Calibrated inference: statistical inference that accounts for both sampling uncertainty and distributional uncertainty

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Abstract

How can we draw trustworthy scientific conclusions? One criterion is that a study can be replicated by independent teams. While replication is critically important, it is arguably insufficient. If a study is biased for some reason and other studies recapitulate the approach then findings might be consistently incorrect. It has been argued that trustworthy scientific conclusions require disparate sources of evidence. However, different methods might have shared biases, making it difficult to judge the trustworthiness of a result. We formalize this issue by introducing a “distributional uncertainty model”, which captures biases in the data collection process. Distributional uncertainty is related to other concepts in statistics, ranging from correlated data to selection bias and confounding. We show that a stability analysis on a single data set allows to construct confidence intervals that account for both sampling uncertainty and distributional uncertainty.

1 Introduction

Statistical inferences can be fragile. If we compare two analyses conducted by different statisticians on different data sets, variation can be due to sampling, due to distribution shift, or due to a change in methodology. These issues raise a fundamental question: How can we draw trustworthy scientific conclusions? A common recommendation is to have independent teams attempt to replicate the findings of others. While replication is critically important, it is arguably insufficient. If a study suffers from biases for some reason and replication studies emulate the study, the findings will be consistently incorrect (Munafò and Smith, 2018). To solve this issue, researchers have advocated investigating independent lines of evidence (Denzin, 1970; Freedman, 1991; Rosenbaum, 2010; Munafò and Smith, 2018). Ideally, these different lines of evidence are susceptible to different biases. Intuitively, if results agree across different methodologies, then a statistical finding is less likely to be an artifact. However, it might be expensive and impractical to ask several researchers to run studies independently.

Can we emulate this strategy on a single data set? In fact, stability analyses have been advocated by many researchers. To be more precise, it has been recommended to evaluate several reasonable modelling choices for one single data set (Leamer, 1983; Rosenbaum, 2010; Patel et al., 2015; Steegen et al., 2016; Yu and Kumbier, 2020). Common practice includes running differently specified regressions or considering the perturbations induced by various forms of data pre-processing. If the estimator-to-estimator variability is high, then the analyst has reason to distrust the estimates.

This warrants an investigation of the theoretical properties of this practice. What mathematical problem do we solve with this approach? What distinguishes a good stability analysis from a bad one? If differently specified regressions return similar estimates, what criterion tells us whether we should be concerned or not? Often the decision what qualifies as a “stable result” is left up to the individual judgements of the analyst. One could analyze the estimators with a random effects model, but since the estimators are computed on the same data set, they might share biases. More concretely speaking, since the structure of the biases is generally unknown, it is not clear how to define a random effects model that captures the correlation structure of the estimators’ biases.

In order to address these questions in a formal framework, we take a distributional perspective. Outliers, sampling bias, confounding, measurement errors, and unknown correlations between units
are omnipresent in data analysis and make it challenging to gather trustworthy results. We consider a setting, where the data is drawn from a “perturbed” or “contaminated” distribution, while the goal is to infer some properties of the uncontaminated distribution. The classical robust statistics literature (Huber, 1981) addresses distributional perturbations by investigating the worst-case behavior of a statistical functional over a fixed neighborhood of the model. More recently, distributional uncertainty sets based on $f$-divergence have been linked to distributionally robust optimization (Ben-Tal et al., 2013; Duchi et al., 2021). In such models, it is challenging to choose the appropriate set of distributions, since the size of the perturbation is generally unknown.

The distributional perturbations we want to model are due to small errors in the data collection process that potentially induce selection bias, confounding, batch effects, or measurement errors. We do not believe that these issues are adversarial in nature. Thus, instead of considering worst-case distributional perturbations, we define a family of random symmetric perturbations. We show that modelling distributional perturbations as random and symmetric has an intriguing consequence: using a stability analysis, it is possible to estimate the strength of the distributional perturbation. Based on an estimate of the distributional perturbation strength, we propose confidence intervals that capture both sampling uncertainty and distributional uncertainty.

1.1 Related work

Considerations of model stability have emerged in Bayesian statistics (Box, 1980; Skene et al., 1986), causal inference (Leamer, 1983; LaLonde, 1986; Rosenbaum, 1987; Imbens and Rubin, 2015) and in discussions about the data science lifecycle (Yu, 2013; Steegen et al., 2016; Yu and Kumbier, 2020). Using different estimation strategies is commonly recommended to corroborate a causal hypothesis (Freedman, 1991; Rosenbaum, 2010; Karmakar et al., 2019). In particular, to evaluate omitted variable bias, it is a common recommendation to consider the between-estimator variation of several adjusted regressions (Oster, 2019). Sensitivity analysis bounds the influence of confounders that have been omitted in a regression or matching procedure and has played an influential role in increasing trustworthiness of causal inference from observational data (Cornfield et al., 1959; Rosenbaum and Rubin, 1983; VanderWeele and Ding, 2017). It has been argued that causal mechanisms are expected to lead to stable associations across settings, if the same mechanism is shared across settings. Based on this observation, stability principles have been employed to discover causal relationships based on heterogeneous data sets (Peters et al., 2016; Rothenhäusler et al., 2015; Bühlmann, 2020; Pfister et al., 2021). Stability principles are heavily used in machine learning, often with the goal of variance reduction. For example, some tree-based methods employ feature bagging, which can be seen as averaging over differently specified prediction models (Breiman, 1996, 2001). Dropout in neural networks is another form of algorithm perturbation (Srivastava et al., 2014). Distributional uncertainty sets based on $f$-divergences have been linked to distributionally robust optimization (Ben-Tal et al., 2013; Duchi et al., 2021). In the context of prediction under distribution shift, stability or invariance principles have been employed to learn prediction mechanisms that generalize to new settings (Schölkopf et al., 2012; Zhang et al., 2013; Rojas-Carulla et al., 2018; Heinze-Deml and Meinshausen, 2021; Rothenhäusler et al., 2021). Quasi-likelihoods (Wedderburn, 1974) are a way to allow greater variability in the data than what is expected from the model. However, uncertainty quantification in quasi-likelihoods still only deals with sampling uncertainty, while we aim to quantify uncertainty due to both sampling and distributional uncertainty. As we show in the appendix, the considered perturbation model implies equicorrelated data marginally. Thus, there is a connection between our perturbation model and the problem of inference in network data (Lee and Ogburn, 2021). The main difference between our approach and other approaches is that we do not model the network structure itself; instead dependencies arise through a symmetric perturbation scheme.

1.2 Outline of the paper

In Section 1.3, we will quickly review standard practice for forming confidence intervals. In Section 2, we introduce the setting of the paper and discuss why standard statistical practice does not account for all types of uncertainty in this setting. The setting of our paper arises under a distributional perturbation model described in Section 2 and sampling procedures described in the Appendix. We then turn to
In Section 3, we discuss how to form confidence intervals in our setting. This completes the picture from a statistical viewpoint. In Section 4, we evaluate the performance of the proposed procedure on a simulated example from causal inference. In Section 5 we demonstrate that the proposed procedure can increase the stability of decision-making based on real-world data. We conclude in Section 6.

