiving epistemic uncertainty in CDE. All details to the theoretical concepts and novel insights are detailed in Section 2.

Before we go into the details of the theoretical background, we want to give a brief overview of the motivation, the exact research questions that we aim to answer in this work and a summary of the contributions. In particular, the practical implications and applications of this work are first discussed below in Section 1.1. Even though this work is not centered around a particular practical application but is more at home in the theoretical part of machine learning the author of this work belives that a motivation in the practical domain is very important to make the work more accessible and to show the relevance of the work. In particular, we aim to show that the methods proposed in this work can be

applied to a broad range of practical tasks and that they can have a significant positive impact on the performance of machine learning models in those tasks.

1.1 Background

Mostly in risk-sensitive practical domains like finance and life science uncertainty estimation is crucial [Abdar et al., 2021; Xia et al., 2020; Ghesu et al., 2021; Mashrur et al., 2020]. Therefore there exist two fundamental approaches to perceive uncertainty. First, there is the uncertainty that is inherent in the data, which means that for a give input, there are multiple possible outputs which are plausible, which also can not be reduced. This is called aleatoric uncertainty and it is the main task of CDE and CP to estimate this kind of uncertainty. Secondly, and less researched in the domain of regression, there is the uncertainty of the model, which could occur if the model is shown a sample that it can not generalize to, based on the training data it was trained on. This uncertainty is termed epistemic uncertainty. In this work we argue that in order to make reliable and informed decisions in high risk tasks, it is crucial to have methods to estimate both kinds of uncertainty, however, most recent works in regression tasks exclusively focus on estimating aleatoric uncertainty [Y. Romano, Patterson, and Candes, 2019; Sesia and Candès, 2020; Angelopoulos and Bates, 2021; Chernozhukov, Wüthrich, and Zhu, 2021; Sesia and Y. Romano, 2021; Oliveira et al., 2022; J. V. Romano, 2022; Izbicki, Shimizu, and Stern, 2022; Gupta, Kuchibhotla, and Ramdas, 2022; Auer et al., 2024]. In particular, methods like CDE, CP and QR can only directly estimate the aleatoric uncertainty, which is also the reason why epistemic uncertainty has been out of focus. However, in this work we argue that a type of epistemic uncertainty is already unknowingly being induced into models in many cases, that is with calibration.

1.1.1 Uncertainty in Finance

Energy Price Prediction

A practical task that we particularly focus on in this work is an energy price prediction task, in cooperation with Voestalpine AG which provided us with the dataset for the scope of this Master's Thesis, where we attempt to estimate the distribution of the

imbalance energy price[1] of Austria given multiple descriptive input variables/features. In particular, the imbalance energy price we aim to predict is unknown at the time of consumption/production and is only much later revealed.

If an entity on the energy market wants to buy or sell electricity at a certain time, this entity does indicate how much electricity it wants to buy or sell for the dayahead price which is known. Hoever, if this entity produces/consumes more energy than agreed on, the energy imbalance price holds for this over-/underestimation, but this price is only known after the fact and heavily depends on what other entities on the market did. In particular, the imbalance energy price is a very volatile price, making it a relevant use case for uncertainty estimation since it can impact the decision if electricity should be bought or produced at a given time.

Stock Price Prediction

In more traditional finance tasks, we mostly try to predict price-trends of assets like stocks [Ritika Singh and Srivastava, 2017], currencies [Hassanpour, 2023], cryptocurrencies [Alessandretti et al., 2018] and other equities. Those predictions are then used either for assisted decision making of analysts or for automated and potentially high frequency trading. Especially when making decisions with high stakes it is crucial to know exactly the risk that is taken with a certain decision, ideally with certain gurantees. For example, it might be essential not to loose more than a specified amount of money with a trading decision with a certain probabilistic confidence level. A known quantity in trading is the Value at Risk (VaR) as introduced by [Jorion, 2007], which is the maximum amount of money that can be lost with a certain confidence level.

1.1.2 Uncertainty in Healthcare and Life Science

In life science uncertainty aware ML methods have also been of increasing interest [Loftus et al., 2022; Lambert et al., 2024]. Often it is of relevance to estimate some regression targets like from personalized drug dosage prediction [Wu et al., 2023], amniotic fluid volume prediction [Csillag et al., 2023], tumor size quantification [Prasad et al., 2023],

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[1]For precise details on this quantity we refer to `https://markttransparenz.apg.at/en/markt/Markttransparenz/Netzregelung/Ausgleichsenergiepreise`

time-to-event prediction [Kvamme, Borgan, and Scheel, 2019; Sloma et al., 2021]. It is crucial for those tasks to not only know the average outcome, but to also be able to see if there are small probability events that could still happen with some plausible probabilitly. For example, if we predict the size of the tumor of a patient, the main probability density peak might be at a certain size, but it might be possible that there is another smaller peak at a much larger size which could lead to a more urgent tratment strategy. In this case, it is crucial to know the full distribution of the target variable and not only the mean. For similar reasons the epistemic uncertainty is also extremely relevant there. The model might not be able to generalize to a certain patient, which could lead to a completely random prediction and thus to a horrible decision if the doctor is not informed about the uncertainty of the model.

1.2 Related Work and Motivation

Many different related works about CDE [Bishop, 1994; Rothfuss, Ferreira, Walther, et al., 2019; Trippe and Turner, 2018; Rothfuss, Ferreira, Boehm, et al., 2019; Ambrogioni et al., 2017], CP [Izbicki, Shimizu, and Stern, 2022; Chernozhukov, Wüthrich, and Zhu, 2021; Y. Romano, Patterson, and Candes, 2019; Papadopoulos, 2008; Angelopoulos and Bates, 2021], QR [Chung et al., 2020] aswell as uncertainty estimation in general [Gal and Ghahramani, 2016; Hüllermeier and Waegeman, 2021; Abdar et al., 2021; Klotz et al., 2022] have been published in recent years. Most of those methods essentially attempt to model certain parts of the uncertainty of target variables given descriptive feature variables. Moreover, there exist works that observe that certain concepts can be transferred from one domain of uncertainty estimation to another [Chernozhukov, Wüthrich, and Zhu, 2021]. We will here provide a brief overview of CDE, CP and QR with focus on the recent works on those topics and a overview over practical methods that are used for those tasks currently. Only later in Section 2 we will give precise definitions of those tasks since there we also have established the notation.

1.2.1 Recent Works in CP

Initially CP was done by simply scaling a homoscedastic interval around the mean estimator of the data [Lei et al., 2018]. However, many limitations come with this approach

and so other approaches that take into account heteroscedasticity have come forth, in particular a very prominent method for a significance level of 2α to estimate the quantiles at α and $1 - \alpha$ [Y. Romano, Patterson, and Candes, 2019]. The most recent works have gone away from this also and now primarily focus on predicting the shortest CP intervals [Sesia and Y. Romano, 2021; Chernozhukov, Wüthrich, and Zhu, 2021; Izbicki, Shimizu, and Stern, 2022] in expectation. In particular, therefore often distributional information is required in order to effectively obtain the shortest CP intervals which has a strong relation to CDE quite obviously. However, no previous work goes into the details of the exact relationship between CP and CDE.

1.2.2 Recent Works in CDE

The most simplistic way of estimating conditional PDFs is probably just estimating the mean and inferring the optimal homoscedastic variance from the data which also aligns with the assumption of a Gaussian error model in the case of the mean squared error. The next step would be to estimate the variance also for each sample to obtain heteroscedasticity. However, since this still comes with major limitations a very fundamental work has been by [Bishop, 1994] where they propose to model the conditional PDF as a mixture of simple distributions like Gaussians/Laplacians. This method is called Mixture Density Networks (MDNs) and is still the most prominent method for CDE. However, it is also very prone to overfitting and so other methods like Kernel Mixture Networks (KMNs) have been proposed [Ambrogioni et al., 2017]. In particular, one of the most recent works in CDE has been done by [Rothfuss, Ferreira, Boehm, et al., 2019] where they propose a method to mitigate the overfitting problem of MDNs by adding noise to the input data. However, no previous work goes into the details of the exact relationship between CDE and CP. Additionally some other recent works on CDE like Normalizing Flow Networks [Trippe and Turner, 2018] exist, however this method still can not outperform MDNs or KMNs in practice.

1.2.3 Recent Works in QR

QR is was already explored in the 70s and 80s [Koenker and Bassett Jr, 1978] and has since then been a very prominent method for estimating quantiles of the target variable by

using the Pinball Loss. Moreover, more recent works in QR exist by [Chung et al., 2020] where they establish some connection between QR, CP and CDE already, which will be discussed in more detail in the theoretical part of this work.

1.2.4 Recent Works in Uncertainty Techniques

In recent years the possibly most prominent topic of uncertainty in machine learning has been the estimation of epistemic uncertainty [Barber and Bishop, 1998; Neal, 2012; Gal and Ghahramani, 2016; Schweighofer et al., 2023; Gawlikowski et al., 2023] where the main task is to estimate the model's confidence, that it's predictions are accurate, given an unseen sample. This is not to be confused with the conditional PDF produced by CDE methods, which only models a different type of uncertainty as discussed in more detail in Section 2.8.

1.2.5 Practial Methods

Methods that are currently used for the purpose of CDE, CP and QR are manifold. We will give an overview over the most prominent and well performing methods in the following.

Mixture Density Networks (MDNs) are probably the most prominent method for CDE by [Bishop, 1994]. They are based on the idea of modeling the conditional PDF as a mixture of simple distributions e.g. Gaussians or Laplacians. In MDNs a NN is used to predict the parameters of the mixture components. In the case of Gaussians, the parameters are the mean, variance and the component weights. The mixture components are then combined to form the full conditional PDF. MDNs are very expressive and can model multimodal distributions very well. However, they are also very prone to overfitting, but recent methods like [Rothfuss, Ferreira, Boehm, et al., 2019] aim to mitigate this problem effectively. MDNs are usually optimized using the negative log likelihood loss function.

Kernel Mixture Networks(KMNs) are a more recent development by [Ambrogioni et al., 2017]. They are based on the idea of selecting kernel centers from the training samples by clustering techniques like K-Means. The kernel centers are then used to form a kernel mixture model, where the kernel centers are the mixture components. The kernel mixture model is then used to estimate the conditional PDF. KMNs are less expressive than MDNs, but they are also less prone to overfitting and can be more robust in practice. Conceptually they are similar to MDNs where the mixture components are formed by the kernel centers. KMNs are also optimized using the negative log likelihood loss function.

Multiple Quantile Regression (MQR) is a method that is based on the idea of estimating multiple quantiles of the target variable. In particular, when doing simple QR we may only have a single quantile, which can be choosen aribtrarily. However, in MQR we estimate multiple quantiles at once. This can be done by using a single NN that outputs multiple quantiles at once or by using multiple NNs that each output a single quantile. MQR has been used to accomplish CP in the past by [Sesia and Y. Romano, 2021] very successfully. In particular, for CP it is the current state-of-the-art method. MQR is optimized by using the Pinball Loss objective function, which is a quantile regression specific loss function.

In conclusion the topic of uncertainty estimation is rapidly growing recently and in works like [Chernozhukov, Wüthrich, and Zhu, 2021] implicitly it has been shown that there is a connection between CP, CDE and QR. However, no previous work has gone into the details of the exact relationship between those methods. Moreover, the conceptual position of epistemic uncertainty in the context of CP, CDE and QR is not well understood.

1.3 Research Questions

Within this work we aim to answer two main questions. The first and most essential question is how exactly CP, CDE and QR are related. As noted previous methods already implicitly show there must be a connection [Sesia and Y. Romano, 2021; Chernozhukov, Wüthrich, and Zhu, 2021; Chung et al., 2020] but lack a precise framwork for their practical application.

Based on this main question other questions arise:

- Can we develop a general framework on which basis techniques from one of those methods can be transferred to another method?

- What optimization strategy should we choose or which ones can we even choose. CDE mostly relies on the MLL objective function, while CP often relies on the pinball loss. Based on the insights we gain in this work, we want to gain more insight into this question.

- Based on the relation between those methods, can we gain more insight into the often made claim that CP and QR are fundamentally distribution free methods? If they are related with CDE, which is often considered a distribution based method, then how can they be distribution free?

The second main question is how uncertainties, in particular aleatoric and epistemic uncertainties, are present in those uncertainty methods and in particular what kinds of in the sense of [Hüllermeier and Waegeman, 2021]. In particular, one major observation is that even on the train data often uncertainty models are not calibrated, but it has not really been extensively treated yet why this is. We often just calibrate CP on the calibration set as in [Sesia and Y. Romano, 2021] but what assumptions are we making when recalibrating. This is also rooted in the realization that in the context of CP, being calibrated alone is actually a trivial task since we can just calibrate on the marginal distribution of the targets.

1.4 Contributions

The main contributions of this work are as follows:

- We show that CDE, CP and QR all have the same goal, that is they all restric the set of possible conditional PDFs, and that all concepts of one task-domain can fully be transferred to the other one.

- We propose a novel way to perceive the MLL objective function, where we show that it is equivalent to the objective function of CP, as we define it. This allows us to split the MLL objective into a constrainted optimization problem, where we

    intuitively minimize the size of the peaks (we make them as narrow as possible) with the constraint that we maintain calibration.

- We show that it might improve CP intervals if we can use properties of inductive biases provided by e.g. a mixture of gaussian estimtated by using MDNs.

- We offer a novel way to estimate epistemic uncertainty in CDE and CP methods, where we show that calibration as often done in CP, actually infuses epistemic uncertainty into the modeled PDF that describes only aleatoric uncertainty.

- Finally we empirically verify our insights on multiple benchmarks and show that our method is competitive with state-of-the-art methods and that it can be applied to a wide variety of tasks. Thereby, we also provide a general overview of hyperparameters that are generally a good choice for CDE,CP and QR tasks. In particular we also propose few new hyperparameters and analyze their impact.

1.5 Structure of the Work

First, in Section 2 we give a thorough introduction into CP, CDE and QR and show they are fundamentally the same task. Moreover, we show how we can infer CP from CDE and how we can estimate epistemic uncertainty in CDE and CP methods. In Section 3 we show how our insights can be applied to a wide variety of tasks and how they improve the performance of CDE, QR and CP methods. Finally, in Section 4 we summarize our insights and give an outlook on future work.

Notably, novel contributions and existing concepts are intervoven in the theoretical part of this work, as tearing them appart would heavily reduce the smooth line of argumentation present in this work and make notation much harder. In particular, this is because we will generalize existing concepts with new interpretations. However, we will always explicitly state if a concept is novel or if it is based on existing concepts.

2 Theoretical Analysis

2.1 Preliminaries

In the rest of this work we will unless stated otherwise always be assuming a machine learning task where samples have the assumption of exchangability. Moreover, for the theoretical part of this paper, we also assume that we have unlimited samples unless stated otherwise which is necessary to make certain theoretical statements and in particular with limted data those statements all hold asymptotically.

Thus, unless stated otherwise, let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. Furthermore, let $\mathbf{Z}_i = (\mathbf{X}_i, \mathbf{Y}_i)$ random variables on the index set $\mathcal{I}$ with $\mathbf{X}_i : \Omega \to \mathbb{R}^n$ and $\mathbf{Y}_i : \Omega \to \mathbb{R}^m$ for all $i \in \mathcal{I}$, where each pair represents one sample. Moreover, let all $(\mathbf{X}_i, \mathbf{Y}_i)$ be exchangable, which means that for any permutation π of the index set $\mathcal{I}$ the join probability distribution remains the same, i.e.

$$\forall \mathbf{x}_i \in \mathbb{R}^n, \mathbf{y}_i \in \mathbb{R}^m : \mathbb{P}\left(\bigcap_{i \in \mathcal{I}}(\mathbf{X}_{\pi(i)} \leq \mathbf{x}_i, \mathbf{Y}_{\pi(i)} \leq \mathbf{y}_i)\right) = \mathbb{P}\left(\bigcap_{i \in \mathcal{I}}(\mathbf{X}_i \leq \mathbf{x}_i, \mathbf{Y}_i \leq \mathbf{y}_i)\right) \quad (2.1)$$

Furthermore, let $I : \Omega \to \mathcal{I}$ be a random variable defined on the probability space that selects an index at random with the further simplification that every index has the same probability to be selected (uniform).