1.3 Standard approach

Let us consider estimation of the mean \( \theta^0 = E[D] \) of a square-integrable real-valued random variable \( D \in D, D \sim P \). Assume that we are given data \((D_i)_{i=1,...,n} \sim i.i.d. P\) with \( \text{Var}(D_i) = \sigma^2 \in (0, \infty) \). We can estimate \( \sigma^2 \) via \( \hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (D_i - \bar{D})^2 \) to form asymptotically valid confidence intervals, that means

\[
P(\bar{D} - z_{1-\alpha/2} \hat{\sigma}/\sqrt{n} \leq \theta^0 \leq \bar{D} + z_{1-\alpha/2} \hat{\sigma}/\sqrt{n}) \to 1 - \alpha,
\]

where \( z_{1-\alpha/2} \) is the \( 1 - \alpha/2 \) quantile of a standard Gaussian random variable. This practice is justified by the central limit theorem which implies

\[
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (D_i - E[D]) \overset{d}{=} N(0, \text{Var}(D)) + o_p(1).
\]

More generally, for some vector-valued data \( D_i \sim i.i.d. P \) consider a parametrized model \( \{ p_\theta, \theta \in \Omega \} \) of positive probability densities \( p_\theta \) with respect to some \( \sigma \)-finite measure \( \mu \). Assume that the parameter space \( \Omega \) is an open subset of \( \mathbb{R}^d \). We consider the maximum-likelihood estimator

\[
\hat{\theta} = \arg \max \sum_{i=1}^{n} \log p_\theta(D_i)
\]

for some unknown target parameter \( \theta^0(P) = \arg \max E[\log p_\theta(D)] \), where \( D \sim P \). Under regularity assumptions (van der Vaart, 2000; Tsiatis, 2006), for \( n \to \infty \),

\[
\sqrt{n}(\hat{\theta} - \theta^0) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} -E[\partial^2 \log p_\theta(D)]^{-1} \partial \log p_\theta(D_i) + o_p(1) \overset{d}{=} N(0, \Sigma) + o_p(1),
\]

where \( \Sigma = E[\partial^2 \log p_\theta(D)]^{-1} \text{Var}(\partial \log p_\theta(D)) E[\partial^2 \log p_\theta(D)]^{-1} \). Thus, based on a consistent estimator \( \Sigma \to \Sigma \), one can form asymptotically valid confidence intervals via

\[
\hat{\theta}_k \pm z_{1-\alpha/2} \frac{\sqrt{\Sigma_{kk}}}{\sqrt{n}}.
\]

A similar approach can be used to construct asymptotically valid confidence intervals for \( M \)-estimators. In the following, we discuss situations in which this approach does not have the desired coverage.

2 Distributional uncertainty

There are several reasons why the coverage in equation (1) might not hold. The main focus of this paper will be violations of (2) due to what we call distributional uncertainty. Due to batch effects, sampling bias, confounding, or other distributional shifts, the data scientist might not draw a sample from the target distribution \( P \) but from some \( P^* \neq P \). The data analyst may try to address this source of bias by re-weighting, regression adjustment, random effect modeling, or other statistical techniques. Our viewpoint is that when using such techniques, it is likely that some residual error remains. Ideally, we would like to construct confidence intervals that detect residual errors due to distributional perturbations, and accounts for it, if necessary. We model the variation due to distributional changes as random. This will allow us to integrate both distributional uncertainty and sampling uncertainty in a natural fashion.
Let us make this more concrete by returning to the example of estimating the mean. Due to unknown sampling bias or other unknown distributional shifts, the data scientist might not draw a sample from the target distribution $P$. Instead, the data $(D_i)_{i=1,...,n}$ might be drawn i.i.d. from some perturbed distribution $P^\xi \neq P$, where $\xi$ is a random variable and $P^\bullet$ is a probability distribution for each fixed $\bullet \in \text{range}(\xi)$. Then the error of the empirical mean can be decomposed:

$$\frac{1}{n} \sum_{i=1}^{n} D_i - \mathbb{E}[D] = \frac{1}{n} \sum_{i=1}^{n} D_i - \mathbb{E}[D] + \mathbb{E}[D] - \mathbb{E}[D]$$

(4)

Equation (2) usually does not hold in this setting as distributional perturbations induce additional variation.

Roughly speaking, in equation (4) we can distinguish three different regimes. If variation due to sampling is much larger than the variation due to distributional perturbations, intuitively one can simply ignore the variation due to the second term and just compute confidence intervals as in the previous section. Secondly, one can consider the setting where both sources of variation are of the same order, that means the case where the distributional variation is of the order $1/\sqrt{n}$. This is the setting we will focus on. Thirdly, in practice one will encounter cases where the distributional variation is of higher order than $1/\sqrt{n}$. In this case, one would have to scale the confidence intervals in equation (3) by a factor that goes to infinity for $n \to \infty$. We restrict ourselves to the second setting mainly for expository reasons: It is desirable to have a methodology that works in all three settings. To facilitate adoption by practitioners, ideally such methodology should be a direct extension of current statistical practice. Thus, it is natural to start with a regime where both types of uncertainty are of the same order. To summarize, we consider the regime where the overall variation is of order $1/\sqrt{n}$.

**A simple model for perturbations.** What is a reasonable model for the distributional perturbation? For an event $A$ we will think about $P^\xi[A]$ as a random variable that depends on the (random) perturbation $\xi$. Perhaps the most simplistic form of distributional perturbation is to randomly up-or down-weight probabilities of events. For example, for a uniform distribution $P(D = k) = \frac{1}{K}$ for $k = 1,\ldots,K$ and an exchangeable set of non-negative weights $\{\xi_k\}_{k=1}^{K}$ with $\sum_{k=1}^{K} \xi_k = 1$ we can define

$$P^\xi(D = k) = \xi_k.$$ 

(5)

If the data $D_i$ is drawn i.i.d. from the perturbed distribution $P^\xi$, then empirical means are unbiased marginally: For any function $\psi(\bullet)$

$$E\left[ \frac{1}{n} \sum_{i=1}^{n} \psi(D_i) \right] = E[\psi(D)].$$

On the left-hand side, we take the expectation over both the randomness due to drawing from $P^\xi$ and the randomness in $\xi$. Thus, marginally, empirical means are unbiased for the respective population quantities. Let us turn to computing the variance of empirical means. Define $s(k) = \sum_{i=1}^{n} 1_{D_i = k}$. Note that under the perturbation model above, the $s(k)$, $k = 1,\ldots,K$ are exchangeable marginally. A short calculation (see Section B.1) shows that

$$\text{Var}_P\left( \frac{1}{n} \sum_{i=1}^{n} \psi(D_i) \right) = \frac{K^2}{n^2(K - 1)} \text{Var}_P(s(1)) \text{Var}_P(\psi(D))$$

$$= \frac{\delta^2}{n} \text{Var}_P(\psi(D)),$$

(6)

where $\delta^2 = \frac{K^2}{n(K - 1)} \text{Var}_P(s(1))$ and $D \sim P$. Interestingly, compared to equation (2), the variance in (6) contains a scaling factor $\delta$ that does not depend on $\psi$. Since $\xi$ and $P$ are unknown in general, also $\delta$ is usually unknown.

At this point, the reader might wonder whether this property is specific for the considered example, and whether a slightly different type of perturbation model for numerical or discrete data would have
led to a different change in the variance. In other words, the reader might wonder, whether this type of perturbation model is “natural”. To not interrupt the flow of exposition, we discuss this question in more detail in the Appendix, Section A.1. The short answer is that our perturbation model arises naturally under a symmetry assumption. The following result is a direct consequence of Theorem 2 in the Appendix.

**Corollary 1** (Uniqueness of perturbation model, informal). Let \( D_1, \ldots, D_n \) be drawn from \( \mathbb{P}^\xi \). Under a symmetry assumption and some regularity conditions on \( \mathbb{P}^\xi \) (stated in Theorem 2), there exists \( \delta > 0 \), such that for all \( \psi \in L^2(\mathbb{P}) \) marginally across distributional and sampling uncertainty we have

\[
\text{Var}_P\left( \frac{1}{n} \sum_{i=1}^n \psi(D_i) \right) = \frac{\delta^2}{n} \text{Var}_P(\psi(D)).
\]

The considered symmetry assumptions also directly imply that \( E[\frac{1}{n} \sum_{i=1}^n \psi(D_i)] = E[\psi(D)] \).

How should we think about the parameter \( \delta \)? Intuitively, the larger \( \delta \) is, the further away \( \mathbb{P}^\xi \) is from \( \mathbb{P} \). Thus, assumptions that hold for the unperturbed distribution \( \mathbb{P} \) will be increasingly violated under \( \mathbb{P}^\xi \). For example, for large \( \delta \) one can think about this model as inducing sampling bias. The perturbations potentially induce other types of issues such as correlated data, and confounding. We discuss this in more detail in the Appendix, Section A.3.