This extensive notation is required mostly in order to define exchangability, however, in many proofs in this paper we will not require the use of the probability space explicitly, in particular with the index set since we often just integrate over the whole sample space $\mathbb{R}^{n+m}$.

The task of the ML methods discussed here is always to predict some property, like the conditional PDF, about the target variable $\mathbf{Y}_I$ given the features $\mathbf{X}_I$. In the more practical case we only have access to a subset of the indices in the index set, which is the observed data set $\mathcal{D} = \{(\mathbf{X}_i, \mathbf{Y}_i)\}_{i \in I_\mathcal{D}}$, with $|I_\mathcal{D}| < \infty$.

Moreover, any model that we discuss here, regardless if it is CDE, CP or QR, will be parameterized by some parameters $\theta \in \Theta$ where Θ is the parameter space. Furthermore, we will make the assumption that the model class can perfectly model the optimal model, which seems like a strong assumption, but considering that we focus on model classes that either can be tweaked to be very expressive or NN's that even are universal function approximators [Hornik, Stinchcombe, and White, 1989], this assumption is not unreasonably strong. The optimal parameter set is indicated by θ^*.

For the above definitions the corresponding PDF of and event $\mathbf{z} = (\mathbf{x}, \mathbf{y}) \sim (\mathbf{X}_I, \mathbf{Y}_I)$ is defined by

$$p(\mathbf{x}, \mathbf{y}) := \frac{d^2 \mathbb{P}(\mathbf{X}_I \leq \mathbf{x}, \mathbf{Y}_I \leq \mathbf{y})}{d\mathbf{x} d\mathbf{y}} \tag{2.2}$$

for $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$. It is left as a hint to the reader that $\mathbb{P}(\mathbf{X}_I \leq \mathbf{x}, \mathbf{Y}_I \leq \mathbf{y})$ in the above equation is the cumulative distribution function (CDF). The marginal and conditional PDFs can then be found by integrating out and normalizing with the marginal respectively.

Finally in order to analytically show certain results we require some standard assumptions of the underlying conditional PDF $p(\cdot \mid \mathbf{x})$ which hold $\forall \mathbf{x} \in \mathbb{R}^n$.

Definition 2.1.1 (Standard Assumptions).   1. The PDF p is continously differentiable a.e.

2. $\forall b \in \mathbb{R}^+ : \mathbb{P}(p(\mathbf{Y}) = b \mid \mathbf{x}) = \lambda(p(\mathbf{Y}) = b \mid \mathbf{x}) = 0$

3. $p > 0$ a.e.

Those assumptions are weak in practice since we can approximate any PDF that does not fullfill those assumptions with a PDF that does fullfill those assumptions arbitrary well. We refer to [Klenke, 2013] for a formal argument why this is true.

In the following we will first detail the three main uncertainty centric tasks already introduced in Section 1.2, namely CDE in Section 2.2, CP in Section 2.4 and QE in Section 2.3. We will then show how those tasks are fundamentally the same in Section 2.5, that optimizing the MLL objective function is equivalent to optimizing the CP objective function as we define it in Section 2.6 and finally a rigorous examination of recalibration where we show that it infuses epistemic uncertainty into the modeled conditional PDF that describes only aleatoric uncertainty in Section 2.7 and Section 2.8. It given as a recommendation to the reader to read the sections in order as certain essential concepts that are introduced in the first sections are used in the later sections.

2.2 Conditional Density Estimation

The goal of CDE methods is to estimate the conditional PDF $p(\mathbf{y} \mid \mathbf{x})$ of samples $(\mathbf{x}, \mathbf{y}) \sim \mathbf{Z}_I$. The objective function used for CDE is usually likelihood function, which is given by $p(\mathbf{y} \mid \mathbf{x})$ for one sample and $\mathbb{E}_\Omega \left[\log p(\mathbf{Y}_I \mid \mathbf{X}_I) \right]$ generally, where we take the logarithm of the likelihood function and thereafter can take the integral (the expectation) over the whole sample space, which is valid since the logarithm is a strictly monotonous function.

The reason we do not restrict ourselves here to a finite sample set is that we want to make general statements about the training objective of CDE methods. The objective in a finite sample set setting is analogous, but we can not make general statements about the whole sample space.

2.2.1 Smoothness Assumptions

As we usually in the context of ML like to obtain a model that can generalize, we need to make smoothness assumptions in the context of CDE, as without them it is easy to define the optimal model as the delta function at the observed data points which is not a useful model as it will not generalize to new data points.

As we can see in the work of [Rothfuss, Ferreira, Boehm, et al., 2019] the objective function of the model equals

$$\arg \max_{\theta \in \Theta} \sum_{i=1}^{n} \log \hat{f}_\theta \left(x_i \right) = \arg \min_{\theta \in \Theta} \mathcal{D}_{KL} \left(p_\mathcal{D} \| \hat{f}_\theta \right) \tag{2.3}$$

where $p_\mathcal{D}$ is the delta distribution with peaks at the observed target locations. If we consider the full sample space in the optimization problem, then $p_\mathcal{D}$ reduces p. Intuitively this equation indicates that MLL estimator is the same as the estimator that has the minimal Kullback-Leibler divergence between the true distribution and itself.

It is easy to see that finding the optimal model for this problem, at least if we limit the number of samples that we can learn from to a finite amount, is meaningless since it will not generalize with the delta function. However, if we make the assumption that the target variable is smooth, then we can assume something like a Gaussian distribution over each observed target and input variable. This is also the apporach that [Rothfuss, Ferreira, Boehm, et al., 2019] introduce in their work where they analytically show that adding noise to the targets and inputs is beneficial for the generalization of the model. In order to gain an intuitive understanding why this is required one needs to imagine the input and output variables as a join probability distribution. If we add noise to each sample than this noise spans thru all dimensions of this distribution and thus we can find reasonable output predictions for unseen input features.

Notably, even if adding noise, the log likelihood and the KL-divergence between the smoothed true distribution and the estimated distribution still remain the optimization objective.

2.3 Quantile Regression

The goal of QR is to estimate specific quantiles of the target variable given the input variables. Formally, that means we want to predict $Q(\mathbf{x})$ for a quantile q and $(\mathbf{x}, \mathbf{y}) \in \mathbf{Z}_I$ such that $\mathbb{P}(\mathbf{Y}_I \leq Q(\mathbf{X}_I)) = q$. The most used objective function for QR is the pinball loss as introduced by [Koenker and Bassett Jr, 1978], which for one sample is defined as $\max((\mathbf{y} - Q(\mathbf{x})) \cdot q, (\mathbf{y} - Q(\mathbf{x})) \cdot (1 - q))$ and where we find the optimal parameters at $\min \mathbb{E}_\Omega \left[\max \left((\mathbf{Y}_I - Q(\mathbf{X}_I)) \cdot q, (\mathbf{Y}_I - Q(\mathbf{X}_I)) \cdot (1 - q) \right) \right]$ where we take the expectation over the whole sample space. [Koenker and Bassett Jr, 1978] show that the pinball loss

is optimal at the true quantile function. There have also been more recent works with different loss functions, like in the work by [Chung et al., 2021], however, for the scope of this work it is sufficient to use the definition of the pinball loss.

In particular, when estimating a tight grid of quantiles, the QR model can be used to estimated the full conditional CDF of the target variables given the input variables. When estimating a tight grid on limited data, it can happen that two quantiles are switched in position. In this case it is a common practice to simply swap the two quantiles out, i.e. we sort the outputs of the model and only then apply the pinball loss. This is a common practice in QR and is also used in the work of [Sesia and Y. Romano, 2021].

2.4 Conformal Prediction

Conformal Prediction generally is the task of finding sets of possible outcomes that in expectation will contain the true outcome with a certain miscoverage level α. Formally, that means we predict sets of possible outcomes $C(\mathbf{x})$ where $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbb{P}(\mathbf{Y}_I \in C(\mathbf{X}_I)) = 1 - \alpha =: a$, where a is the confidence level that we will often use for the ease of notation. In practice, we will often not be able to fullfill the equality and in this case we generally prefer overcoverage, i.e. $\mathbb{P}(\mathbf{Y}_I \in C(\mathbf{X}_I)) \geq 1 - \alpha$.

This rather general definition has moreover been extended to methods where we aim to find some specific sets of outcomes and not just any kind of set that fullfills the miscoverage level. There have been many different methods proposed to achieve this [Sesia and Y. Romano, 2021; Chernozhukov, Wüthrich, and Zhu, 2021; Balasubramanian, Ho, and Vovk, 2014; Shafer and Vovk, 2008], a very popular method being quantile regression on the central 90% of density. There we aim to predict the invervals given by $[Q(\frac{\alpha}{2}), Q(1 - \frac{\alpha}{2})]$, where Q is the quantile function. However, in more recent works [Sesia and Y. Romano, 2021; Chernozhukov, Wüthrich, and Zhu, 2021] more advanced methods have been proposed that aim to estimate the shortest possible intervals for a given miscoverage level α. However, those approaches both are still aiming to predict single intervals which might not be desireable if the true distribution is multimodal. In particular, [Sesia and Y. Romano, 2021] argue that it is often not desirable to predict multiple intervals for the reason that they are harder to interpret for domain experts. In another work by [Izbicki, Shimizu, and Stern, 2022] they propose a method 'hpd-split' that can predict multiple intervals with the

highest probability density, but they do not argue why this is actually desireable from a practical point of view.

In this work however, later in Section 2.6, we will give argumentations why it is actually desirable to predict multiple intervals in the case of multimodal distributions and how this can be achieved by means of CDE. Moreover, we show that even when predicting single intervals using our method, it is almost as powerful as previous methods and more interpretable. Before we dive into this, we will show in the next section how CDE and CP are fundamentally the same task that will allows us to gain a powerful perspective on CP, QR and CDE methods.

2.4.1 Trivial CP

CP can be degenerated to a trivial task where we only predict the marginal distribution of the target variable and apply a way to construct a CP interval on that basis. However, this would completely neglect the information in the input variables and would not be a useful model. In particular, that is why we usually extend the core definition of CP as described in Section 2.4 to find specific sets of outcomes that are based on the input variables and not only the target variables.

2.5 CP, CDE and QR are the Same Task

Before going into details why this is the case, the motivation behind showing this result is mainly that it gives us a strong foundation on which we can use techniques used for one of the methods also directly for the other methods. In Section 2.7 we will based on that show that we can apply recalibration which is mainly used in CP also for QR and CDE.

To give an intuitive introduction into this section one can see that one could argue that CDE is the most general of the three tasks and both CP and QR are sub-tasks of CDE. Sub-tasks in this context means that the two methods only model information also used for constructing CDE models and possibly less. For the connection between CDE and QR, we can argue that the QR predicts points on the conditional CDF, which can be fully described by the conditional PDF which is predicted by CDE. For the connection between QR and CP, we can argue that since CP regions need to capture, in expectation over $\mathbf{Z}_I$, a

specific proportion of the target variable, the difference between high and low quantiles[1] that produce the borders of the CP regions must in expectation sum up to the desired proportion. This means with a very dense QR grid we can find any CP regions of interest with asymptotic precision.

The precise analysis in how those uncertainty methods are the same task will be explained in two steps on different conceptual levels. First, we show that the establishment of models, that is the model producing functions, that do one of the tasks are deeply connected between the methods in Section 2.5.1. Secondly, we show that in the results that those methods produce they also share a common goal in Section 2.5.2.

2.5.1 Connection between the Model Producing Functions

A model producing function is a any function that takes the training data and produces a model. In particular, we focus on the set of model producing functions $\mathcal{G}$ that can consistently produce models that can accurately do any of the three tasks with asymptotic gurantees and gurantees that the models are not over- or underfit. While those are strong assumptions, there exist techniques to approximately gurantee those like adding noise for avoiding overfitting [Rothfuss, Ferreira, Boehm, et al., 2019].

Notably $\mathcal{G}$ is a bit of a philosophical instance since it also includes the researchers who construct the model or other factors like this. This is also based on the insight that after a model has been produced, it does not really make any assumptions about the problem, but the model producing function does. To be clear, yes, a model that has as output e.g. Gaussian component parameters can be seen as making assumptions about the problem, however, without the model producing function that produces this model, we do not have any gurantees or knowledge about how those components are related to the data or the problem; They might as well be random. Moreover, the researcher who decided to use a MDN also belongs already to the model producing function in this instance, in particular, without the knowledge/assumptions of this researcher, the model architecture of the model which could represent a MDN is also unknown.

Without diving more into the philosophical nuances of this, we will now show that any

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[1]When we talk about high and low quantiles of CP regions we mean that any CP method produces for a given sample certain regions that can be described by the borders of the intervals within this region. For example, a region might be described by $[3.4, 5.1] \cup [7.2, 7.3]$ and for those borders there also exist quantiles that describe the borders of the regions, i.e. it could be $Q(0.05) = 3.4$ and $Q(0.5) = 5.1$ etc

function $g(\mathcal{D}) \in \mathcal{G}$ that can consistently produce models that can accurately do any of the three tasks all only need to model the same true probability density function $p(\mathbf{x}, \mathbf{y})$ or parts of it.

In practice, the task that produces a model is often specified as an optimization problem that is solved to find the model parameters i.e. gradient descent in NNs or also hyperparameter search alogrithms which might include Bayesian hyperparameter optimization. Mostly, the task is to find a model that is most optimal for an evaluation function.

Theoretical Bridge: CDE and CP

By definition, CP is any method that aims to predict regions, that in expectation should contain the true label with a significance level α. Formally, $\mathbb{P}(\mathbf{Y} \in U(\mathbf{X})) = 1 - \alpha$. It is essential to notice here that the PDF is explicitly part of the definition of any CP method.

The evidence for the claim that we can provide here is based on the No Free Lunch (NFL) theorem [Wolpert and Macready, 1997]. The NFL theorem states that for any learning algorithm to perform well on a broad class of problems, it must necessarily make some implicit or explicit assumptions about the nature of those problems. This theorem tells us that for any algorithm $g \in \mathcal{G}$ to work well for CP it must contain some assumptions about the problem. The limitation of the NFL are that we can not directly say that it must be the PDF.

However, it appears a reasonable conclusion that the PDF or parts of it are those assumptions made via the NFL theorem since the CP problem is defined thru it and it would not need any other assumptions to fullfill the requirement. Moreover, it would seem unreasonable that a method that can fullfill the constraint could completely ignore the structure of the PDF, since it would basically be random then. It was not possible to find an existing work that provides a general theorem that lets us make statements about that if a model producing function is defined thru a certain property, like the PDF, then it must be biased with this information and it is out of the scope of this work to proof such a general statement, so we will leave it as a very reasonable hypothesis and for a rather technical mathematical future work to prove this statement.

Knowing this and also knowing that as CDE fully models the PDF, we can conclude that producing a CP model is a sub-task of producing a CDE model. In particular, sub-task is

meant in the sense that the model producing function $g \in \mathcal{G}$ that produces a CP model must implicitly consider only parts of what a method that produces a CDE model must consider. Notably, this is also quite philosophical since it is unclear what it means to consider the PDF or parts of it, but we suppose that it must be encoded in the loss function that can identify certain characteristics of the PDF.

Theoretical Bridge: CDE and QR

Analogous to CP we know that QR is defined as any method that can predict quantiles q of the target space where we have that $\mathbb{P}(\mathbf{Y} \leq Q(\mathbf{X})) = q$. Again, the PDF is explicitly part of the definition of any QR method and with the NFL and the argumentation in Section 2.5.1 it follows that QR is a sub-task of CDE.

## 2.5.2 CDE can fully be modeled by CP and QR

We know from Section 2.5.1 and Section 2.5.1 a way to understand how QR and CP are sub-tasks of CDE. However, we do not know yet what the practical implications of this are. In particular, we do not know if we can fully model the PDF with CP and QR. In this section, we will show that this is indeed the case.

Let $\mathcal{P}$ denote the set of all possible PDFs over $\mathbb{R}^m$. We define a function $\mathscr{P} : \mathbb{R}^n \to 2^{\mathcal{P}}$, where $2^{\mathcal{P}}$ represents the power set of $\mathcal{P}$ (i.e., the set of all subsets of $\mathcal{P}$). This definition will be used from now on in this work. Moreover, $\mathscr{P}$ is parameterized by θ as $\mathscr{P}_\theta$. Conditional Density Method (CDM) refers to any method that imposes a restriction on the conditional PDFs which contains CP, QR and CDE. The level of restriction can differ between CDMs. In particular, the restriction is always at least to the extent that the desired target type can be obtained uniquely from the restricted set of PDFs. For CDE only a single element is contained in this sets for each $\mathbf{x} \sim \mathbf{X}_I$ and for QR all PDFs that have the integral up to a specific quantile of probability mass and for CP it is a set of PDFs that make it possible to infer that a specific region contains a certain amount of probability mass. In Figure 2.1a and Figure 2.1b we can see how the restriction on a CDF can look like for different quantiles.

We can now infer quite clearly what information is required in a $\mathscr{P}_\theta$ in order to do CP, QR or CDE. For QR, we only need to know that $\forall \mathbf{x} \in \mathbb{R}^n \exists q \in (0,1) \forall p \in \mathscr{P}_\theta(\mathbf{x}) : \int_{-\infty}^{Q(\mathbf{x})} p d\mathbf{y} = q$
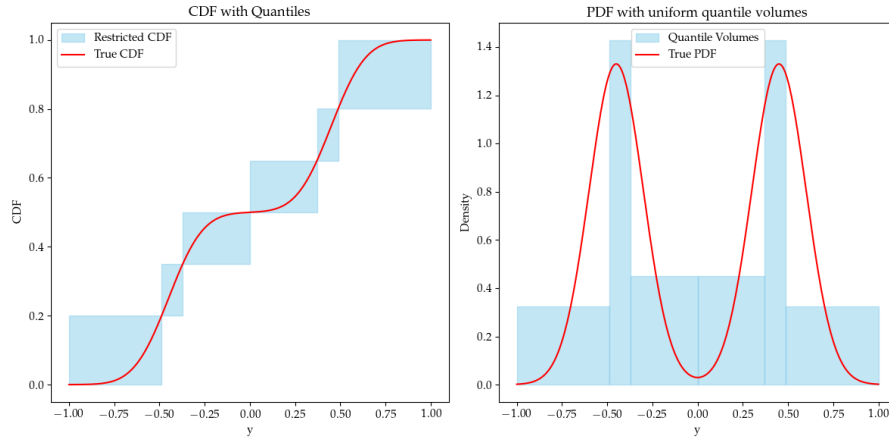
(a) Restricted CDF with 5 quantiles
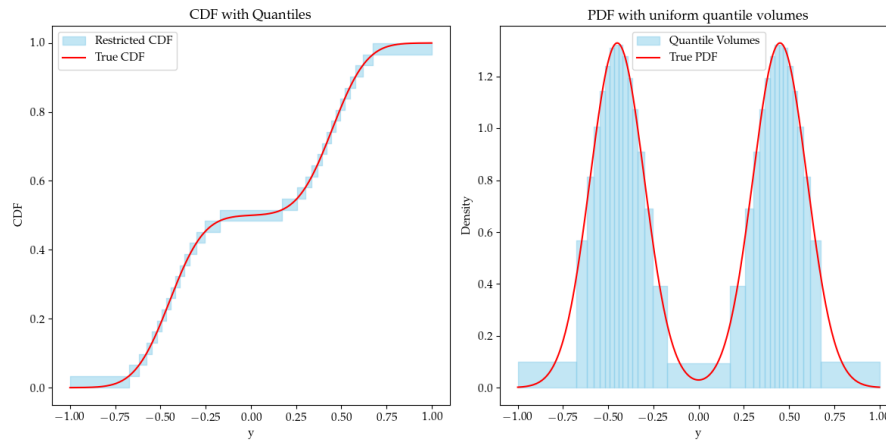
(b) Restricted CDF with 30 quantiles

Figure 2.1: We can see that if we increase the number of quantiles that we predict, the restriction on the CDF becomes more and more strict and we approach the true PDF on the right side.

which can also be intuitively understood from Figure 2.1a. Even tho we do not know the full PDF when only looking at the restricted PDF we can still infer certain quantile levels precisely. For CP, if we want to be conditionally calibrated as in [Sesia and Y. Romano, 2021], we need to know that $\forall \mathbf{x} \in \mathbb{R}^n \exists \alpha \in (0,1) \forall p \in \mathscr{P}_\theta(\mathbf{x}) : \int_{C(\mathbf{x})} p(\mathbf{y}) d\mathbf{y} = 1 - \alpha$. In Figure 2.1a we can see that this could simply be an interval between two quantile levels that we predict. If we only require marginal calibration we only need to know that this is true in expectation over $\mathbb{R}^n$ which is a weaker restriction but less commonly of interest in the literature. For CDE we need to know that $\forall \mathbf{x} \in \mathbb{R}^n : |\mathscr{P}_\theta(\mathbf{x})| = 1$. Because of this, also practically it is quite clear that there is no ambiguity in predicting qunatiles or CP regions and we can just choose any quantile or region if we have a CDE model.

However, in order to be able to obtain $\mathscr{P}_\theta$ such that it is valid for CDE via CP or QR we need to be able to restrict it to be a single element. Therefore, we need to observe that we can just apply multiple QR or CP restrictions to $\mathscr{P}_\theta$ by performing multiple CDM that only partially restrict $\mathcal{P}$ for each $\mathbf{x} \in \mathbb{R}^n$:

$$\forall x \in \mathbb{R}^n : \mathscr{P}_\theta(x) = \bigcap_{i=1}^{n} \mathscr{P}_{\theta_i} \tag{2.4}$$

Where each $\mathscr{P}_{\theta_i}$ is a restriction on $\mathcal{P}$ that is valid for CDE, CP or QR. Thereby one needs to be careful in the definition of each restriction not to have two restrictions that contradict each other and thus produce the empty set, however this is generally approximately possible in practice because of the asymptotic properties of the CDMs. Moreover, even if we have two model producing functions that contradict each other, practically that often is not a problem. For example if we do multiple quantile regression and observe quantile inversion, then it is a common practice to simply swap the two quantiles out. In this case in is common practice to just take this then as the final $\mathcal{P}_\theta$.[2] Moreover, combining restrictions of $\mathcal{P}_\theta$ implicitly is already a common method in the literature, e.g. [Sesia and Y. Romano, 2021] where multiple quantile regression is used in order to obtain a grid of quantiles that can be used to infer CP regions.

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[2]This common practice, while it results in a valid $\mathcal{P}_\theta$ does generally and also in literature lack a theoretical foundation an is more a "trick of the trade". We will not analyze the theoretical validity of doing this.

We can arbitrarily restrict $\mathcal{P}_\theta$ if we can make those restrictions arbitrarily tight with a method as we can also see in Figure 2.1b. In the case of QR we can simply make an infinitely dense quantile grid which accomplishes that. That is, in the limit of the number of quantiles torwards infinity the requirement for CDE will be fullfilled. It is easy to see, since in the limit for each quantile $q \in (0, 1)$ we will have a unique quantile and from that we can clearly infer the PDF uniquely, that is, from the quantile function we can recover the PDF.

For CP it is a bit less obvious since we could define CP intervals anywhere and it is unclear how we would make sure that we still restrict everything even if we increase/decrease the confidence level. However, most if not all CP methods in the literature (e.g. [Sesia and Y. Romano, 2021; Chernozhukov, Wüthrich, and Zhu, 2021]) are based on methods that allow for a nested way of increasing/descreasing CP regions which relates to how calibration works in CP as we can see in Section 2.7. Nested regions essentially allow that we indirectly also obtain all quantile levels precisely and thus also the PDF.

Notably those methods to obtain CDE from QR or CP all only work approximately and asyptotically. However, CDE methods also only work asyptotically and are practically not fully expressive, in particular if they can not overfit, which is an assumption. This implies that also CDE practically can not be accurate completely and thus there must be basically some freedom in the restriction of the PDF even for CDE methods. This completes the argument that CDE, CP and QR are fundamentally the same task, that is restricting the PDF $\mathcal{P}$ in a way that we can infer the desired target type from it and we can use techniques from one method for the other methods or more generally that implicitly we are always only restricting the PDF $\mathcal{P}$ and from that we can under certain conditions infer the desired target type.

Moreover, if we now want to obtain the CDE target from a not fully restricted $\mathcal{P}$ we can simply make smoothness assumptions, since we need to do that anyways as described in Section 2.2.1 and implicitly also designated CDE methods do that as can be seen from the argment above that also CDE methods practically need some freedom in the restriction of the conditional PDF.

2.5.3 CDM to improve current CP

In this work we argue, that by first estimating a more complete picture of the true conditional density via the CDM-theory instead of only restricting it partially we can improve the performance of CP and QR. In particular, by restricting $\mathcal{P}$ more we argue that this provides a regulatory effect where unreasonable partial predictions are purged. This is conceptually a bit similar to the concept of ensembles if we do this by means of multiple quantile regression.

For example, if we were to predict a quantile at a specific position that might not be perfectly accurate, then by having a tight quantile regression grid over the whole space $(0, 1)$ we will stabilize this since it is likely in that case that quantile inversion appears and by swapping/sorting the quantiles we can obtain a valid PDF. The same applies to CP.

This implicitly also means that given that the CP/QR method only needs to model a subset of the information of the PDF, it will not worsen the performance if we also try to model other parts of the PDF $\mathcal{P}_{\theta'}$ and use it as regularizer in practice. I.e. if we only want the median then it would not hurt the performance in practice if we also predict the 0.1 and 0.9 quantiles and use them as regularizer.

2.5.4 CP methods are practically not distribution free methods

In the literature it is often stated for the benefit of CP that it is distribution free [Angelopoulos and Bates, 2021] which means that we do not make any distributional assumptions within the model. Moreover, if we were to infer CP by means of first estimating a CDE e.g. with a MDN then we on first glance directly make distributional assumptions since a MDN is based on distributional components. In the literature it is argued that freedom of distribution has certain benefits, e.g. that we can predict any arbitrary PDF.

However, even if we introduce distributional assumptions, in fact, it can be shown that when using MDNs for CDE with an infinite number of Gaussian components, we can predict any arbitrary PDF [Bishop, 1994]. Moreover, socalled distribution free CP methods, when limited to a finite number of model parameters, as it is always the case in practice, similarly have distributional assumptions introduced by the modeling limitations of NNs. Those modeling limitations of neural networks or any other finitely expressive model.

For NNs those are present in the initialization of weights with a certain distribution and the distribution of activations after linearities and activation functions. Each activation function imposes a certain distribution on the model. So both, CP and CDE, are not distribution free methods when limiting the expressivity of model dispite common literature suggesting CP is or can be made distribution free. Moreover, being distribution free does not really bring any practical benefits. Further, one could argue that being distribution free just means being infinitely expressive in the model which clashes with the requirement of smoothness as described in Section 2.2.1. In conclusion, we can say that no pracitcal CP methods are distribution free and that it is not a benefit to be distribution free in practice anyways.

2.5.5 Limitations of the Bridge between CDMs

While the statements made about CDE, CP and QR being the same task, they all only directly apply under our standard assumptions. However, even without the standard assumptions, without proof, we reasonably suspect that the same statements hold in a practical scope. In those cases it might be that the conditional CDF has discontinuities, flat spots or zero distribution spots for which of course all three methods will struggle. For example QR might behave strangely since we have a jump in the CDF at this point or on points between the quantile level QR is trying to predict. However, since we can approximate any PDF that does not fullfill our standard assumptions with a PDF that does, we can still argue that the same statements hold approximately and in practice anyways.

Moreover, when combining restrictions on the PDF, current methods, like swapping quantiles with quantiles inversion, to combine them while maintaining a valid PDF are not well studied and also impose assumptions on the PDF which are often quite arbitrary and of practical nature. However, as all CDMs are asymptotically consistent, cases where the restrictions contradict are an artifact of limited data and there approximate solutions are used anyways making it not really a limitation. However, it would be good to have a more theoretical foundation for those methods.

The final limitation is that we only showed a very reasonable hypothesis in Section 2.5.1 with clear evidence why the model producing function should do sub-tasks of CDE in CP and QR, however, we admit that a rigorous mathematical proof is missing, which is

left for future work. However, we argue that the evidence is strong enough to make this claim.

2.5.6 Conclusion on the Bridge between CDE, CP and QR

By Section 2.5.1 and Section 2.5.1 we can see that in the background of each CDM the restriction on all PDFs f_θ stands. This has two major implications:

Firstly, any technique on a CDM also implicitly (and actually primarely) acts on f_θ and thus can be thru $\mathscr{P}_\theta$ translated to any other CDM. For example if we were to decide that the standard deviation of a CDE model is to be inceased a bit by a particular function (for all $\mathbf{x} \in \mathbb{R}^n$ for simplicity), e.g. $h(p) = 2p$, then this will clearly be reflected in the restricted distributions $\mathscr{P}_\theta$ which means we also could find the generalized form of h which explicitly acts on $\mathscr{P}_\theta$ and thus can be applied to any CDM. In this case it would be for an $\mathbf{x} \in \mathbb{R}^n$ $h(\mathscr{P}_\theta(\mathbf{x})) = \left\{ 2p : p \in \mathcal{P} \wedge \frac{p}{2} \in \mathscr{P}_\theta(\mathbf{x}) \right\}$, i.e. we just apply the f to each element in $\mathscr{P}_\theta(\mathbf{x})$. So we see that any technique that acts on a CDM can be translated to any other CDM with that logic.

Secondly, any CDM goal can be done with any other CDM e.g. we can get a full conditional PDF from a method that does QR or CP.

2.6 Optimal Conformal Prediction

In this section we first define what we mean by optimal CP and then show how we can infer optimal CP from CDM by using a novel method in this context. We will give a new perspective on the optimization objective of CDMs, which often is likelihood, and show how it relates to the definition of optimal conformal prediction that we give here. This relationship is of theoretical interest and also has practical implications as we will show in Section 2.7.

In order to develop our argument we first define what we mean when we say that a CP method is optimal. We orient ourselves on the work of [Sesia and Y. Romano, 2021] where they define the optimal CP method as the one that predicts the shortest intervals for a given miscoverage level α. However, instead of only predicing single intervals, we argue

that it is simpler and more practical to simply the shortest possible regions of the target space that contain the target variable in expectation with the required confidence level.

Let $\alpha \in (0,1)$ be a significance level. Then the goal of conformal prediction is to find a function $C : \mathbb{R}^n \to \mathcal{B}(\mathbb{R}^m)$ that can predict the subsets with the smallest Lebesgue measure λ marginalized over Ω with significance α. That means we want $\mathbb{P}(\mathbf{Y}_I \in C(\mathbf{X}_I)) = 1 - \alpha$ with $\int_\Omega \lambda(U(\mathbf{X}_{I(\omega)}(\omega)))d\mathbb{P}(\omega)$ small.