To conduct statistical inference, it is not sufficient to just compute the variance. We have to think about the distributional change as a superposition of small changes, then marginally across both sampling uncertainty and distributional uncertainty we get a central limit theorem, albeit with a non-standard variance formula.

**CLT for the isotropic perturbation model.** We have already introduced a random perturbation model for the special case of discrete data and for a fixed perturbation size. Now we will construct a general isotropic perturbation model for multivariate continuous or discrete random variables and consider the case where the change in measure is a superposition of small incremental changes. We will see that under such a model, we will get a non-standard CLT in the sense that sample means are asymptotically normal, with a different variance formula compared to the i.i.d. case.

To recap, in the random perturbation model, the data is not directly drawn from the target distribution \( \mathbb{P} \), but from some random probability measure \( \mathbb{P}^\xi \), where \( \mathbb{P}^\xi \) is close to \( \mathbb{P} \). The idea is that due to small batch effects, measurement error, or convenience sampling, the actual sampling distribution \( \mathbb{P}^\xi \) randomly differs from the target distribution \( \mathbb{P} \). Under \( \mathbb{P}^\xi \), probabilities of events are slightly up-weighted or down-weighted compared to \( \mathbb{P} \).

We want to construct a random perturbation model that includes many commonly encountered situations such as distributions on \( \mathbb{R}^d \) or the (infinite-dimensional) space of continuous functions on \( \mathbb{R} \). A result from probability theory shows that any random variable \( D \) on a finite or countably infinite dimensional probability space can be written as a measurable function \( D \overset{d}{=} h(U) \), where \( U \) is a uniform random variable on \([0, 1]\).

Thus, without loss of generality we will construct distributional perturbations for a uniform distribution on \([0, 1]\). With the transformation \( h(\cdot) \) defined above, this construction generalizes to the general cases by setting

\[
\mathbb{P}^\xi(D \in \bullet) = \mathbb{P}^\xi(h(U) \in \bullet).
\]

Let us now construct the distributional perturbation for a uniform random variable. Take \( m \) bins \( I_k = [(k-1)/m, k/m] \) for \( k = 1, \ldots, m \). Let \( W_1, \ldots, W_m \) be i.i.d. positive random variables with finite variance. Set \( \xi = (W_1, \ldots, W_m) \). We define the randomly perturbed distribution \( \mathbb{P}^\xi \) by setting

\[
\mathbb{P}^\xi(U \in \bullet) = \sum_k \mathbb{P}(U \in I_k \cap \bullet) \cdot \frac{W_k}{\sum_{k=1}^m W_k/m}.
\]

\(^1\text{For any Borel-measurable random variable } D \text{ on a Polish (separable and completely metrizable) space } \mathcal{D}, \text{ there exists a Borel-measurable function } h \text{ such that } D \overset{d}{=} h(U) \text{ where } U \text{ follows the uniform distribution on } [0, 1] \text{ (Dudley, 2018).}\)
Let \( m = m(n) \) such that \( \frac{m}{m(n)} \) converges to some limit \( r \in (0, \infty) \). Note that \( \xi \) depends on \( m \) and thus also on \( n \). Conditionally on \( \xi \), let \( (D_1^n, \ldots, D_n^n) \) be i.i.d. from \( \mathbb{P}^\xi \).

**Lemma 1** (Asymptotic behaviour of means). Under the assumptions mentioned above, for any Borel-measurable square-integrable function \( \psi : \mathcal{D} \mapsto \mathbb{R}^l \), we have

\[
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D_i^n) - \mathbb{E}[\psi(D)] \xrightarrow{d} N(0, \delta^2 \text{Var}_\psi(\psi(D))) + o_p(1),
\]

with

\[
\delta^2 = 1 + \frac{r \text{Var}(W)}{E[W]^2}.
\]

In other words, the marginal distribution of \( \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D_i^n) \) is asymptotically Gaussian with asymptotic variance containing a scaling factor \( \delta \).

The proof can be found in the Appendix, Section B.2. The reason we consider a triangular array of data sets is that we want both the sampling uncertainty and distributional uncertainty to be of the same order (see discussion above). As \( n \) goes to infinity we thus have to consider distributional perturbations that go to zero. We believe that the proposed methodology is also useful in cases where the distributional perturbations have constant order, but a formal investigation of this setting is beyond the scope of this work.

The asymptotic behaviour shown in equation (7) arises not only under the distributional perturbation model but other types of sampling procedures that induce dependence between observations. In Appendix B.3, we discuss other sampling models that give rise to (7).

Unless explicitly mentioned otherwise, in the following we assume that the data scientist has access to one such data set \( (D_1^n, \ldots, D_n^n) \) for some large \( n \). Note that if the data \( (D_1, \ldots, D_n) \) is i.i.d. \( \mathbb{P} \), then equation (7) holds for \( \delta = 1 \) and \( D_i^n = D_i \). Thus, equation (7) is weaker than assuming that the data is drawn i.i.d. from \( \mathbb{P} \).

In the following, we will discuss how estimators behave asymptotically under equation (7). It turns out that under some regularity assumptions, maximum likelihood estimators are still consistent and asymptotically normal, but with the scaling factor \( \delta^2 \) in the variance formula.

**Asymptotic behaviour of M-estimators.** Here we will consider the asymptotic behaviour of estimators of type \( \hat{\theta} = \arg \min_{\theta \in \Omega} \frac{1}{n} \sum_{i=1}^{n} L(\theta, D_i^n) \) for a target defined via

\[
\theta^0 = \arg \min_{\theta \in \Omega} \mathbb{E}[L(\theta, D)],
\]

where \( L(\theta, \cdot) \) is a Borel-measurable loss function and \( \Omega \) is an open subset of \( \mathbb{R}^d \). These estimators include maximum likelihood estimators with \( L(\theta, D) = -\log p_0(D) \). In classical statistical theory, uncertainty quantification is usually based on showing that the estimator is asymptotically Gaussian. Since we have a different two-stage sampling model, one has to verify that a similar approximation – with a different variance formula – still holds in our setting.

First, we will discuss consistency. Instead of aiming for maximal generality, we will adapt a simple consistency proof from the literature. In particular, we will adapt the classical consistency result in van der Vaart (2000), Section 5.2.1. We expect that other consistency proofs can be adapted similarly. The main difference in the proof is that since the data is not i.i.d. from the target distribution we cannot directly rely on the law of large numbers. The proof can be found in Appendix B.7.

**Lemma 2** (Consistency of M-estimators). Consider the M-estimator \( \hat{\theta} = \arg \min_{\theta \in \Omega} \frac{1}{n} \sum_{i=1}^{n} L(\theta, D_i^n) \) and the target \( \theta^0 = \arg \min_{\theta \in \Omega} \mathbb{E}[L(\theta, D)] \), where \( \Omega \) is a compact subset of \( \mathbb{R}^d \). Furthermore assume that \( \theta \mapsto L(\theta, D) \) is continuous and that \( \inf_{\|\theta-\theta\|_2 \leq \delta} L(\theta, D) \) is square-integrable under \( \mathbb{P} \) for every \( \delta \) and \( \theta' \) and that \( \inf_{\theta \in \Omega} L(\theta, D) \) is square integrable. We assume that \( \mathbb{E}[L(\theta, D)] \) has a unique minimum. Then,

\[
\hat{\theta} - \theta^0 = o_p(1).
\]
Now let us turn to asymptotic normality. We will modify the proof in van der Vaart (2000), Section 5.6. Similarly as above, the main difference in the proof is since the data is not i.i.d. from the target distribution we cannot directly rely on the law of large numbers or a standard CLT. The proof can be found in Appendix B.7.