Formulated as a proper constrained optimization problem, we can rewrite this as:

$$\min_U \quad \int_{\mathbb{R}^{m+n}} p(\mathbf{z})\lambda(C(\mathbf{x}))d\mathbf{z} \tag{2.5}$$

$$\text{s.t.} \quad \int_{\mathbb{R}^{m+n}} \mathbb{1}_{\mathbf{y} \in C(\mathbf{x})}d\mathbf{z} = a \tag{2.6}$$

2.6.1 New perspective on MLL and Optimal CP

The method to infer the intervals that will be used by us is the highest density regions method. Using this we can, given a PDF, infer the set of intervals with the shortest summed Lebesgue measure. In particular, we are shifting our focus from looking at the shortest regions to looking at the regions that contain the most probability mass, even tho that is very similar and mostly the same with HDR there are some delicate differences. This is partiulary beneficial since regions with high densities should usually not be ignored in practice as they often indicate important events as we will discuss in depth in Section 2.6.2

If C is being calculated by first using a CMD to sufficiently restrict $\mathscr{P}_\theta$ in the sense of Section 2.5.2 and then using Highest Density Regions (HDRs) as defined by [Hyndman, 1996] to obtain a significance level of α, then C is a function of the CDM and the significance level α. HDR is by [Hyndman, 1996] defined as:

$$H(f_a) = \{\mathbf{y} : f(\mathbf{y}) \geq f_a\}$$

with

$$f_a = \max_{f_a} \left\{ f_a \in \mathbb{R}^+ : \mathbb{P}\left(\mathbf{y} \in H(f_a)\right) \geq a \right\}$$

but it can be written equivalently as below. The below formulation is also the one being used in this work from now on.

$$H\left(f, a\right) := \left\{ \mathbf{y} \in \mathbb{R}^m : f(\mathbf{y}) \geq \max_{b} \left\{ b \in \mathbb{R}^+ : \mathbb{P}\left(\{\hat{\mathbf{y}} \in \mathbb{R}^m : f(\hat{\mathbf{y}}) \geq b\}\right) \geq a \right\} \right\} \quad (2.7)$$

where f is an arbitrary probability density function (PDF) and $a := 1 - \alpha$ is the confidence level. Note that $\mathbb{P}$ here is different from the one defined in the beginning and only here for defining HDRs. As the CDM in my case is parametric like MDNs it is more reasonable to write C a function of the parameterization of the CDM and the coverage level. So considering that, the initial goal of conformal prediction can be rewritten as:

$$\min_{\theta \in \Theta} \quad \int_{\mathbb{R}^{m+n}} p(\mathbf{z}) \lambda(H(p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta), a)) d\mathbf{z} \quad (2.8)$$

$$\text{s.t.} \quad \int_{\mathbb{R}^{m+n}} \mathbb{1}_{\mathbf{y} \in H(p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta), a)} d\mathbf{z} = a \quad (2.9)$$

where it is important that the $\hat{\mathbf{y}}$ is not the one we integrate over but more a demonstrative artefact we write to denote that $p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta)$ is a conditional density. Moreover Θ is the space of all parameters of the CDE method.

In the following if we write $p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta)$ we mean the PDF that can be inferred from a restriction of a CDM method parameterized with θ(see Section 2.5.2 for more details) and if we write $p(\hat{\mathbf{y}} \mid \mathbf{x})$, the true conditional density is meant. Notice, that the goal of this optimization problem is to optimize w.r.t. θ as it is basically the component that completely defines $p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta)$. This in turn means we need to find the argmin of the optimization in Equation 2.8.

Let θ^* be the argmin of the equation in Equation 2.8, we would like to show that

$$\theta^* = \arg\max_{\theta \in \Theta} \int_{\mathbb{R}^{m+n}} p(\mathbf{z}) \log p(\mathbf{y} \mid \mathbf{x}; \theta) d\mathbf{z} \tag{2.10}$$

which is the maximum likelihood estimator (MLE). This is of great importance if we wish to optimize a CDE method w.r.t. the maximum likelihood objective function in order to implicitly optimize for the conformal prediction objective function when using HDRs. In order to show this powerful statement we first need to develop some insight into the workings of the components in conformal prediction.

First, we require to show that $\lambda(H(p,a))$ is continously differentiable a.e. in order to make sensible statements. Its not that the intuition does not hold if its not continous, however, it complicates things and makes the statemtent more difficult. First in Lemma 2.6.1 below we show that this is fullfilled if the PDF fullfills our standard assumptions in Assumptions 2.1.1.

Note that the second assumption is fullfilled if it holds that p is changing a.e. or the area with derivative 0 is of measure 0 which is left without proof.

Lemma 2.6.1. *Let $p : \mathbb{R}^m \to \mathbb{R}$ be a probability density function for which Assumptions 2.1.1 hold where we neglect the $\mathbf{x}$ for breefity.*

Furthermore let p be for the random variable $\mathbf{Y}$ (for breefity we neglect the index) and let $g(b) := \mathbb{P}(p(\mathbf{Y}) \geq b)$. Moreover, $\lambda_p : [0,1] \to \mathbb{R}$ with $\lambda_p(a) = \lambda(H(p,a))$. Then the following statements hold for $a \in (0,1)$:

1. *$g(b)$ is strictly monotonic on the set $g^{-1}((0,1))$.*

2. *$g(b)$ is continous.*

3. *$g(b)$ is bijective on the set $g^{-1}((0,1))$.*

4. *$g(b)$ is continously differentiable a.e.*

5. *$B(p,a)$ is strictly monotonous on the set $B^{-1}((0,1))$.*

6. *$B(p,a)$ is continous.*

7. *$B(p,a)$ is bijecitve on the set $B^{-1}((0,1))$.*

8. $B(p, a)$ is continously differentiable a.e.

9. $\lambda_p(a)$ is strictly monotonous.

10. $\lambda_p(a)$ is continous.

11. $\lambda_p(a)$ is bijective on the set $\lambda_p^{-1}((0, \infty))$.

12. $\lambda_p(a)$ is continously differentiable a.e.

It is in particular required to not have any flat-splots in the PDF because otherwise per definition of HDR we can sometimes not obtain the shortest possible intervals for a confidence level *a* since we would not know which part of the flat-spot to include in the interval and which to leave out. In practice this would hardly be a problem.

Proof. 1. Monotonicity itself is obvious since we can not make the set $\mathbf{Y} \geq b$ larger when increasing b. For strict monotonicity on $g^{-1}((0,1))$ we require that $\forall b \in g^{-1}((0,1))$: $\frac{\partial \mathbb{P}(p(\mathbf{Y}) \geq b)}{\partial b} > 0$.

Let b be in $g^{-1}((0,1))$. We essentially need to show that for any $b' > b$ there exists a $\epsilon > 0$ such that $\mathbb{P}(p(\mathbf{Y}) \geq b + \epsilon) = \epsilon + \mathbb{P}(p(\mathbf{Y}) \geq b')$ which essentially means that there is change in g no matter how tight we choose the interval which comes directly from the definition of the derivative. So let b' be like so, and choose any $b'' \in (b, b')$, then continuity of p implies there exists a dense neighborhood around b'' which lies in $p(\mathbf{Y}) \in (b, b')$. In particular the fact that this neighborhood is dense also implies via the Lebesgue Density Theroem that this neighborhood has a positive Lebesuge measure and the assumption that $p > 0$ implies that it does also have positive probability measure. This implies the result of strict monotonicity.

2. To show continuity of g we use that it is because of monotonicity and boundedness of the $\mathbb{P}$ measure, that for any $\tilde{b} \in \mathbb{R}^+$

$$\lim_{b \downarrow \tilde{b}} g(b) = \mathbf{P}(\mathbf{Y} > \tilde{b}) \tag{2.11}$$

and also

$$\lim_{b\uparrow\tilde{b}} g(b) = \mathbf{P}(\mathbf{Y} \geq \tilde{b}) \tag{2.12}$$

where implicitly the continuity of p from above and below are used. This means the two limits are always the same if $\mathbb{P}(\mathbf{Y} = \tilde{b}) = 0$ which is an assumption and thus continuity of g is shown.

3. Bijectivity follows from strict monotonicity directly. To be exact why actually $g^{-1}((0,1))$ exists for every $a \in (0,1)$ we can use the monotonicty of g and the intermediate value therem since we can clearly find a b such that $g(b)$ is arbitrarily close to 0 and to 1 because of the PDF property of p and the fact that continuity of p implies boundedness of p.

4. Differntiability a.e. follows from the Lebesgue's Theorem for Monotonic Function as g is monotonic. Continous differentiability a.e. follows from the fact that g is uniformly continous due to the Heine-Cantor Theorem and this implies that the derivative is continous a.e. as well.

5. This follows by observing that g is bijective on $g^{-1}((0,1))$ which implies that the maximum of b where g is still greater-equal a will always exactly reach a. Then since g is $g^{-1}((0,1))$ is well defined and g is strictly monotonic we see that increasing a will always increase the possible b.

6. Continuity follows from the fact that g is also continous and bijective.

7. Bijectivity follows directly from 5. and 6. similar to 3.

8. Follows with the same logic as 4.

9. Strict monotonicity of B and the same argument as in 1. (Lebesgue density theorem) imply this.

10. This can also be shown by the same argument as 2. and continuity of B in 6.

11. Bijectivity follows from 9. The fact that the image is $(0,\infty)$ follows from the fact that $p > 0$ and thus in order to go with $a \to 1$ we will require infinite area in the Lebesgue sense. That we also approach 0 in the image follows easily from bijectivity of B on $(0,1)$.

12. Follows with the same logic as 4. □

From this lemma we can see that iff the PDF is continously diffentiable a.e., also the length of the HDR w.r.t. *a* will be continously differentiable a.e.. This is required because otherwise we can not show the following lemma about convexity of the HDR length w.r.t. *a*:

Lemma 2.6.2. *Let $p : \mathbb{R}^m \to \mathbb{R}$ fullfill Assumption 2.1.1. Then, the function $\lambda_p(a)$ is strictly convex, i.e.,*

$$\frac{\partial^2 \lambda_p(a)}{\partial a^2} > 0. \tag{2.13}$$

Proof. Without loss of generality, assume $a_1 < a_2$ with both $a_1, a_2 \in (0, 1)$. For any $\alpha \in (0, 1)$, let $a := \alpha a_1 + (1 - \alpha)a_2$. By the definition of H_p in Equation 2.7, the set $H(p, a)$ encompasses points up to the highest densities corresponding to coverage *a*. Taken from the definition in Equation 2.7 we define this highest density as

$$B(p, a) := \max \left\{ b \in \mathbb{R}^+ : \mathbb{P}\left(\{\hat{\mathbf{y}} \in \mathbb{R}^m : p(\hat{\mathbf{y}}) \geq b\}\right) \geq a \right\} \tag{2.14}$$

This implies that $\lambda_p(a_1) \leq \lambda_p(a) \leq \lambda_p(a_2)$. Define $k_1 = a - a_1$, $k_2 = a_2 - a$. Consequently, $H(p, a_1) \subset H(p, a)$, indicating that to transition from $H(p, a_1)$ to $H(p, a)$, only points with density less than $B(p, a_1)$ can be utilized. In contrast, if we go from *a* to a_2 only points with a density less than $B(p, a)$ can be utilized.

As we know that

$$\lambda_p(a) = \lambda(H(p, a_1) \cup (H(p, a) \setminus H(p, a_1))) = \lambda_p(a_1) + \lambda(H(p, a) \setminus H(p, a_1)) \tag{2.15}$$

and we know that $\lambda(H(p, a) \setminus H(p, a_1)) \leq k_1 \cdot B(p, a)$ and $\lambda(H(p, a_2) \setminus H(p, a)) \geq k_2 \cdot B(p, a)$ we can see that we can approximate the gradient by dividing the change of λ_p by the change of *a*, which is in k_1 and k_2 we see that the gradients are bounded from above and below respectively for the invervals (a_1, a) and (a, a_2). Moreover strict monotonicity of *B* as shown in Lemma 2.6.1 implies that the gradient is strictly increasing for λ_p which implies a postive second derivative and thus convexity.

In particular, the second derivative exists by the use of the Lebesgue's Theorem for Monotonic Function a.e. since the first derivative exists continuously a.e. and is strictly monotonic as we know from Lemma 2.6.1 which implies absolute continous derivative a.e. and thus twice differentiability a.e.. □

Lemma 2.6.3. *For any PDFs $f : \mathbb{R}^m \to \mathbb{R}$ and $p : \mathbb{R}^m \to \mathbb{R}$, where p must fullfill Assumptions 2.1.1, with the same coverage size under confidence levels a_p and a_f, that is,*

$$\lambda_f(a_f) = \lambda_p(a_p)$$

it holds that if we measure the coverage of those HDRs with points distributed w.r.t. p, that the coverage measured with $H(p,a)$ will be greater-equal. Moreover, the coverage level of $H(p,a)$ will be exactly a_p. Formally:

$$\int_{\mathbb{R}^m} p(\mathbf{y}) \mathbb{1}_{\mathbf{y} \in H(f,a_f)} d\mathbf{y} \leq \int_{\mathbb{R}^m} p(\mathbf{y}) \mathbb{1}_{\mathbf{y} \in H(p,a_p)} d\mathbf{y} = a_p$$

Note that it is absolutely possible that $a_p = a_f$.

Proof. We split $H(p,a_p)$ and $H(f,a_f)$ into subsets: $H(f,a_f) = A \cup B$ and $H(p,a_p) = A \cup C$ with $H(f,a_f) \cap H(p,a_p) = A$, $H(f,a_f) \setminus A = B$ and $H(p,a_p) \setminus A = C$.

$$\int_{\mathbb{R}^m} p(\mathbf{y}) \mathbb{1}_{\mathbf{y} \in H(f,a_f)} d\mathbf{y} = \int_{H(f,a_f)} p(\mathbf{y}) d\mathbf{y} = \int_A p(\mathbf{y}) d\mathbf{y} + \int_B p(\mathbf{y}) d\mathbf{y} \tag{2.16}$$

$$\int_{\mathbb{R}^m} p(\mathbf{y}) \mathbb{1}_{\mathbf{y} \in H(p,a_p)} d\mathbf{y} = \int_{H(p,a_p)} p(\mathbf{y}) d\mathbf{y} = \int_A p(\mathbf{y}) d\mathbf{y} + \int_C p(\mathbf{y}) d\mathbf{y} \tag{2.17}$$

since the A part of the integrals is equal we can ignore it for comparing $H(f,a_f)$ and $H(p,a_p)$ coverage. So, we need to show:

$$\int_B p(\mathbf{y})d\mathbf{y} \leq \int_C p(\mathbf{y})d\mathbf{y} \tag{2.18}$$

This can be shown by proofing $\forall \mathbf{y}_B \in B \forall \mathbf{y}_C \in C : p(\mathbf{y}_B) \leq p(\mathbf{y}_C)$ because $\lambda(B) = \lambda(C)$. So, let $\mathbf{y}_B$ and $\mathbf{y}_C$ be arbitrary from the corresponding sets. Then we know that $\mathbf{y}_B \in H(p, a_p)$, which means that $p(\mathbf{y}_C) \geq B(p, a_p)$ where $B(p, a_p)$ is the maximum density bound such that the coverage level of a_p is still given w.r.t. p. However, since $\mathbf{y}_C \notin H(p, a_p)$ this means that $p(\mathbf{y}_C) < B(p, a_p)$, which shows the first part of the proof.