**Lemma 3** (Asymptotic normality of M-estimators). For each \( \theta \) in an open subset of \( \Omega \), let \( \theta \mapsto \partial_\theta L(\theta, d) \) be twice continuously differentiable in \( \theta \) for every \( d \). Assume that the matrix \( \mathbb{E}[\partial^2_\theta L(\theta_0, D)] \) exists and is nonsingular. Assume that third order partial derivatives of \( \theta \mapsto L(\theta, d) \) are dominated by a fixed function \( h(\cdot) \) for every \( \theta \) in a neighborhood of \( \theta_0 \). We assume that \( \partial_\theta L(\theta_0, D), \partial^2_\theta L(\theta_0, D) \) and \( h(D) \) are square-integrable under \( \mathbb{P} \). Let \( \hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} L(\theta, D^n_i) \). Assume that \( \hat{\theta} - \theta_0 = o_p(1) \), where \( \theta_0 \) satisfies the estimating equation \( \mathbb{E}[\partial_\theta L(\theta_0, D_i)] = 0 \). Then,

\[
\sqrt{n}(\hat{\theta} - \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[\partial^2_\theta L(\theta_0, D_i)]^{-1} \partial_\theta L(\theta_0, D^n_i) + o_p(1).
\]

In particular, by Lemma 1 we have that \( \sqrt{n}(\hat{\theta} - \theta_0) \) is asymptotically normal with mean zero and covariance matrix \( \delta^2 \Sigma \), where

\[
\Sigma = \mathbb{E}[\partial^2_\theta L(\theta_0, D)]^{-1} \mathbb{E}[\partial_\theta L(\theta_0, D)^\top \partial_\theta L(\theta_0, D)] \mathbb{E}[\partial^2_\theta L(\theta_0, D)]^{-1}.
\]

The upshot is that M-estimators are asymptotically unbiased, marginally across both sampling uncertainty and distributional uncertainty. However, the variance formula changes in the sense that there is an (unknown) scaling factor \( \delta^2 \).

**The standard mode of inference fails.** Let us quickly sketch why the standard mode of inference fails. Let’s consider the case of estimating the mean \( \theta_0 = \mathbb{E}[D] \) via \( \hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} D^n_i \). One may be tempted to use the standard variance estimate \( \delta^2_{\text{naive}}/n \), where

\[
\delta^2_{\text{naive}} = \frac{1}{n} \sum_{i=1}^{n} (D^n_i - \frac{1}{n} \sum_{i=1}^{n} D^n_i)^2.
\]

However, a short calculation shows that

\[
\delta^2_{\text{naive}} = \frac{1}{n} \sum_{i=1}^{n} (D^n_i - \frac{1}{n} \sum_{j=1}^{n} D^n_j)^2 = \frac{1}{n} \sum_{i=1}^{n} (D^n_i)^2 - (\frac{1}{n} \sum_{j=1}^{n} D^n_j)^2 = \text{Var}_P(D) + o_P(1).
\]

Here, we used equation (7) for \( \psi(D) = D \) and \( \psi(D) = D^2 \). However, as shown in Lemma 1, the asymptotic variance of \( \hat{\theta} \) is \( \frac{\delta^2}{n} \text{Var}_P(D) \). Thus, the standard approach drastically underestimates variance in our setting. If \( \delta \) is known, one can simply stretch the confidence intervals discussed in Section 1.3 accordingly. However, in general \( \delta \) will be unknown and has to be estimated from data. We will discuss the estimation of \( \delta \) in Section 3.

**Notation.** Let \( \mathbb{P} \) denote a probability measure on \( \mathcal{D} \). For each fixed \( n \) the random variable \( \xi(n) \in \Xi \) encodes the distributional perturbation. Formally, \( \mathbb{P}^n, \bullet \in \Xi \), is a stochastic kernel with the target space \( \mathcal{D} \). Conditionally on \( \xi(n) \), we draw an i.i.d. sample \( (D^n_1, \ldots, D^n_n) \) from \( \mathbb{P}^\xi(n) \). \( \xi(n) \) might depend on \( n \) but we suppress this in the notation and simply write \( \xi \). Similarly, we sometimes suppress the dependence of \( (D^n_1, \ldots, D^n_n) \) on \( n \) and simply write \( (D_1, \ldots, D_n) \). We write \( P \) for the marginal distribution of \( (D_1, \ldots, D_n, \xi) \). We write \( \text{Var}_P \) for the variance under \( P \) and \( \text{Var}_F \) for the variance under \( \mathbb{P} \).

## 3 Calibrated inference

We will now discuss how to estimate \( \delta \) and form asymptotically valid confidence intervals for \( \theta_0 \). As discussed earlier, data analysts often have not just one reasonable estimator for a given parameter \( \theta_0 \), but potentially several reasonable estimators \( \theta^1, \ldots, \theta^K \). For example, these estimators can arise from using different specifications in generalized linear models or by running the analysis for subgroups of the observations.
Example 1 (OLS with several specifications). Let us consider a setting in which the data analyst wants to estimate the causal effect of some variable $X_1$ on a target variable $Y$. On observational data, this is often done by invoking suitable assumptions and regressing $Y$ on $X_1$ and a suitable set of covariates. Often, the analyst has several reasonable choices for the set of covariates. Suppose that the data analyst performs ordinary least-squares on $K$ different subsets of $X$ that include $X_1$, denoted by $X^{S_1}, X^{S_2}, \ldots, X^{S_K}$. For example, $X^{S_1}$ can be $(X_1, X_2, X_3)$. Now the data analyst has $K$ different regression coefficients of $X_1$, $\hat{\theta}^1, \ldots, \hat{\theta}^K$ where

$$\hat{\theta}^k = \left( \sum_{i=1}^{n} X^{S_k}_i (X^{S_k}_i)^\top \right)^{-1} \sum_{i=1}^{n} X^{S_k}_i Y_i.$$ 

If the empirical variation between the estimators $\hat{\theta}^1, \ldots, \hat{\theta}^K$ is low, then the analyst may feel more confident about conclusions drawn from these estimates than if the variation between these estimators is very large. As an example, in Chiappori et al. (2012) the authors write “It is reassuring that the estimates are very similar in the standard and the augmented specifications”. We will now look at this practice under the isotropic perturbation model. We will see that in this setting it is possible to construct a consistent estimator of $\delta$ and form asymptotically valid confidence intervals that account for both sampling uncertainty and distributional perturbations.

Let us investigate the behaviour of these estimators in more detail. First, if the estimators $\hat{\theta}^k = \hat{\theta}^k(D_1, \ldots, D_n)$ are M-estimators, by Lemma 2 and Lemma 3 the estimators are asymptotically linear in the sense that

$$\hat{\theta}^k - \theta^k = \frac{1}{n} \sum_{i=1}^{n} \phi^k(D_i) + o_p\left(\frac{1}{\sqrt{n}}\right)$$

for some deterministic $\theta^k = \arg \min \mathbb{E} [L^k(\theta, D)]$, where $L^k$ is the loss function of estimator $\theta^k$. Here the functions $\phi^k$ are assumed to satisfy $\mathbb{E} [\phi^k(D)] = 0$ and $\text{Var}_\mathbb{P}(\phi^k(D)) \in (0, \infty)$. Since $\phi^k(D)$ is square integrable, by Lemma 1 the sequence $\sqrt{n}(\hat{\theta}^k - \theta^k)$ is asymptotically normal with mean zero and covariance $\hat{\sigma}^2 \text{Var}_\mathbb{P}(\phi^k(D))$. We summarize this behaviour of the estimators as the following assumption for the convenience of reference later.

**Assumption 1** (Asymptotic linearity). The estimators $\hat{\theta}^k, k = 1, \ldots, K$ are asymptotically linear, that is they satisfy equation (8) for functions $\phi^k$ with $\mathbb{E} [\phi^k(D)] = 0$ and $0 < \text{Var}_\mathbb{P}(\phi^k(D)) < \infty$.

As discussed above, for the case of M-estimators, this assumption can be justified via Lemma 2 and Lemma 3. We will now formalize the premise that the data analyst considers each of the $\hat{\theta}^k$ a reasonable estimator for the parameter of interest, $\theta^0$.

**Assumption 2** (Agreement). We have $\theta^k = \theta^0$ for $k = 1, \ldots, K$.

This assumption must be justified with scientific background knowledge. Intuitively, the assumption states that if both sampling uncertainty and distributional uncertainty were negligible, the estimators would agree. In Section 4, we discuss in a numerical example how the choice of such estimators can be justified and study the behaviour of our method in cases where the estimators do not agree asymptotically. If the data scientist does not believe in asymptotic agreement of the estimators, we present conservative confidence intervals in the Appendix, Section C.

### 3.1 Confidence intervals

Now let us turn to constructing confidence intervals for $\theta^0$. Assume that the data analyst has access to $K$ different estimators $\hat{\theta}^1, \ldots, \hat{\theta}^K$ that are asymptotically linear for estimating $\theta^0$ with influence functions $\phi^1(D), \ldots, \phi^K(D)$. For expository simplicity, for now we assume that their influence functions $\phi^1(D), \ldots, \phi^K(D)$ are uncorrelated and have the same variance $\sigma^2 > 0$ under $\mathbb{P}$. Later in the section, we discuss how to construct confidence intervals for general cases where influence functions are possibly correlated and have different variances. Since the estimators are asymptotically unbiased, uncorrelated, and have the same variance, as final estimate we consider the mean of estimators, $\hat{\theta}^{\text{pooled}} = \frac{1}{K} \sum_k \hat{\theta}^k$. In the following, we will investigate the asymptotic behaviour of this estimator.
By Assumption 1, 2 and Lemma 1, for \( k = 1, \ldots, K \),

\[
\sqrt{n} (\hat{\theta}^k - \theta^0) \overset{d}{=} \delta \sigma Z_k + o_P(1),
\]

where \( Z_k \) are independent standard normal random variables. Thus,

\[
\sqrt{n} (\hat{\theta}^{\text{pooled}} - \theta^0) \overset{d}{=} \delta \sigma \bar{Z} + o_P(1).
\]  \( \text{(9)} \)

On the other hand, define the between-estimator variance

\[
\hat{\sigma}^2_{\text{bet}} = \frac{1}{K-1} \sum_{k=1}^{K} (\hat{\theta}^k - \hat{\theta}^{\text{pooled}})^2.
\]

Then,

\[
\hat{\sigma}^2_{\text{bet}} \overset{d}{=} \frac{\delta^2 \sigma^2}{n} \frac{1}{K-1} \sum_{k=1}^{K} (Z_k - \bar{Z})^2 + o_P(1/n) \overset{d}{=} \frac{\delta^2 \sigma^2}{n} \chi^2(K-1) + o_P(1/n)
\]  \( \text{(10)} \)

where \( \chi^2(K-1) \) is a chi-square random variable with \( K-1 \) degrees of freedom. Let us assume for a moment that \( \sigma^2 \) is known to the data scientist. In this case, the data scientist may estimate \( \delta^2 \) via

\[
\hat{\delta}^2 := \frac{n \hat{\sigma}^2_{\text{bet}}}{(K-1)\sigma^2} \overset{d}{=} \delta^2 \frac{\chi^2(K-1)}{K-1} + o_P(1).
\]

Combining equations (9) and (10), we get

\[
\frac{\hat{\theta}^{\text{pooled}} - \theta^0}{\hat{\sigma}_{\text{bet}} / \sqrt{K-1}} \overset{d}{=} t(K-1) + o_p(1).
\]

where \( t(K-1) \) is a \( t \)-distributed random variable with \( K-1 \) degrees of freedom. Note that \( \delta, \sigma \) cancel out.

Without direct estimation of \( \delta \) or \( \sigma \), we have an \( 1 - \alpha \) confidence interval of \( \theta^0 \):

\[
\hat{\theta}^{\text{pooled}} \pm t_{K-1,1-\alpha/2} \frac{\hat{\sigma}_{\text{bet}}}{\sqrt{K-1}},
\]

where \( t_{K-1,1-\alpha/2} \) is the \( 1 - \alpha/2 \) quantile of the \( t \)-distribution with \( K-1 \) degrees of freedom. Note that the size of the confidence intervals goes to zero with rate \( 1/\sqrt{n} \) as \( \hat{\sigma}_{\text{bet}} = O_P(1/\sqrt{n}) \). Computing the between-estimator variance has some similarities with random effect models. We discuss some of the differences in Remark 3.

Let us make this argument more general. We will now discuss the case where the estimators \( \hat{\theta}^k \) have potentially different asymptotic variances \( \text{Var}_P(\hat{\phi}^k(D)) \). Instead of using \( \hat{\theta}^{\text{pooled}} = \frac{1}{K} \sum_k \hat{\theta}^k \) as the final estimate, we recommend inverse variance weighting. Thus, we first need to estimate \( \text{Var}_P(\hat{\phi}^k(D)) \) consistently. While estimating \( \text{Var}_P(\hat{\phi}^k(D)) \) is straightforward under i.i.d. sampling, we also have to verify that this works in our model class. We estimate \( \text{Var}_P(\hat{\phi}^k(D)) \) using plug-in estimators of the influence function \( \hat{\phi}^k(D) \) as

\[
\text{Var}_P(\hat{\phi}^k(D)) = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\phi}^k(D_i) - \frac{1}{n} \sum_{i=1}^{n} \hat{\phi}^k(D_i) \right)^2.
\]  \( \text{(11)} \)

The following proposition shows that \( \text{Var}_P(\hat{\phi}^k(D)) \) is a consistent estimator of \( \text{Var}_P(\phi^k(D)) \).

**Proposition 1** (Consistency of \( \text{Var}_P(\hat{\phi}^k(D)) \)). Suppose that the \( \phi^k(D) \) has finite fourth moments. Furthermore, suppose that the estimation of the influence function is consistent in the sense that

\[
\frac{1}{n} \sum_{i=1}^{n} (\hat{\phi}^k(D_i) - \phi^k(D_i))^2 = o_p(1).
\]  \( \text{(12)} \)

Then, \( \text{Var}_P(\hat{\phi}^k(D)) \) defined in (11) satisfies that

\[
\text{Var}_P(\hat{\phi}^k(D)) = \text{Var}_P(\phi^k(D)) + o_P(1).
\]
Remark 1 (OLS). Note that equation (12) is expected to hold for the plug-in estimators of the influence function under regularity assumptions. Revisiting Example 1, a plug-in estimator of the influence function is

$$\hat{\phi}^k(D_i) = \left(\frac{1}{n} \sum_{j=1}^{n} X_j^S_i (X_j^S_i)^\top \right)^{-1} X_i^S (Y_i - (X_i^S)^\top \hat{\theta}^{k,OLS}),$$

where $\hat{\theta}^{k,OLS}$ is the OLS estimator computed with covariates $X^S_k$. One can now justify equation (12) via Lemma 2.

Now we construct asymptotically valid confidence intervals for $\theta^0$ using $K$ different estimators $\hat{\theta}^1, \ldots, \hat{\theta}^K$ that are asymptotically linear for estimating $\theta^0$. In the following theorem with Remark 2, influence functions of $K$ different estimators can be correlated and have different variances.