The second part of the proof is to show that

$$\int_{\mathbb{R}^m} p(\mathbf{y}) \mathbb{1}_{\mathbf{y} \in H(p, a_p)} d\mathbf{y} = a_p \tag{2.19}$$

which follows from the fact that with our Assumption 2.1.1 $B(p, a_p)$ is bijective and thus $\mathbb{P}(\mathbf{Y} \geq B(p, a_p)) = a_p$. In particular, $H(p, a_p)$ is per construction a set where this is fullfilled. $\qquad \square$

In order to finally be able to use this lemma efficiently we need to define something like an inverse of the HDR w.r.t. the significance, which based on the input $\mathbf{x}$ and the length $\lambda(H(p(\mathbf{y} \mid \mathbf{y}), a))$ gives us the significance level that we would need to insert in H together with the true distribution at x to obtain the same size of the distribution but with the above lemma always has a larger or equal coverage.

Definition 2.6.1 (HDR Transform). Let $f, p : \mathbb{R}^m \to \mathbb{R}$ be two probability density functions and let $a \in (0, 1)$ be some coverage level. Then we define the HDR Transform as:

$$H_p(f, a) := \max \left\{ b \in (0, 1) : \lambda_p(b) \leq \lambda_f(a) \right\} \tag{2.20}$$

In words, the HDR Transform gives us the maximal significance level that we can insert under the distribution p while maintaining a coverage size lower-equal than what we obtain by inserting the significance level a under the distribution f.

In particular, if we evaluate the actual coverage of $H(f, a)$ with samples drawn from p, then the coverage will be always lower-equal a which follows from Lemma 2.6.3. The HDR transform then gives us basically the confidence level that we need to insert into the HDR with the true distribution to obtain the same coverage size but are guranteed to have higher-equal coverage.

Using this definition together with Lemma 2.6.3 establishes a very powerful tool to make proofs related to HDR.

Lemma 2.6.4. *With f, p as in Definition 2.6.1 and Assumption 2.1.1 on p, it always holds that:*

$$H_p(f, a) = \max \left\{ b \in (0, 1) : \lambda_p(b) = \lambda_f(a) \right\} \tag{2.21}$$

and that the right hand side exists.

Proof. Bijectivity of $\lambda_p(a)$, under the assumptions, with Lemma 2.6.1 implies that exactly one b exists such that $\lambda(H(p, b)) = \lambda(H(f, a))$ which finishes the proof. $\square$

Now we have all tools in order to proof the important statement. From now on, if the expectation $\mathbb{E}$ is used, it is always w.r.t. the whole space $\mathbb{R}^{m+n}$ and with the random variables $\mathbf{Y}$ and $\mathbf{X}$ which have PDF $p(\mathbf{y}, \mathbf{x})$. Moverover, if $\hat{\mathbf{y}}$ is written, it is not an input to the function but a demonstrative artefact to show that the function maps to a conditional density on the same space as $\mathbf{Y}$ is defined.

Theorem 2.6.5 (MLL is equivalent with Optimal Conformal Prediction)**.** *We want to show that if we have definitions as in Section 2.4, the space of all parameters Θ and $\forall \mathbf{x} \in \mathbb{R}^n : p(\mathbf{y} \mid \mathbf{x})$ fullfills Assumption 2.1.1 and that*

$$\forall \mathbf{x} \in \mathbb{R}^n : \max_{\theta \in \Theta} p(\mathbf{y} \mid \mathbf{x}; \theta) = p(\mathbf{y} \mid \mathbf{x}) \tag{2.22}$$

then it holds that:

$$\arg\max_{\theta \in \Theta} \mathbb{E}\left[\log p(\mathbf{Y} \mid \mathbf{X}; \theta)\right] \qquad (2.23)$$

equals

$$\arg\min_{\theta \in \Theta} \mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X};\theta)}(a)\right] \qquad (2.24)$$

$$s.t. \quad \mathbb{E}\left[\mathbb{1}_{\mathbf{Y} \in H(p(\hat{\mathbf{y}}|\mathbf{X};\theta),a)}\right] = a \qquad (2.25)$$

Importantly under our assumption in Equation 2.22 we have that Equation 2.23 is the true underlying conditional distribution as a property of the MLE, i.e. $\forall \mathbf{x} \in \mathbb{R}^n : p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta^*) = p(\hat{\mathbf{y}} \mid \mathbf{x})$. So this is not only an equality between the MLE and optimal CP but also an equality between the true underlying distribution and optimal CP.

Proof. Let $\theta \neq \theta^*$ be arbitrary but fixed. If we can show that for this θ it holds that if

$$\mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X};\theta)}(a)\right] < \left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}(a)\right] \qquad (2.26)$$

it implies

$$\mathbb{E}\left[\mathbb{1}_{\mathbf{Y} \in H(p(\hat{\mathbf{y}}|\mathbf{X};\theta),a)}\right] < a \qquad (2.27)$$

then it would finish the proof, since it'd show that for any parameter set θ, that produces a smaller average HDR than the the MLE, the constraint would be violated and it is clear that if using the MLE, which is the same as the true PDF, we would fulfill the constraint because of Lemma 2.6.3. We will show now that Equation 2.26 $\implies$ Equation 2.27. So θ is such that Equation 2.26 holds.

First, we can upper bound the coverage with the HDR transform in Definition 2.6.1:

$$\mathbb{E}\left[\mathbb{1}_{\mathbf{Y}\in H(p(\hat{\mathbf{y}}|\mathbf{X};\theta),a)}\right] \leq \mathbb{E}\left[\mathbb{1}_{\mathbf{Y}\in H(p(\hat{\mathbf{y}}|\mathbf{X}),H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}}|\mathbf{X};\theta),a))}\right] \tag{2.28}$$

$$= \mathbb{E}\left[H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}}\mid\mathbf{X};\theta),a)\right] \tag{2.29}$$

The upper bound follows directly from Lemma 2.6.3 and the monotonicity property of integrals. The equality in Equation 2.29 follows from the fact that if we evaluate the coverage w.r.t. underlying distribution p we will always get the same coverage level as the one we inserted in the HDR if we fullfill Assumption 2.1.1.

We know that:

$$\mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}(a)\right] > \mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X};\theta)}(a)\right] \tag{2.30}$$

and

$$\mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X};\theta)}(a)\right] = \mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}\left(H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}}\mid\mathbf{X};\theta),a)\right)\right] \tag{2.31}$$

where the second equality follows from Lemma 2.6.4. This upper bound gives via Lemma 2.6.4 the highest coverage level for the same coverage size that is possible. If we can show the desired result for this upper bound, then we have shown the desired result.

Due to convexity and with the Jensen inequality we now have that then we can appended to the equation in Equation 2.31 the following inequality on the right:

$$\geq \mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}\left(\mathbb{E}\left[H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}}\mid\mathbf{X};\theta),a)\right]\right)\right] \tag{2.32}$$

and thus:

$$\mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}(a)\right] > \mathbb{E}\left[\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}\left(\mathbb{E}\left[H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}}\mid\mathbf{X};\theta),a)\right]\right)\right] \tag{2.33}$$

In words, what this means is that given the same distribution $p(\hat{\mathbf{y}} \mid \mathbf{x})$, we obtain a strictly larger average coverage size when using coverage a, then when we use coverage $\mathbb{E}\left[H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}} \mid \mathbf{x}; \theta), a)\right]$. By monotonicity of the coverage size function, this means a.e. that

$$\lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}(a) > \lambda_{p(\hat{\mathbf{y}}|\mathbf{X})}\left(\mathbb{E}\left[H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}} \mid \mathbf{X}; \theta), a)\right]\right) \tag{2.34}$$

since it can a.e. not be that the inequality is reversed, and thus:

$$a > \mathbb{E}\left[H_{p(\hat{\mathbf{y}}|\mathbf{X})}(p(\hat{\mathbf{y}} \mid \mathbf{X}; \theta), a)\right] \tag{2.35}$$

which, as we can see in Equation 2.28, upper bounds the coverage of the actual $p(\hat{\mathbf{y}} \mid \mathbf{X}; \theta)$. This completes the proof.

□

This now shows our desired result, that in fact, by maximizing the likelihood of a CDE model to afterwards apply HDR to obtain small but calibrated regions is equivalent to directly trying to minimize the size of the HDR while maintaining calibration. When assuming that our CDE models can reasonably well approximate the true underlying distribution this is a powerful result that allows us to focus fully on optimizing the likelihood for CDE and we get optimal conformal prediction with HDR for free. In particular, this is a bit more evolved than standard CP as described in Section 2.4 since we have a more complex requirement on the model, that is it must be the shortest possible HDR for a given coverage level.

Moreover, we can see that this means the MLE can be decomposed into a constrained optimization problem which is related to insights from [Chung et al., 2021]. In particular this is true because not only the MLE is the ideal model for optimal CP, but also the inverse is true, the optimal CP model is also the optimal MLE model which follows directly from the equality that was just shown in Theorem 2.6.5. While in the context of this work we leave it as a theoretical insight, it is possible that this can be used in future work for new

relevant findings. Arguably this fact has some mathematical beauty to it, as we realize the MLE inherently is looking for the tightest possible peaks while maintaining calibration.

2.6.2 Focusing on Density instead of the Coverage Level

As hinted in Section 1.2 in this work we argue that it is practically more reasonable to move the focus to the probability mass/density instead of only the length of the inverval while maintaining calibration. The difference is subtle, but via Figure 2.2 we aim to provide a clear understanding of the difference through two distinct arguments.

Firstly, when performing CP, the focus is solely on minimizing the length of the single interval in the prediction while maintaining calibration, without considering the actual shape of the distribution. In particular, if it were possible to obtain significantly more mass with just a very slight increase the interval size it would be ignored. In the figure this can be observed when comparing the connected HDR with the shortest interval CP. We can see that when we first use HDR but then simply connect it, with the argumentation of [Sesia and Y. Romano, 2021](multiple intervals can be confusing in practice), we will capture the second peak of the distribution while we do not capture low density parts of the first bigger peak. This example demonstrates that focusing exclusively on the length of the interval can lead to suboptimal results.

Secondly, although we currently lack empirical evidence, we argue that including a second predicted peak in the CP prediction is justified because if the model identifies a second distinct modality at a specific point, there is likely a meaningful reason for it, whereas a heavy tail might be an artifact of the modeling method. We are looking for further research to confirm this hypothesis.

Primarily for the first reason, and to a lesser extent the second, we argue that our approach (first applying HDR, then connecting the regions) offers advantages in practical scenarios such as healthcare and finance.
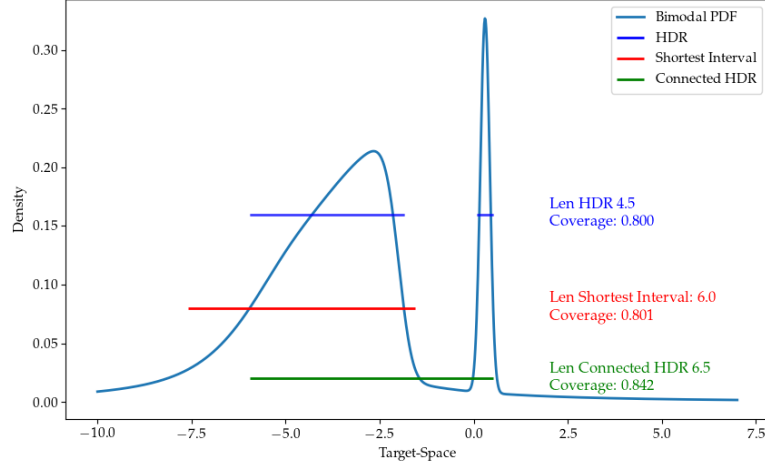
Figure 2.2: Comparison of HDR, connected HDR and Shortest Interval CP for a bimodal distribution. We can see that although the connected HDR slightly overcoves, we obtain significantly more coverage with only a slightly larger interval and also intutively this interval is more meaningful.

2.7 Calibration and Recalibration

Calibration, while a core property of CP as described in Section 2.4, can in a more general way also be a desireable property of CDMs. In particular, we are calibrated in the context of $\mathscr{P}_\theta$ if for any quantile $q \in (0,1)$ that we choose, in expectation the proportion of the target that falls into the quantile really is q. CDMs often suffer from poor calibration in practice due to limited data, model misspecification, overfitting, or underfitting. For this section of our work we assume a limited training set $\mathcal{Z} = (\mathcal{X}, \mathcal{Y})$ that is used to train the CDM model. The probably most important realization on this is, that even tho the objective functions CDMs use in practice are optimal in theory, in practice we mostly need to resort to gradient based optimization methods, which require a step wise optimization and will only find local optima. Especially this insight is important because that means, even tho globally optimal models w.r.t. objective functions of CDMs will be calibrated, those objective functions do not guarantee calibration at all times during optimization. The reason is that the constraint of those optimization problems is an implicit one in practice and we will violate it usually with CP.

This is the reason why in practice recalibration methods exist and are at this time mostly applied to CP methods. From Section 2.5 it follows that we can apply the same methods to all CDMs that are used currently only for CP. However, since recalibration methods are mostly explored in CP methods, we will first introduce them in the context of CP in Section 2.7.1 and step-wise extend the methods till we reach full generalization of recalibration in all CDMs in Section 2.7.4.

2.7.1 Calibration in CP

Generally, calibration of CP refers to the requirement of the defining property of CP to be fullfilled as described in Section 2.4. In particular, since today most CP methods don't aim to estimate any CP intervals but specific ones, during optimization the calibration requirement is often overshadowed. However, calibration in the context of CP is basically the whole point of CP to begin with and because it is in practice often not fullfilled, recalibration methods are employed.

In any case, if doing recalibration we have that the estimated conformal intervals do in expectation not capture the desired $1 - \alpha$ proportion of the target in the calibration set. However, this can be tackled by recalibration for which a large possible number of methods exist, each depending on the method used to estimate the CP intervals.

To formally define calibration within CPs, consider the calibration objective function given by:

$$\min_{\psi \in \Psi} |(1 - \alpha) - \mathbb{P}(\mathbf{Y}_I \in C(\mathscr{P}_\theta(\mathbf{X}_I), \psi))| \tag{2.36}$$

This function aims to minimize the discrepancy between the desired confidence level $1 - \alpha$ and the proportion of data within the CP interval predicted by the model, reflecting the model's calibration accuracy. Here C is the map to the CP regions. $\psi \in \Psi$ is a configuration of the method used that can be optimized w.r.t. objective function and can be quite arbitrary and might dependent on the form of $\mathscr{P}_\theta$ which we argue for in Section 2.7.4. In particular, ψ is something that we apply after the CDM model has been estimated. We usually assume that we already have learned a CDM model estimated with parameters θ but that it is possibly not calibrated.

In the following we will describe a variation of C and θ where we simplify the optimization problem in Equation 2.36 to one that we can practically easily optimize, that is, it is a method that induces a misconformity score of sorts. The method we focus on here is heavily inspired by [Sesia and Y. Romano, 2021] and can be used if C and θ fullfill certain sufficient conditions:

Definition 2.7.1 (Recalibration Requirements)**.** Recalibration requirements with which we can easily optimize Equation 2.36 are:

1. $C(\cdot, \psi)$ must be such that $(C(\cdot, \psi_r))_{r \in \mathbf{R} \subsetneq \mathbb{R}}$ where $\mathbf{R}$ is bounded and $(C(\cdot, \psi_r))$ are strictly nested sets on the target space where the smallest set $(C(, \psi_0)) = \varnothing$ is the empty set and the largest one contains the full target space, i.e. we have $\forall r_1, r_2 \in \mathbf{R}:$ $r_1 < r_2 \implies C(\cdot, \psi_{r_1}) \subset C(\cdot, \psi_{r_2})$.