**Theorem 1.** (Asymptotic validity of calibrated confidence interval). Suppose Assumption 1 and 2 hold and the influence functions $\phi^1(D), \ldots, \phi^K(D)$ are uncorrelated. Let $\hat{\theta}^W = \sum_{k=1}^{K} \hat{\alpha}_k \hat{\theta}^k$ be the inverse-variance weighted estimator where the weights are

$$\hat{\alpha}_k = \frac{1}{\sum_{j=1}^{K} \frac{1}{\text{Var}_0(\phi^j(D))}}$$

with $\text{Var}_0(\phi^j(D)) = \text{Var}_0(\phi^j(D)) + o_p(1)$ for $k = 1, \ldots, K$. Let $\hat{\sigma}_{bet}$ be the weighted between-estimator variance defined as

$$\hat{\sigma}_{bet}^2 = \sum_k \hat{\alpha}_k (\hat{\theta}^k - \hat{\theta}^W)^2.$$

Then for any $\alpha \in (0, 1)$, for fixed $K$ and as $n \to \infty$ we have

$$P\left( \theta^0 \in \left[ \hat{\theta}^W \pm t_{K-1,1-\alpha/2} \cdot \frac{\hat{\sigma}_{bet}}{\sqrt{K-1}} \right] \right) \to 1 - \alpha,$$

where $t_{K-1,1-\alpha/2}$ is the $1 - \alpha/2$ quantile of the $t$ distribution with $K-1$ degrees of freedom. To be clear, here we marginalize over both the randomness due to sampling and the randomness due to the distributive perturbation.

**Remark 2** (Correlated estimators). In practice, the components of $(\phi^1(D), \ldots, \phi^K(D))$ may be correlated. Then, we can apply a linear transformation to the estimators to obtain uncorrelated estimators that are asymptotically unbiased for $\theta^0$. We define the transformation matrix $T_{ij} = \frac{1}{\sum_{j'} (\hat{\Sigma}^{-1/2})_{ij'}},$ where $\hat{\Sigma}$ is an estimate of the covariance matrix of $\hat{\theta}^1, \ldots, \hat{\theta}^K$. We can then define $(\hat{\eta}^1, \ldots, \hat{\eta}^K)^\top = T \cdot (\hat{\theta}^1, \ldots, \hat{\theta}^K)^\top.$ If $||\hat{\Sigma} - \Sigma||_2 = o_p(1)$ and $\Sigma$ is invertible, then the estimators $\hat{\eta}^1, \ldots, \hat{\eta}^K$ also satisfy Assumption 1 with influence functions that are pairwise uncorrelated. Furthermore, if the $\hat{\theta}^k$, $k = 1, \ldots, K$ satisfy Assumption 2, then also $\hat{\eta}^k$, $k = 1, \ldots, K$ satisfy Assumption 2.

**Remark 3** (Random effect models). The proposed method shares some similarity with random effect models, since both can be seen as investigating variability across estimators. In a random effect model, estimator-to-estimator variability can be modeled as random additive terms with a correlation structure given by a user-defined model matrix. This model matrix is usually justified by background knowledge. In our setup, we capture estimator-to-estimator variability through a multiplicative term. This multiplicative term is justified by symmetry assumptions on the sampling and perturbation process. We believe that these procedures will be used in different scenarios: if the data scientist has sufficient background knowledge to model the dependency of biases of $\hat{\theta}^k$ with a model matrix, one can use a random effect model. If such knowledge is not available, using a random effect model is prohibited. In this case, in our view adjusting confidence intervals with scaling factors is more justifiable than assuming that the data is i.i.d. from the unperturbed distribution $p$. In some cases, the data analyst may trust one of the estimators $\hat{\theta}^k$ more than others. For example, the data analyst may be convinced that $\hat{\theta}^1 = \theta^0$, but may not be sure whether $\theta^k = \theta^0$ for $k \geq 2$. In this case, it is possible to construct variance estimates that are upwardly biased in the sense that
the resulting confidence intervals are expected to be conservative. In this case, the data analyst may report the confidence interval for $\theta^0$ using $\hat{\theta}^1$ instead of $\hat{\theta}^W$ with $\delta$ estimated by computing the between-estimator variance of the remaining $K - 1$ estimators. As a result, they would lose one degree of freedom in their confidence intervals. The details can be found in the Appendix, Section C.

In the final variance estimate, there are two effects that are counteracting each other. Inverse-variance weighting reduces the variance of the final estimate compared to each of the individual estimators $\hat{\theta}^k$. On the other hand, the new variance formula accounts for distributional uncertainty and thus potentially inflates the variance.

Practical implications for stability analyses. The proposed model not only leads to a recommendation on how to summarize the between-estimator uncertainty in confidence intervals but also lets us give some additional guidance.

First, note that if all estimators $\hat{\theta}^k$ have similar influence functions, the proposed method will be unstable since in Remark 2 we invert the estimated covariance matrix. This coincides with the following intuition: Reporting that a large number of extremely similar estimators return similar results does not automatically increase the trustworthiness of a result. To corroborate a hypothesis one should have estimators that are susceptible to different sources of biases. In our model, this corresponds to estimators that are not highly correlated. Ideally, the estimators are independent. Similar arguments have appeared in other parts of the literature. For example, Rosenbaum (2021) writes: “An observational study has two evidence factors if it provides two comparisons susceptible to different biases that may be combined as if from independent studies of different data by different investigators, despite using the same data twice”.

In practice, it may happen that calibrated confidence intervals are very large compared to traditional sampling-based confidence intervals. Apart from the estimation error and small $K$, there are two possible explanations.

First, it could be that distributional uncertainty is very large. If distributional uncertainty is much larger than sampling uncertainty, conventional (unadjusted) confidence intervals are of limited value. Similar points have been made in different parts of the literature. For example, Meng (2018) argues that as the sample size grows, data quality becomes more important than data quantity and that standard confidence intervals have to be inflated to account for issues of data quality. In this vein, distributional confidence intervals can be used as a warning signal that we might be in a regime where data quality issues are more pressing than sampling uncertainty.

Secondly, it could be that the assumptions are violated (that means $\theta^k \neq \theta^{k'}$ for some $k, k'$). If the assumptions are grossly violated, inference will be more conservative. If the assumptions are correct, inference will be more precise. In other words, the precision of calibrated inference depends on whether Assumption 2 is satisfied or not.

If the number of estimators $K$ is very small, then there is an inferential price to pay for estimating distributional uncertainty in terms of power. This is reflected in the degrees of freedom of the $t$-distribution.

4 Simulation study

In this section, we evaluate the performance of the proposed method via a simulation study. The estimation accuracy of $\delta$ and the marginal coverage of calibrated confidence intervals are evaluated on simulated data sets generated by random perturbation models. In this simulation, we emulate the situation where a data scientist uses linear regression with an adjustment set to estimate a causal effect.

Setup. The unperturbed distribution of $D = (X, Y)$ with covariates $X \in \mathbb{R}^5$ and response $Y \in \mathbb{R}$ is generated from the following structural causal model (Bollen, 1989; Pearl, 2009):
The goal is to estimate the direct causal effect of $X_1$ on $Y$, which in this setup corresponds to the regression coefficient of $X_1$ in a regression of $Y$ on the set $S = (X_1, X_2)$. Practitioners often conduct such regressions for different choices of sets $S$ to evaluate the overall stability of the procedure (Leamer, 1983; Oster, 2019).

In this example, the structural causal model can be used to construct multiple valid estimators. We look at the case where the data analyst considers $K = 8$ different adjustment sets which all include the confounding variable $X_2$. In this case, $K = 8$ different regression-adjusted estimators estimate the same quantity, the direct causal effect of $X_1$ on $Y$, under the unperturbed distribution. We consider following adjustment sets: \{$X_1, X_2\}, \{X_1, X_2, X_3\}, \{X_1, X_2, X_4\}, \{X_1, X_2, X_5\}, \{X_1, X_2, X_3, X_4\}, \{X_1, X_2, X_3, X_5\}, \{X_1, X_2, X_4, X_3\}, \{X_1, X_2, X_4, X_5\}, \{X_1, X_2, X_5, X_3\}.

We now want to model a random shift between the target and the sampling distribution due to issues during the sampling procedure. We generate randomly perturbed data sets in two ways. First, we adopt the random perturbation model in Lemma 1. We partition the support of the joint distribution of $X$ and $Y$ into $m^{p+1}$ equal probability bins and perturb the probability of each bin with i.i.d. random weights $Z \sim \text{Gamma}(1,1)$ and $Z \sim \text{Ber}(1/m^p)$. For sufficiently large $m$, this procedure can be seen as randomly selecting $m$ bins out of $m^{p+1}$ bins and perturbing the probability of each selected bin with i.i.d random weights $W \sim \text{Gamma}(1,1)$. In our simulations, we generate $n$ i.i.d. data points $D_1, \ldots, D_n$ from this randomly perturbed distribution. The strength of the perturbation is given as $\delta^2 \approx 1 + 2 \cdot n/m$. Secondly, we employ the random perturbation model described in Example 5 in the Appendix. We sample $m$ data points from the original distribution and let randomly perturbed distribution be the empirical distribution of $m$ samples. The strength of the perturbation is given as $\delta^2 \approx 1 + n/m$.

Our method is carried out for sample sizes $n = 200, 500, 1000$ and for $m = 200, 500, 1000$ which determines the strength of the perturbation, each with $N = 1000$ replicates. In each replicate, we generate $n$ samples from the randomly perturbed distribution, obtain $K = 8$ different regression-adjusted estimators from the perturbed data set, and estimate $\hat{\delta}^2$. Then we construct non-calibrated and calibrated $(1 - \alpha)$ confidence intervals for each regression-adjusted estimator. Note that we use max($\delta, 1$) instead of $\delta$ to adjust confidence intervals. We evaluate the accuracy of $\hat{\delta}$ compared to the ground truth $\delta$ and the marginal coverage of calibrated confidence intervals compared to that of non-calibrated confidence intervals for each regression-adjusted estimator.

Accuracy of $\hat{\delta}$. The estimation accuracy of $\hat{\delta}$ compared to the ground truth $\delta$ is illustrated in Figure 1. We also look at the case where the data analyst fails to adjust for the confounding variable $X_2$ in one of the regressions as they consider the adjustment set $\{X_1, X_3, X_4\}$ instead of $\{X_1, X_2, X_3, X_4\}$. In this case, $K = 8$ different estimators do not agree asymptotically and therefore $\hat{\delta}$ is upwardly biased, which leads to overcoverage.

Marginal coverage of calibrated CI. The marginal coverages of calibrated confidence intervals and non-calibrated confidence intervals are given in Figure 2. We see that calibrated confidence intervals have much improved coverage compared to non-calibrated confidence intervals, especially when $n$ is large and $m$ is small as the variance due to distributional perturbations dominates the marginal variance.

5 Real-world data

Ultimately, the goal of our procedure is to increase stability and trustworthiness of decision-making. In this section, we demonstrate that our method can improve stability on a real data set. We will see that...
Figure 1: Accuracy of $\hat{\delta}$: The left panel shows results under the perturbation model in Lemma 1 and the right panel shows results under the perturbation model in Example 5 from the Appendix. Mean, 2.5% and 97.5% quantiles of the estimated $\hat{\delta}$ for each $m = 200, 500, 1000$ and $n = 200, 500, 1000$ are provided for two cases when $K$ different estimators agree asymptotically and when they do not. The dashed lines indicate the true values of $\delta$.

Figure 2: Marginal coverages of calibrated confidence intervals: The left panel shows results under the perturbation in Lemma 1 and the right panel shows results under the perturbation model in Example 5 in the Appendix. Marginal coverages of calibrated confidence intervals and non-calibrated confidence intervals are presented for $m = 200, 500, 1000$ and $n = 200, 500, 1000$. The dashed lines indicate the nominal coverage 0.95.

even in situations without distributional perturbations, the proposed method can increase stability of decision-making. The data set (Cortez and Silva (2008)) was collected by using school reports and questionnaires for the estimation of final grades of students in secondary education of two Portuguese schools. The data attributes include student grades, demographic, social and school related features. It is available at the UCI machine learning repository (Dheeru and Karra Taniskidou (2017)). We adopt 20 covariates in the data set. The response $Y$ is the final year grade in Portuguese language. There are 649 students in total.
The goal is to determine the relative importance of \( L = 7 \) selected binary covariates: 1) parents’ cohabitation status, 2) whether the student received extra educational support from the school, 3) whether the student received family educational support, 4) whether the student is in a relationship, 5) whether the student had extra paid classes within the course subject, 6) whether the student’s mother had secondary or higher education, and 7) whether the student’s father had secondary or higher education. The relative importance is determined by the rank order of the covariates’ effect sizes in a linear regression.

In the simulation setup, we want to emulate a situation where as baseline the analyst has several reasonable choices to conduct a statistical analysis, and makes these decisions randomly. On the other hand, as a comparison the analyst aggregates the estimators and conducts uncertainty quantification as proposed above.

Suppose we are given multiple sets of covariates, all containing the 7 covariates of our interest. We consider the following two methods. In method 1, a statistician randomly chooses one of the sets of covariates, performs a linear regression, and ranks the effect sizes of 7 covariates. In method 2, a statistician employs our method. In particular, they perform linear regressions with multiple sets of covariates and for each covariate, calculate an inverse-variance weighted estimator and its effect size in consideration of distributional perturbations as described in Section 3. Then, they rank these effect sizes.

We evaluate the two methods’ stability in ranking effect sizes. To evaluate method \( i \), we randomly split the data set into two, perform method \( i \) on each split, and compare the rankings resulting from each split. To measure the stability of the ranking, we compute the set similarity measure between \( S_{1,\ell} = \{ \text{Top } \ell \text{ covariates by the effect size on split 1} \} \) and \( S_{2,\ell} = \{ \text{Top } \ell \text{ covariates by the effect size on split 2} \} \) for each \( \ell = 1, \ldots, L = 7 \) as \(|S_{1,\ell} \cap S_{2,\ell}|/L\). We repeat this procedure \( N = 500 \) times and record the average set similarity measure. In each replicate, we randomly generate \( K = 10, 20 \) sets of covariates that include the 7 covariates of our interest. The results can be found in Table 1. Overall, we see our method (Method 2) improves the stability of the ranking, notably outperforming Method 1 for \( \ell = 1, 2, 3 \). Note that the method 1 gives slightly worse results than random guessing for small \( \ell \). One possible explanation is that sample splitting introduces small negative correlations between splits: If a regression coefficient is close to zero on the entire data set and on one split by chance the coefficient is large, then the coefficient is expected to be small on the other split.

| \( \ell \) | 1  | 2  | 3  | 4  | 5  | 6  | 7  |
|----------|----|----|----|----|----|----|----|
| Method 1 \((K = 10)\) | 0.102 | 0.203 | 0.407 | 0.648 | 0.817 | 0.898 | 1.000 |
| Method 2 \((K = 10)\) | 0.210 | 0.296 | 0.449 | 0.658 | 0.828 | 0.912 | 1.000 |
| Method 1 \((K = 20)\) | 0.090 | 0.203 | 0.417 | 0.659 | 0.817 | 0.893 | 1.000 |
| Method 2 \((K = 20)\) | 0.235 | 0.313 | 0.445 | 0.679 | 0.845 | 0.912 | 1.000 |

Table 1: The stability of the ranking: The table above shows results with \( K = 10 \) sets of covariates and the table below shows results with \( K = 20 \) sets of covariates. Mean over \( N = 500 \) iterations of the computed set similarity measure between \( S_{1,\ell} \) and \( S_{2,\ell} \) for each \( \ell = 1, \ldots, 7 \) is provided for each method.

Additionally, we compare the length of calibrated and non-calibrated confidence intervals for each selected binary covariate. From the results provided in Figure 3, one sees that our method is not so conservative given that we are adjusting confidence intervals with scaling factor \( \max(\hat{\delta}, 1) \). Moreover, the variance of the length of calibrated confidence intervals tends to decrease as we increase the number of sets of covariates from \( K = 10 \) to \( K = 20 \).