2. We require that the sequence is continous in a way if we want to be able to gurantee that we can come arbitrarily close the the desired calibration in expectation, i.e. $\forall a \in (0,1) \exists \psi \in \Psi : a = \mathbb{P}(\mathbf{Y}_I \in C(\mathscr{P}_\theta(\mathbf{X}_I), \psi))$

Let r be from the context of Definition 2.7.1. Then, in words, requirement one means that we can, by tweaking r, obtain at least the empty set or the full target space and thus 0 or 1 coverage respectively. Requirement two means that we can interpolate r such that we can reach any desired calibration in expectation. For example, the HDR with $a = r \in (0,1)$ fullfills this requirements under our standard assumptions Assumption 2.1.1 as explain in more detail in Section 2.7.2.

If condition two in Definition 2.7.1 is not fullfilled we can only gurantee that the calibration in expectation will be larger-equal the desired proportion. This is because there is guranteed to an a close to 1 that we can reach with an $r \in \mathbf{R}$ because of assumption one, so we might need to do with a converage larger than the desired one. When condition one is not fullfilled, we can not gurantee anything about the calibration in expectation, not even that it will be larger-equal the desired proportion. This is because there might be sets that are never part of the sequence but contain probability mass and thus we can never gurantee that we come even close to the desired calibration in expectation there.

If we optimize Equation 2.36 on the calibration set, which is easily doable in practice with various methods since its just a convex univariate optimization problem with bounded

domain, we can gurantee that the model is calibrated in expectation on the calibration set when assuming exchangability.

The *r* required for a specific calibration sample in this Defintion 2.7.1 is basically a form of misconformity score. Thus the method used by [Sesia and Y. Romano, 2021; Chernozhukov, Wüthrich, and Zhu, 2021] and others is to basically sort the *r* that are required for each single one of the calibration samples to be included in the CP interval. Then we take the upper $(1 - \alpha)$ quantile of this sorted list as the *r* that we use for the CP interval. We refer to [Sesia and Y. Romano, 2021] for a more detailed explanation of the method and of it's validity, but it gurantees in expectation of both, the training and the validation set, that the CP interval will contain the desired proportion of the target. In particular, in this case *r* acts as the conformity score of the sample as usually defined in CP literature like in the work by [Sesia and Y. Romano, 2021].

It is noteworthy, that if we have only few calibration samples, then the method will not work well, since the quantile will be very noisy. In this case the common choice is to resort to an overestimation, which means we take *r* larger than the $1 - \alpha$ quantile would suggest.

2.7.2 Recalibration of CDE on CP when using HDR

As the HDR for a given confidence level *a* is actually a sequence of nested sets which conform with assumptions from Definition 2.7.1 with $a = r \in (0, 1)$ if we also have Assumption 2.1.1 applicable, for which it holds that those subintervals will contain *a* proportion of the probability mass on the estimated conditional PDF, which can also be seen from Lemma 2.6.1, which implies that we basically have a set of quantile intervals that sum up to *a*, we can see that a calibrated model will actually contain the true value in the HDR with a probability of *a*. Thus, if we are not calibrated, we can directly utilize the concepts described in Section 2.7.1 when using HDR.

2.7.3 Common Implicit Assumptions on the CP-Region Fuction

It is common practice in the CP literature to do calibration without of considering the implict assumptions that are being actually made when doing so. In particular the

assumptions imposed on the $\mathscr{P}_\theta$ that we do CP with. One example would be that often in the literature we predict the 5% and 95% quantiles, and if we have a miscalibration we simply recalibrate the model by moving those two quantiles by the same amount in or outwards. Many assumptions are made there, in particular we assume that the conditional PDF is symmetric and that the densities of all samples look similar which are extremely strong assumptions also in practice. Furthermore, those assumptions might be orthorgonal to the optimization objective of CDM, i.e. to precisely model the true PDF asymptotically. We will now establish below in Section 2.7.3 a framework that allows us to do recalibration with theoretically justified assumptions.

Likelihood and the Relation to CDMs

It is clear that for CDE methods the likelihood is a very relevant metric and very often also the objective function in the optimization problem, e.g. for MDNs or KMNs. Moreover, from Section 2.5 we can directly see that the likelihood must thus also be relvant for CDMs in general. Importantly, likelihood only directly can be evaluated on a specific PDF, but from Section 2.5.2 we inferred that CDM in general need to make smoothness assumptions anyways with arumentation from Section 2.2.1 which at least makes directly sense if the CMDs are very restrictive on $\mathscr{P}_\theta$. However, the question arises how we can conceptualize likelihood if CDMs are not restricting $\mathscr{P}_\theta$ very much. In particular, can we make a statement that in any case a more accurate CDM method will allow for higher likelihoods in terms of the restrictive set of $\mathscr{P}_\theta$?

The optimization objectives of CDMs all have asymptotic gurantees on the restrictions they impose. Moreover, it is obvious that the likelihood and all other CDM metrics are optimal if the CMDs are restricted on the true conditional PDF as a property implicit in those metrics. However, it is not clear how exactly likelihood corresponds to other metrics used for restricting CDMs, like the pinball loss and it goes beyond the scope of this work to investigate which metrics are not only optmial at the same parameters but which are truly equivalent in terms of restrictions. For example, will a restriction that is better for the one metric always be better for the other metric?

In any case, we will leave it as a hypothesis that we generally have that good CDMs will have high likelihood which means in the scope of this work we designate likelihood as the general metric for CDMs. A good liklihood has certain desireable implications as

properties of likelihood. In particular, we have the gurantee that in expectation on the entire target space the density will be close to the true density and if we have a model that generalizes, which we assume, then we also have that gurantee on unseen data.

2.7.4 Calibration of CDMs in General

We have in Section 2.7.1 seen that it is possible in practice to recalibrate CP models. Now Section 2.5 directly implies that we can generalize this concept to all CDMs, i.e. also to CDE and QR which is a core contribution of this work. Thereby we will with Section 2.7.3 also underpin the justification for common recalibration methods used in the literature [Sesia and Y. Romano, 2021].

In order to rigoriously utilize the theoretical framework that we have established, we first need to reformulate calibration for CP to a more general form that can be applied to all CDMs. Therefore we need to develop what recalibration means in the context of $\mathscr{P}_\theta$, i.e. the constrainted set of PDFs that any CP method is acting on.

As a sidenote, we want to make the connection to the foundational work of [Gneiting, Balabdaoui, and Raftery, 2007], in particular to the concept of probabilistic calibration which when applicable to CMDs also implies that it is calibrated in the CP context in Section 2.7.1.

When we recalibrate, we essentially always admit that the current model $\mathscr{P}_\theta$ does not describe the true PDF accurately and in order to obtain a certain property, calibration that is, we effectively intend to change $\mathscr{P}_\theta$. In other words, we need to formulate what $C(\cdot, \psi)$ does in Equation 2.36 as part of θ, which defines the model, itself. This means we apply a function to the constrained sets of PDFs $\mathscr{P}_\theta$ to obtain a new set of PDFs $\mathscr{P}_{\theta'}$ that is calibrated or more generally that we apply the optimization problem in Equation 2.36 to. By optimizing this we are essentially transforming this $\mathscr{P}_\theta$ w.r.t. $C(\cdot, \psi)$ such that a certain nested set gets assigned a different probability mass as before, in expectation, in the sense of Definition 2.7.1. In a more general context of CDM, we have that when recalibrating we are moving quantiles within $\mathscr{P}_\theta$. As the quantiles directly encode all information required for producing the target types for the CDM that is the generalized interpretation of CP recalibration.

Practical Considerations for Recalibration of CDMs

Practically to use this for e.g. CDE, one would simply define a dense grid of quantiles and then shift them all at once to recalibrate the model which will squeeze and stretch the model in the right places to obtain calibration. However, in order to realize a reasonable calibration with an infinitely dense grid of quantiles, we need to have an infinitely large calibration set. Interestingly, this limitation is not new to the general version of recalibration but actually also applies to CP which is easy to see. In practice we thus need to approximate recalibration. Moreover, it is noteworthy that, since recalibration acts on the quantiles and thus on the conditional CDF and not directly the PDF, we basically loose some amount of the smoothness of the estimated PDF when using designated CDE methods since we basically need to convert the PDF to a CDF by numerical integration and then after recalibration reconstruct the PDF from the CDF. However, we have observed with a large enough grid size for inegration of the CDF that this is not a big problem in practice. Moreover, a practical considerations that could be made is that there are more samples at denser areas so we could use a denser grid there and a less dense grid in less dense areas for recalibration. Quantiles induced by the HDR as the quantile limits for recalibration fit this description well and this is also why we used the HDR for recalibrating empirically. Furthermore, the strongest limitation lies in the number of samples if the calibration set. In particular, if we only have few calibration samples it we can of course not precisely find the calibrated quantiles on a dense grid. Empirically we saw that it is helpful to do a smoothing operation with a filter size depending on the number of calibration samples after we recalibrate whole CDE models which can be justified with Section 2.2.1. A visualization of this can be seen in Figure 2.3.

A Pseudo Code where we use HDR to recalibrate a CDE model is provided in Algorithm 3.

Implicit Assumptions when Recalibrating CDMs

An important consideration for this whole Section 2.7 is, that if we are changing θ arbitrarely in order to fullfill the optimization problem then, without considering the setting in a more general context, the only gurantee that we have is that the new $\mathscr{P}_{\theta'}$ is calibrated but might other than that not contain any relation to the true conditional PDF. Further,
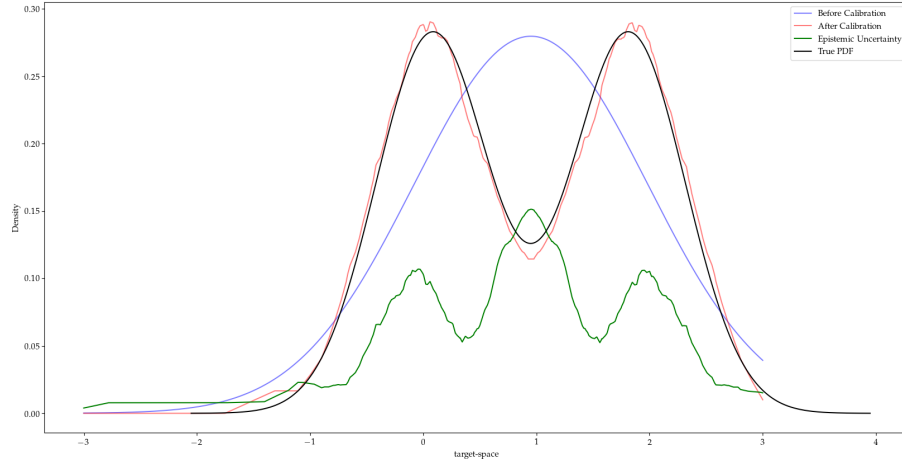
Figure 2.3: Recalibration of a bimodal CDE model. The model is recalibrated by shifting the quantiles of the HDR according to marginal misconformity quantile levels as in Algorithm 3.

this without a more general context this would be not more meaningful than trivial CP as described in Section 2.4.1.

However, with Section 2.7.3 we find that we must be close everywhere in the target space in expectation. With this methods like proposed by [Sesia and Y. Romano, 2021] make sense, as the idea is to navigate the estimated density in a way that, e.g. for underestimation for a specific confidence level in CP, we have that we increase our CP interval where we estimated more density and not just arbitrarily, which is now justified. Moreover, the same applies to recalibrating CP with HDR as described in Section 2.7.2.

2.8 Uncertainty and Calibration: The Connection

The general area of uncertainty estimation has been growing drastically in recent years. This is because of the increasing complexity of models and the need to understand the models better as well as the requirement in risk-sensitive applications to understand when and how much the model can be trusted. Generally, as described by [Hüllermeier and Waegeman, 2021] there exist a lot of different types and perspectives on uncertainty. Most importantly there exists a distinction between so called aleatoric and epistemic uncertainty. Not all defintions of those two fully agree but generally aleatoric uncertainty

is the inherent stochtasticity of the data while epistemic uncertainty is the unsureness of the model if only a limited amount of data is observed.

For example, if we try to model the coinflip of a biased coin with 75% probability of landing on the head and 25% on tails, then epistemic uncertainty would be if we did only observe 10 coinflips and we are unsure yet about the exact porbabilities within the coin. Aleatoric uncertainty would be the the inherent randomness of the coin that we might try to model. This means the 75% and 25% themselves are the aleatoric uncertainty. Differences of interpretation of those two kinds of uncertainty are in practice often inherent in how we expect the true model of the data to be and how it really is. For example, if we were to expect for the coinflip experiment that the coin is always landing on the same side with the intention to learn this side,and differences in what we observe is simply noise, then we might not be able to model either uncertainty properly. In particular we might in this case predict that the coin always lands on head and there is simply 25% noise which is of of course not true. A slight variation in definitions between aleatoric and epistemic uncertainty within works [Hüllermeier and Waegeman, 2021] is often whether aleatoric uncertainty is only noise or if it also contains stochtasticity of the data that might be reducible with more features like hidden variables that are not really observable. In this work, we do not want to dive into the philosophical interpretation of this and define that aleatoric uncertainty is always the randomness of the targets, given a fixed set of features, without of considering that there might be hidden variables that actually could reduce this uncertainty.

CDMs' task is to model the aleatoric uncertainty when we try to predict targets given features. The CDM model $\mathscr{P}_\theta(x)$ that we estimate is supposed to come as closely as possible to the inherent randomness of the targets given the features. One particular aspect that rarely has been acknowledged is, that those models can, at least with the optimization objective alone, not learn epistemic uncertainty. This implies, that the model might actually give overestimations in the preciseness of outcomes. Moreover, since in this kind of setting model the aleatoric uncertainty itself and usually do not assume that there is such a thing as a second-order aleatoric uncertainty, we actually assume that the conditional distribution of a target given features is deterministic i.e. there is no (second-order) aleatoric uncertainty. This also directly implies that all error of a model which has certain asymptotic gurantees stems from epistemic uncertainty alone.

In this work we provide a novel perspective on how one can estimate full uncertainty which not only includes the directly modeled aleatoric uncertainty but also the epistemic uncertainty. In the context of CDE, aleatoric uncertainty asks the question how the targets are distributed, given the features, while epistemic uncertainty asks to which extent we can actually accurately predict that. Especially for CDE where we need to predict very specific details about the distribution of the data, this is a very important question, as we realistically in real world settings can never model the distribution with full accuracy.

The tool that we propose for this is a novel method that highlights calibration in a new way. In particular, we argue that recalibration of models can be used to accurately infuse the prediction with a lower bound on epistemic uncertainty. Thereby we can reestimate the whole distribution with both epistemic and aleatoric uncertainty which thus gives us a more accurate perspective on what we really know about the distribution of a target.

2.8.1 All Model Error corresponds to Epistemic Uncertainty

Our proposed method relies on two key insights. First, all error in CDM models is exclusively due to epistemic uncertainty if the model is asymptotically correct and does not over-/underfit. Secondly, if we observe that a model is miscalibrated, it is a direct implication that the model is suboptimal and thus that there is error. In particular what that tells us is, if a model is misaclibrated there is epistemic uncertainty. Moreover, we claim that the amount of miscalibration is in a direct relationship with the amount of epistemic uncertainty and we also claim that if we can recalibrate the whole model, we can estimate a lower bound of the epistemic uncertainty as the difference between the distribution of the uncalibrated and the calibrated model.

In order to solidify those claims and insight we need to define a variant of epistemic uncertainty where we can show those relationships. In particular, in our case we aim to express the amount of epistemic uncertainty in the output space of the model, i.e. in the space of the conditional PDF that we estimate. Therefore we observe that it is a fair statement to say that if the likelihood of the data given the model increases, the model is closer to the true model. The reason why this insight is non-trivial in the context of CDMs is that we generally do not have information about the optimal likelihood that could be obtained which is due to the fact that we need to make smoothness assumptions as described in Section 2.2.1 and have limited data.

Lemma 2.8.1. *If we have a model $\mathscr{P}_\theta$ that is miscalibrated w.r.t. HDR on $\mathbf{Z}_I$, then there must exist a model $\mathscr{P}_{\theta'}$ that can be obtained by recalibration of all quantiless and is calibrated and where we have a higher likelihood if the true $p(\mathbf{Y} \mid \mathbf{X})$ fullfills* *Assumptions 2.1.1.*

Proof. Let $\mathscr{P}_\gamma$ be an arbitrary but fixed subset of $\mathscr{P}_\theta$ where for each input $\mathbf{x} \sim \mathbf{X}_I$ it holds that $|\mathscr{P}_\gamma(\mathbf{x})| = 1$, i.e. we are maximally restricted. Recalibration means that we move the quantiles of $\mathscr{P}_\gamma$ such that the model is calibrated. Let q be a quantile and q' be the recalibrated quantile, i.e. it holds that

$$\mathbb{E}\left[\mathbb{1}_{\mathbf{Y}_I \in H(\mathscr{P}_\psi(X), q)}\right] = q' \tag{2.37}$$

if now we change ψ to ψ' by recalibrating q, and we do that with all quantiles, the question is what happens to the likelihood. We approximate $\mathscr{P}_\psi$ with quantile sized step functions, i.e. for each possible $\mathbf{x} \sim \mathbf{X}_I$ we approximate:

$$\mathscr{P}_\psi(\mathbf{x})(\mathbf{y}) \approx \sum_{i=1}^{N} \mathbb{1}_{\mathbf{y} \in [q_i, q_{i+1}]} \cdot (q_{i+1} - q_i) \cdot \frac{1}{N} \tag{2.38}$$

By the monotone convergence theorem this can be fit as tight as we want if we increase N since we could just approach $(q_{i+1} - q_i)$ from below. Note that the q are specific to the $\mathbf{x}$; so each $\mathbf{x}$ has its corresponding q which is omitted due to breevity. When recalibrating we are changing the q to q' in the proportion of $q_i - q_{i-1}$. So when changing q in expectation to q', then what happens is that we look for the appropriate ratio between the $q_i - q_{i-1}$ which is for all $\mathbf{x}$ the same and move the quantile to q'_i. Note that if q'_i is moved over q_{i-1} then q_{i-1} will also be moved implicitly.

The expected likelihood is can then also be approximated by this as:

$$\mathbb{E}\left[\log(\sum_{i=1}^{N} \mathbb{1}_{\mathbf{Y}_I \in [q(\mathbf{X}_I)_i, q(\mathbf{X}_I)_{i+1}]} \cdot (q(\mathbf{X}_I)_{i+1} - q(\mathbf{X}_I)_i) \cdot \frac{1}{N})\right] \tag{2.39}$$

where we can pull the sum outside log since only 1 summand is not zero (since the quantile grid is disjoint) and we can also pull the sum out the expectation.

$$\sum_{i=1}^{N} \mathbb{E}\left[\log(\mathbb{1}_{\mathbf{Y}_I \in [q(\mathbf{X}_I)_i, q(\mathbf{X}_I)_{i+1}]} \cdot (q(\mathbf{X}_I)_{i+1} - q(\mathbf{X}_I)_i) \cdot \frac{1}{N})\right] \tag{2.40}$$

if we now move one quantile within this sum this implies that in one summand the term in the logarithm will become larger and in one smaller but also the smaller will have less coverage etc. We can only look at those two summands to decide how the likelihood changes. So let *i* be the changed quantile. The question is whether:

$$\mathbb{E}\left[\log(\mathbb{1}_{\mathbf{Y}_I \in [q(\mathbf{X}_I)_{i-1}, q(\mathbf{X}_I)_i]} \cdot (q(\mathbf{X}_I)_i - q(\mathbf{X}_I)_{i-1}) \cdot \frac{1}{N})\right] + \mathbb{E}\left[\log(\mathbb{1}_{\mathbf{Y}_I \in [q(\mathbf{X}_I)_i, q(\mathbf{X}_I)_{i+1}]} \cdot (q(\mathbf{X}_I)_{i+1} - q(\mathbf{X}_I)_i) \cdot \frac{1}{N})\right]$$

$$\tag{2.41}$$

where we note that the $i + 1$ and $i - 1$ quantiles also are actually transformed but they are the same as the q in our case. The difficulty now is that we do not exactly know the shape of the true conditional density; with the exception that calibration-wise it is the same in this quantile *i*. However, we can also approximate the true conditional PDF with step functions which we can also chunk such that the quantiles align. We approximate between q_{i-1}, q_i', q_i and q_{i+1} and obtain a step function. On this step function we need that the likelihood is larger after recalibrating. We know that after recalibration, in expectation, the interval between q_i' and q_{i+1} becomes appropriately lower and between q_{i-1} and q_i' becomes appropriately higher for all **x**.

$\square$

Lemma 2.8.1 shows us that if we are not calibrated than we know that we still have an error in the model i.e. that we have epistemic uncertainty to some extent. Moreover, it shows that if we racalibrate the model, it will have less epistemic uncertainty and so the difference between the recalibrated and the uncalibrated model is a lower bound on the epistemic uncertainty that we have for the problem at hand. In particular, one way to

quantify this epistemic uncertainty is to use distributional measures of difference like the average Hellinger Distance, KL-divergence or the Wasserstein distance.

This measuring of epistemic uncertainty works if we assume smoothness in the true model, in particular in way that if we have a wrong model and we shift its quantiles, which is what we are doing when recalibrating, that intermediate results of this transition of quantiles are smoothly related to the optimization alogorithm itself. In particular, this is true since we assume that the model does not overfit and thus the model must be to some extent smooth w.r.t. epsitemic uncertainty, i.e. it will not have sharp edges in the distribution of the targets and, in particular, it approaches the true distribution in a smooth way from a less sharp distribution. For a more detailed understanding on the relation between overfitting and smoothness we refer to the work of [Bishop, 2006].

3 Empirical Study

In order to practically verify the validity of the novel theoretical findings as described in Section 2.5 and the approach to use the HDR as described in Section 2.6 for finding the best conformal regions we did a series of experiments with two different stages and a multitude of benchmark datasets. In particular, the first stage was a extensive hyperparameter search with Bayesian optimization on eight datasets with over 1000 hyperparameter configurations on each. Thereby nested cross validation was utilized. The goal of this stage was to get a better understanding of the hyperparameters, including novel hyperparameters and to find a good starting point for the next stage. The second stage then was to do a more detailed hyperparameter search with a smaller grid but with multiple test set splits to get a better understanding of the generalization of the hyperparameters. In this chapter we will describe the results of the first stage and the setup of the second stage. In particular we will discuss mutliple novel hyperparameters that we experimented with and highlight the ones that significantly improved the performance of the models empirically.

3.1 Core Model Classes

In the course of this work we experimented with a multitude of different CDM model classes. In particular, insights gained from Section 2.5 establish that we can use any model class in the literature that has been used from CDE, QR or CP which opens up a wide range of options. Model classes experimented with in this work include Mixture Density Networks (MDNs) by [Bishop, 1994], Kernel Mixture Networks (KMNs) [Ambrogioni et al., 2017], Multiple Quantile Regression (MQR) [Gupta, Kuchibhotla, and Ramdas, 2022; Moon et al., 2021], Normalizing Flow Networks (NFNs) by [Trippe and Turner, 2018] and conventional Regression as a baseline. However, in the latter experimental stages we

restricted ourselves to MDNs, KMNs and MQRs as they showed the best performance in the first stage and also have significantly lower computational requirements than NFNs which is also why we restrict the reports to those three model classes in this work.

3.2 Experimental Setup

For the experiments done in the course of this work a python setup with standard libraries like PyTorch [Paszke et al., 2019], NumPy [Harris et al., 2020], Pandas [team, 2020], Scikit-Learn [Pedregosa et al., 2011] and others was utilized. The hardware consisted of NVIDIA TITAN X (Pascal) GPUs, each with 12GB memory.

3.3 Hyperparameters

Architectures in this regime of ML offer an extremely wide range of possible hyperparameter settings. In particular, this is due to the fact that in the output space there is a lot of freedom in how we can model the distribution. While not the main focus of this work, it is an interesting realization that CDMs have possibly the most degrees of freedom in their output compared to any other ML task. In particular, it is impossible to fully output in all those degrees of freedom but any output must necissarly be an abstraction of the true PDF. For example we just output model parameters of a mixture of Gaussians instead of the infinitely dense PDF which is very obviously not possible. The elegance now comes in how we decide to make this abstractions and many options with the help of CDMs exist.

In this section first we will discuss the known hyperparameters and how the performance seems to be affected by them with a rigorious empirical analysis of good settings for those in the regime of CDMs. Then we will discuss novel hyperparameters that we experimented with and how they affected the performance of the models. In particular we found that there is no existing literature that discusses in depth the possible hyperparamters for CDMs and their impact. This is a very important contribution of this work as it gives a good starting point for future research in this area as well as a good starting point for practical applications of CDMs in the industry.

3.3.1 Known Hyperparameters - General

Learning Rate

A learning rate of around `2e-4` gave us good performance accross all datasets. Moreover, for some of our experiments we utilized a learning rate scheduler `ReduceLROnPlateau` with a patience of 5 epochs, cooldown of 3 and a factor of 0.5. This gave us a slight performance boost when using MDN and KMN models, but not with MQR models.

Batch Size

This hyperparameter varies a lot between datasets. Some datasets had a better performance with a size around 32 and others performed best with as high as 512 with a significant impact on performance. We suggest that this hyperparameter should be tuned for each dataset individually. We did not experiment with a batch size scheduler.

Number of Epochs

We found the models had a rather quick convergence with mostly lower than 50 epochs and performance not improving with more epochs. Furthermore we used early stopping by monitoring the negative log likelihood loss for all models as this loss is the most important one for CDMs.

Dropout

We experimented with a wide range of dropout rates and found that the models are extremely sensitive to this hyperparameter. In particular a dropout rate of more than 0.05 will lead to a significant performance decrease for most instances. However, there are some exceptions, in particular when using KMN. Moreover we observed a correlation between the Dropout rate, number of components in MDN, number of layers and number of units. A more expressive architecture allows for a slight increase in dropout which is to be expected. Moreover, we suspect that the higher dropout preference in KMN is due to the reduced degrees of freedom in the KMN model compared to MDN and MQR.

Weight Decay

We initially did experiment with this hyperparameter, tuning it in many ways. However, we found that setting it to 0 consistently yields the best performance.

Base Architecture

The base architecture used was a multi layer perceptron (MLP). We experimented with a wide range of depths and widths and the most performant architecture was one with four hidden layers with sizes $[64, 128, 128, 64]$; however it is possible that with significantly more or complex data a deeper architecture might be beneficial.

Activation Function

The different activation functions we tried were ReLu, Leaky ReLu, TanH, Sigmoid, SELU and ELU. The three best performing ones were ReLu, Leaky ReLu and TanH, however, the differences were not very significant and there are some slight variations between datasets. We decided to use ReLu as it was the most stable one. It is noteworthy that when using ReLu we utilized a He initialization and when using TanH we utilized a Xavier initialization as best practice.

Input-/Output Noise

A hyperparamter that to the best of our knowledge is novel to the CP model literature and was first introduced to CDE methods by [Rothfuss, Ferreira, Boehm, et al., 2019] is the input/output noise to the models. This hyperparameter boosts the performance very significantly and it essential for performance in all CDMs. We found an input and output noise of around 0.03 the most consistent, however, tuning this hyperparameter for each dataset can improve the performance even further by a significant margin. In particular when using KMN a higher noise level is sometimes beneficial with values up to 0.3.

Layer Norm

Layer Norm was tried in the later course of the experiments and we found it does reduce the performance of all our models. We did not investigate this further.

Component Entropy Loss

This additional regularization loss which can be used in MDNs and KMNs essentially aims to decrease the entropy of the different mixture components. We found adding a small amount of around 0.125 tends to slightly increase the performance of the models.

Number of Components

The number of components in both MDN and KMN make a significant difference. For MDN a number of components around 35 was the most performant across all datasets. For KMN a higher number of 90 was the best performing one. Moreover, we we had two kernels in the KMN model. This makes an effective number of components of 180. For MQR generally a higher quantile number is better always since with a higher number basically we can model the conditional CDF better. However, we restricted ourselves to 256.

Component Distribution

We experimented with Laplacian and Gaussian mixture components. Both have their advantages and disadvantages depending on the dataset. However, the differences were not very big and since Gaussian components were slightly more performant we decided to use those.

Kernel Width

We initialized the kernel width with 0.3 and 0.7 but decided to make them learnable hyperparameters, which means that we optimize them with the model parameters which slightly boosted the performance.

3.3.2 Novel Hyperparameters

Additional Target Noise

As explained in the theoretical part of this work, in order to be a reasonable prediction that can also be calibrated effectively, certain conditions need to be fullfilled on the distributions. In particular, it is required to have a certain amount of density everywhere. Moreover, we suspected that it might be helpful to enforce the marginal target distribution component on the CDE-models since then during calibration we can be sure that for each possible target there is at least a small amount of density in the model. In particular we decided to implement this by swapping certain targets which implicitly should enforce that the model has a certain amount of density everywhere on the marginal distribution. Furthermore, a theory was that if we have more samples then we have less empistemic uncertainty which implies that we would need to inforce less density on the marginal distribution and thus we made the number of swaps per epoch.

Another suspicion, especially for MDNs, was that some components can never "reach" the density where they want to go during training. In particular this came from the assumption, that if initially all mixture componens are somewhat in the center and we have a smaller density more on an outside location, that in order for a component to move to this location it would need to bridge the gap betweeen the high density in the center to the lower peak on the outside which might be very low density. We suspected that if a component needs to do that it might cause degenerative behaviour since if a component is at a location with low actual density the loss should enforce a lower weight on the component, which, in turn will decrease the general gradient imposed on this component. We suspected that it might happen that a component will then just stay in a gap with a negicible amount of weight so that it will never move again. In order to counteract this we decided to initialize the training with a large amount of uniform noise in the space of the targets and let it decay rather quickly over time. This procedure slightly improved the performance on all tasks but it is hard to say if there might be better ways to do it.

Learn MQR Quantile Distribution Std

MQR asymptotically with an increase in quantile components can as shown in Section 2.5 model the true PDF fully. However, since we have a limited amount of training data and also a limited amount of compute we needed to resrict the number of components to 256. In order to still be able to efficiently calculate the density at a point we decided to treat each quantile as a component with equal weight in a mixture of gaussians. Thereby we decided to learn the standard deviation. However, the standard deviation in this case can not be learned with the Pinball loss that is used for MQR. Thus we decided to use the NLL loss for the standard deviation only but without impacting the quantiles. We did this by detaching the means from the computational graph of the gradient in the loss function.

3.4 Datasets

In the course of this work we experimented with a multitude of different datasets. In particular, we tried to orient ourselves at the literature in CP and CDE [Rothfuss, Ferreira, Boehm, et al., 2019; Sesia and Y. Romano, 2021] and used most of the datasets that were used there. Moreover we tried to have datasets with some different properties to gain more insight into strenghts and weaknesses of different models. Thereby we used `Boston Housing`, `Concrete`, `Energy Efficiency` as smaller datasets in order to elaborate performance with lower number of samples. Moreover, we used larger datasets `Meps19`, `Meps20`, `Meps21`, `CASP`, `Blog`, `Facebook1`, `Facebook2`. Finally, we used two versions of a time series dataset provided by VoestAlpine AG about energy price prediction. In particular `VoestRealistic` and `VoestIdeal` are two variations of the same data where we used realistic features and features as if we could look into the future respectively. This dataset was used to investigate the performance of CDMs on time series data.[1] In Table 3.1 we provide an overview of the characteristics of each dataset.

---

[1]The features used for the Voest datasets were all taken from `https://transparency.entsoe.eu/dashboard/show` in a time windows from November 2022 till November 2023 but will not be directly disclosed.

Table 3.1: Comparison of Different Used Datasets

Dataset	# Samples	# Features	Description
Boston Housing	506	13	Housing prices in Boston
Concrete	1030	8	Concrete compressive strength
Energy	768	8	Energy efficiency of buildings
CASP	45730	9	Protein structure prediction
Blog	52397	280	Blog popularity prediction
Facebook1	40948	53	Facebook user engagement
Facebook2	81311	53	Facebook user engagement
Meps19	15785	139	Medical Expenditure Panel Survey
Meps20	17541	139	Medical Expenditure Panel Survey
Meps21	15656	139	Medical Expenditure Panel Survey
VoestRealistic	35001	42	Realistic Features Voest Dataset
VoestIdeal	35001	42	Ideal Features Voest Dataset

3.5 Calculation of the HDR

Calculating the HDR is a straightforward procedure which is described in the PseudoCode below in Algorithm 1 where we assume that the target grid is spaced equally but that is not required technically. The output are the elements of the target grid that are in the HDR. To obtain the actual intervals we just need to go half the step size to the left and right of each element in the HDR but it is left out the algorithm for inconvenience of writing that down. Moreover it is possible to add an improvement step into Algorithm 1 where we can smooth the HDR via linear interpolation between the consecutive densities. This is a very important step as it can significantly improve the performance of the models in particular if it is expensive to evaluate the density at each point by using the model itself. Moreover when we want a single interval as region than as argued in Section 2.6.2 we just connect the largest and smallest border of the HDR which is guranteed to have more than α probability mass. Note that if we have after the $I_{HDR} + 1$ item other items that have the same density as the $I_{HDR} + 1$ item technically also should include those in the HDR but we decided to not do that for simplicity.

Algorithm 1 HDR Calculation

Input: CDM model f, Features x, Significance Level α, Target Grid y
Output: HDR H
$p \leftarrow f(x, y)$
$p_{\text{normalized}} \leftarrow \frac{p}{\text{sum}(p)}$ We normalize the density
$I_{\text{sorted}} \leftarrow \text{argsort}(p_{\text{normalized}})[:: -1]$ We sort in descending order
$p_{\text{sorted}} \leftarrow p_{\text{normalized}}[I_{\text{sorted}}]$
$p_{\text{cumsum}} \leftarrow \text{cumsum}(p_{\text{sorted}})$
$I_{\text{HDR}} \leftarrow \text{sum}(p_{\text{cumsum}} < 1 - \alpha)$ We look how many elements we need to take
$H \leftarrow y[I_{\text{sorted}}[: I_{\text{HDR}} + 1]]$ We take the elements in the HDR on the overestimated side
return H

3.6 Calculating the Calibrated Conditional PDF

For calibrating the whole PDFs of a dataset we need to find the adjustment for a grid of quantile levels similar to how we would do it for calibrating CP for a sigle level. Therefore we can use Algorithm 3 below which expects calibration samples. In practice we observed that even when inputting the training samples for calibration it increases the general performance. Moreover, it is almost necessary to do smoothing because otherwise the result will be very noisy. In the second for loop we basically reconstruct the PDF from the calibrated HDR by assigning each HDR level the same density. Even tho this algorithm will marginally increase the performance it is possible that on single samples the performance is significantly worse. Moreover, we can obtain a quantification of the epistemic uncertainty by integrating the returned value.

Algorithm 2 Calibrating a HDR at a specific level

Input: Density Grids p, Calibration Targets y, Significance Level α, Target Grid $\bar{y}$
Output: Calibrated Significance Level α'
$p_{\text{normalized}} \leftarrow \frac{p}{\text{sum}(p)}$ We normalize the density
$I_{\text{sorted}} \leftarrow \text{argsort}(p_{\text{normalized}})[:: -1]$ We sort in descending order
$p_{\text{sorted}} \leftarrow p_{\text{normalized}}[I_{\text{sorted}}]$
$\text{cumsum} \leftarrow \text{cumsum}(p_{\text{sorted}})$
$\hat{alpha} \leftarrow \text{cumsum}[\arg\min(|p_{\text{cumsum}} - \alpha|)]$ We find the required quantile levels
$\alpha' \leftarrow 1 - \text{quantile}(\hat{alpha}, 1 - \alpha)$ We find the quantile level of the closest level
return α'

Algorithm 3 Calibrating the Conditional PDF

Input: CDM model f, Calibration Features x, Calibration Targets y, Significance Level Grid α, Target Grid $\bar{y}$

Output: Calibrated Conditional PDF grid p', Epistemic Uncertainty p_e

$p \leftarrow f(x, \bar{y})$

$\bar{y}_{\text{spacing}} \leftarrow \bar{y}[1] - \bar{y}[0]$

for α_i in α **do**

   $\alpha_i' \leftarrow$ HDR-Calibrate$(p, y, \bar{y}, \alpha_i)$ Here we use Algorithm 2 to calibrate the HDR

   $H_i \leftarrow$ HDR$(p, \alpha_i', \bar{y})$

end for

$H_0 \leftarrow \varnothing$

$H_{N+1} \leftarrow$ ones$(\text{len}(\bar{y}))$

for i in $1, \ldots, \text{len}(\alpha) + 1$ **do**

   $H_i \leftarrow H_{i-1} \cap H_i$ We take the intersection of the HDRs to get the elements for this level

   $p'[H_i] \leftarrow \frac{1}{\text{len}(\alpha) \cdot \text{sum}(H_i) \cdot \bar{y}_{\text{spacing}}}$ We adjust the density for the elements in the HDR

end for

$p_e \leftarrow$ p - p' We calculate the epistemic uncertainty grid

$p' \leftarrow$ smooth(p') Optional smoothing because of finite samples and finitely fine grids

$p_e \leftarrow$ smooth(p_e) Optional smoothing because of finite samples and finitely fine grids

return p', p_e

3.7 Experiment Results

3.7.1 Recalibration of the Whole CDE

We incoperate recalibration of the whole CDE in some of our experiments (not all due to time-constraints) where we can observe also an increase in performance on real world datasets. In particular by choosing the smoothing window appropriately we can consistently increase the performance on validation sets even when calibrating on the train set itself which shows the utility of this method. Figure 3.1 shows examples of recalibration on the concrete dataset where we smooth with $\frac{1}{16}$ of the grid size. In terms of likelihood, the recalibrated method shows a slight but significant increase in likelihood on the test set, in particular -3.202 instead of -3.224 in average log likelihood.

Moreover, we can observe that recalibration of the full CDE can empirically compensate for a significant amount of model misspecification. In particular, as we can also see in Figure 2.3 where the model was specified as an unimodal gaussian distribution but the true distribution is multimodal. In this case the recalibration can compensate for the misspecification as can even recover the bimodal distribution which makes it more than just a nice utility but a powerful tool that can be used to compensate and potentially identify model misspecification.

3.7.2 Main Benchmark Results

Here we show the results of the final experiments on the 12 datasets. The main experimental procedure consisted for each dataset except for the two Voest ones of five-fold nested cross validation to obtain a robust estimate of the actual performance. On the two Voest Datasets instead we decided to always use the same train-test split where we consider the time dependence in the data by using the chronologically first 80% of the data as training data and the last 20% as test data. For the other datasets we used 80%-20% train-test spilts which is notably different from [Sesia and Y. Romano, 2021] who used a fixed test set of 2000 samples, 2000 for calibration and the other part for training. In particular, on all datasets that we have the same, we have signlificantly less train dat but still competitive results. Moreover, we do cross-validation on a time series split where we expand the training data and use the chronolocially last part for validation. For the
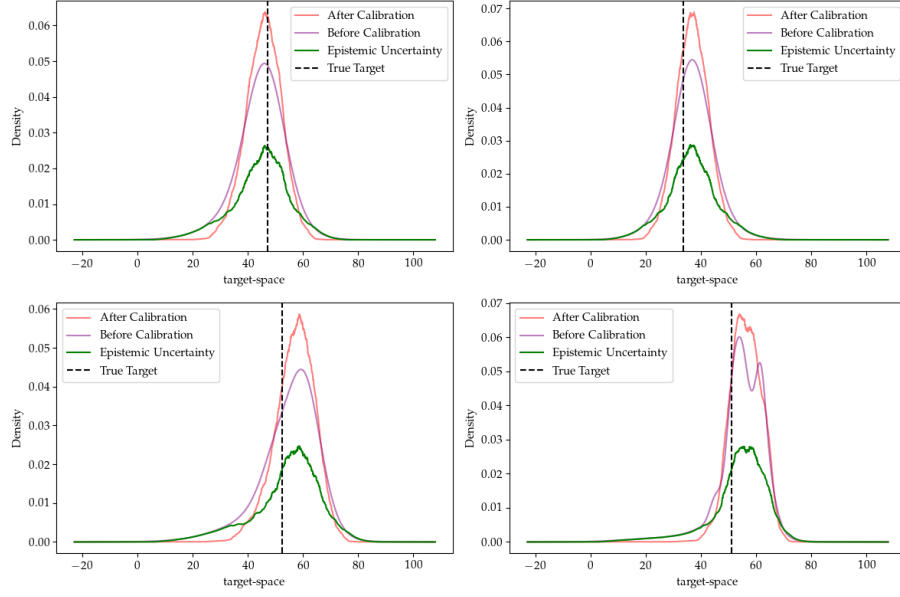
Figure 3.1: Recalibration of the whole estimated conditional PDF on the Concrete dataset. Calibrated on the train dataset and evaluated on the test dataset.

exact implementation we refer to our code. The Algorithm used for the evaluation can be seen in Algorithm 4. This algorithm inspired by [Rothfuss, Ferreira, Boehm, et al., 2019] is a nested cross validation algorithm over multiple seeds and hyperparameters that gurantees a robust estimate of the performance of the models on the test set. In particular, the test set is only used for the final evaluation and the hyperparameters are tuned on the training set which we do CV on.

The results final benchmark results are shown in Table 3.2 and Table 3.3. As expected, resuls in the table with connected intervals are only slightly larger than the true HDR. Comparing our results to the current state of the art which is [Sesia and Y. Romano, 2021] to our best knowledge, we can see that mostly we beat the results with pure HDR and even in some instances like the CASP dataset when using connected intervals which proofs that our methods and hyperparameters are very competitive.

Algorithm 4 Evaluation of the Models

Input: Hyperparameter Grid H, Model Class M, Dataset D, Number of Folds K, Number of Nested Folds L
Output: Performance Metrics P
for k in $1, \ldots, K$ **do**
  $D_{\text{train},k}, D_{\text{test},k} \leftarrow \text{split}(D, k)$
  $CVSplits \leftarrow \text{split}(D_{\text{train},k}, L)$
  for h in H **do**
    for $D'_{\text{train}} D'_{\text{val}}$ in $CVSplits$ **do**
      $M_h \leftarrow \text{fit}(M, D'_{\text{train}}, h)$
      $P_h \leftarrow \text{score}(M_h, D'_{\text{val}})$
    end for
  end for
  $h_{\text{best}} \leftarrow H[\text{argmax}(P)]$ Also set calibrated hyperparameters like epoch and α for CP
  $P_k \leftarrow \text{fit}(M, D_{\text{train}}, h_{\text{best}})$
  $P_k \leftarrow \text{score}(M_k, D_{\text{test}})$
end for
$P \leftarrow \text{mean}(P)$
return P

Table 3.2: CDE Experiment Result CP with HDR Interval Size (lower is better)

Dataset	MDN	KMN	MQR
Boston Housing	9.45 ± 0.70	9.79 ± 0.35	9.32 ± 0.37
Concrete	19.72 ± 0.71	19.37 ± 0.97	17.56 ± 0.55
Energy	6.26 ± 0.18	3.99 ± 0.28	3.89 ± 0.27
CASP	8.41 ± 0.17	7.81 ± 0.15	9.47 ± 0.18
Blog	11.96 ± 0.76	11.83 ± 0.72	12.46 ± 0.77
Facebook 1	12.19 ± 0.64	11.33 ± 0.64	11.34 ± 0.53
Facebook 2	12.81 ± 1.72	12.02 ± 1.69	12.18 ± 1.55
Meps 19	19.41 ± 1.59	19.49 ± 1.22	21.13 ± 1.22
Meps 20	19.26 ± 1.00	18.53 ± 0.96	19.98 ± 0.89
Meps 21	19.02 ± 1.17	18.85 ± 0.87	20.65 ± 0.78

Table 3.3: CDE Experiment Result CP with HDR Connected Interval Size (lower is better)

Dataset	MDN	KMN	MQR
Boston Housing	9.60 ± 0.77	10.23 ± 0.55	9.32 ± 0.37
Concrete	19.88 ± 0.72	19.39 ± 0.96	17.56 ± 0.55
Energy	6.53 ± 0.23	4.22 ± 0.29	3.89 ± 0.27
CASP	11.29 ± 0.26	11.05 ± 0.20	10.27 ± 0.26
Blog	12.12 ± 0.77	17.89 ± 1.33	15.57 ± 1.43
Facebook 1	12.27 ± 0.64	15.81 ± 1.31	13.21 ± 0.93
Facebook 2	12.84 ± 1.71	15.22 ± 1.62	13.78 ± 1.85
Meps 19	19.86 ± 1.66	29.67 ± 2.40	22.90 ± 1.59
Meps 20	19.59 ± 1.15	27.32 ± 2.28	21.34 ± 1.14
Meps 21	19.75 ± 1.46	28.31 ± 1.72	22.37 ± 1.14

4 Conclusion

5 ToDos

1. Show that calibration is the same as in Gneiting et a. (probabilistic calibration). 1a. Show that there are 2 sub-parts then for CP: fitting-calibration and overfitting-calibration Fitting Calibration: the model is probabilistically calibrated to the training data (is fit well) Overfitting Calibration: The model is basically the same way calibrated to the training data as to the test data -> time series and distributional differences come in here too but is a further subchapter then

2. Then show what my recalibration method does mathematically and how it is different from the other recalibration methods

This all contains that CP is a special case of CDE!

3. I should mention in the thesis the stages of my experiemnts. I first did basically only the stuff I did in my practical work (but not sure if that should even be mentioned). Then I should also mention that I did 1000 runs with bayesian optimization on all datasets with a very high variable range of possible hyperparameters with the goal to get a good understanding of the hyperparameters (as there are some novel ones and complex ones). The next stage that I will now start is the stage where I basically start with reasonably good parameters infered by the previous runs and from there basically a. do very specific experiments for the novel hyperparameters to find out there effectiveness (small grid) b. do hyperparameter runs with a smaller grid but multiple test set spilts (with nested cv).

4. As CP is a special case of CDE, also the synthetic reasoning that we basically need them to make real statements about the performance of methods is also valid for CP. So I should also mention that in the thesis. And from there I can basically start finding out the best hyperparameters for CP methods and then also do the same for CDE methods and also possibly new methods that defeat ceavats on the synthetic sets that I only now can find out.

5. It might be interesting to look into the question if when there is some kind of monotonicity between the hyperparameters and the performance of the model, if that is a good synthetic dataset to infer strategies from. I think that is a very interesting question and I should look into that. => "using hyperparameter performances as a measure of the quality of a synthetic dataset."

6. Can I do more advanced recalibration strategies if the data is not IID? (e.g. time series data)

->->-> After those are done its time to look into the strategy part where I look how those CDE/CP can be practically used.

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