6 Discussion

In practice, data analysts often compute not just one estimator but multiple estimators for a single target quantity. These estimators are often based on equally reasonable assumptions. For example, in causal inference from observational data, it is common to compute regression-adjusted estimators
for different choices of adjustment sets. Often, it is recommended study the estimator-to-estimator variability between sensible choices of adjustment sets. If the estimator-to-estimator variability is high, then the analyst might have reason to not trust the estimates. In these cases, such stability investigations may be more informative than traditional $p$-values or confidence regions. This warrants an investigation of the theoretical properties of this practice. Does this practice have any guarantees and if so, which? Can we integrate this type of stability analysis into statistical inference?

We study a variant of this procedure from a distributional perspective. If the data analyst has access to different estimators that are supposedly estimating the same quantity, estimator-to-estimator variability can be used to scale confidence intervals. These scaled confidence intervals can be shown to account for both sampling uncertainty and distributional uncertainty in an isotropic perturbation model. This perturbation model assumes that the distribution shift is a superposition of many small random distributional changes. Such uncertainty quantification seems desirable, especially in settings where the sampling uncertainty is of similar or lower order than other types of uncertainty.

We have shown in the Appendix A.3 that distributional uncertainty is related to other issues that are common in data analysis, such as violations of the i.i.d. assumption, confounding, and sampling bias. That being said, the calibration procedure is not meant to replace existing methods that address confounding or selection bias via direct modelling (such as regression adjustment, or weighting procedures, a random effect model, or by bounding errors). In contrast, the proposed calibration technique allows you to deal with residual “dense” distributional errors that you are unable to capture with direct modelling approaches.

The isotropic perturbation model is a strong assumption, but it is a weaker assumption than assuming that the data is i.i.d. from the target distribution, which is a commonly made. Thus, the proposed calibration procedure works under strictly less assumptions on the data generating process than the most common inferential strategy. Instead of relying on i.i.d. sampling from $\mathbb{P}$, inference in the proposed model is based on a symmetry assumption and on scientific background knowledge for finding multiple reasonable estimators.

Of course, in practice perturbations might affect parts of the distribution differently. In such cases the proposed method can potentially have over-coverage or under-coverage. Looking forward, it would be desirable to extend the isotropic perturbation model (which has only one single parameter $\delta$) to more flexible models that depend on multiple parameters. Such perturbation models would allow

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**Figure 3:** The length of calibrated and non-calibrated confidence intervals: Mean, 2.5% and 97.5% quantiles of the length of calibrated (Method 2) and non-calibrated (Method 1) confidence intervals for each selected binary covariate over $N = 500$ iterations are provided for $K = 10$ and $K = 20$. 
training different uncertainty models for different parts of the distribution, potentially leading to more realistic and flexible uncertainty quantification than existing approaches.

A companion R package, calinf, is available at https://github.com/rothenhaeusler/calinf. Our package allows to draw data under the distributional uncertainty model and calibrate inference in generalized linear models. We provide an example of calibrated inference where the data analyst computes regression-adjusted estimators for different choices of adjustment sets. If multiple estimators are not available, it is also possible to estimate $\delta$ using other types of scientific background knowledge. On the GitHub page, we discuss an example where the data analyst has background knowledge of population parameters.

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Appendix

In Section A, we discuss additional properties of the isotropic perturbation model. Section B contains
the proofs. Section C discusses how to form robust confidence intervals if the data analyst trusts one
of the estimators \( \hat{\theta}^k \) more than others.

A Properties of the isotropic perturbation model

Recall that conditionally on \( \xi \), the data \( (D_1)_{1\leq i \leq n} \) are drawn i.i.d. from the perturbed distribution
\( P_{\xi} (D = \bullet) \), where \( \xi \) is an unobserved random variable. Note that an estimator \( \hat{\theta} = \hat{\theta}(D_1, \ldots, D_n) \) for
some parameter \( \theta^0(P) \) now has two sources of uncertainty: the uncertainty due to sampling and the
uncertainty due to the random perturbation.

\[
\hat{\theta} - \theta^0(P) = \underbrace{\hat{\theta} - \theta(P_{\xi})}_{\text{variation due to sampling}} + \underbrace{\theta(P_{\xi}) - \theta^0(P)}_{\text{variation due to random perturbation}}
\]

We refer to the second component as **distributional uncertainty**. In this section we will study such
distributional perturbation models in more detail. In Section A.1 we will show that under a sym-
metry assumption, there exists only one class of perturbation models that is characterized by a one-
dimensional parameter \( \delta_{\text{dist}} \). In Section A.2 we will sketch an extension of the random perturbation
model that allows different parts of the distribution to be affected by different perturbations. In Sec-
tion A.3 we discuss how the perturbation model relates to other issues with data, such as sampling
bias and confounding.

A.1 Uniqueness of distributional perturbation model

The distributional perturbation models introduced earlier raise the question whether other distribu-
tional perturbation models are reasonable. Let us go back to the construction of a discrete perturbation
model in Section 2. In the example described in Section 2, \( P \) is the uniform probability measure on
\( \{1, \ldots, K\} \). In equation (5), we constructed the perturbed distribution by setting
\( P_{\xi}(D = k) = \xi_k \).

for an exchangeable set of random variables \( \xi_1, \ldots, \xi_K \geq 0 \) with \( \sum \xi_k = 1 \). Analogously as in Section
B.1 it can be shown that for any function \( f : \{1, \ldots, K\} \to \mathbb{R} \),
\[
\text{Var}(E_{\xi}[f(D)]) = \delta_{\text{dist}}^2 \text{Var}_{P}(f(D)),
\]

where \( \delta_{\text{dist}}^2 = \frac{K^2}{K-1} \text{Var}(\xi_1) \). Thus, under this model, the variance of the perturbation is proportional to
the variance in the unperturbed distribution. This raises the question whether this property is specific
for the considered example or whether it holds in more generality. We will see that under a symmetry
assumption, there exists only one type of perturbation model, which is equivalent to the one considered
above. Roughly speaking, the symmetry assumption states that two events that have equal probability
under \( P \) are perturbed in a similar fashion. In the following, we write \( Q \) for the marginal distribution
of \( (D, \xi) \), where first the perturbation \( \xi \) is drawn and then \( D \sim P_{\xi} \). The proof of the following result
can be found in Section B.6.

**Theorem 2** (Characterization of isotropic perturbation models). Let \( (D, \xi) \sim Q \) and assume that
there exists a function \( h(\bullet) \) such that \( h(D) \) is uniformly distributed on \( [0,1] \). Let \( P_{\xi} = Q(\bullet | \xi) \) and let
\( P \) denote the marginal distribution of \( D \) under \( Q \). Assume that for any \( D \)-measurable events \( A \) and \( B \)
with \( P(A) = P(B) \),
\[
\text{Var}(P_{\xi}(A)) = \text{Var}(P_{\xi}(B)).
\]
Furthermore, assume that for every sequence of \( D \)-measurable events \( A_j \) with \( P(A_j) \to 0 \),
\[
\text{Var}(P_{\xi}(A_j)) \to 0.
\]
Then for any $\phi(D) \in L^2(\mathbb{P})$

$$\text{Var}(\mathbb{E}^\xi[\phi(D)]) = \delta_{\text{dist}}^2 \text{Var}_\mathbb{P}(\phi(D)), \quad (14)$$

for some fixed $\delta_{\text{dist}} \geq 0$.

Let us discuss what this result means for the behaviour of empirical means. Let $D_1, \ldots, D_n$ be i.i.d. drawn from $\mathbb{P}^\xi$. Then, for all square-integrable functions $\psi(D) \in L^2(\mathbb{P})$ marginally across sampling uncertainty and distributional uncertainty we have

$$\text{Var}_\mathbb{P}(\frac{1}{n} \sum_{i=1}^n \psi(D_i))
= \left(\frac{1}{n} + \delta_{\text{dist}}^2 - \frac{\delta_{\text{dist}}^2}{n}\right)\text{Var}_\mathbb{P}(\psi(D)).$$

$$= \frac{\delta^2}{n} \text{Var}_\mathbb{P}(\psi(D)),$$

with $\delta^2 = 1 + n\delta_{\text{dist}}^2 - \delta_{\text{dist}}^2$. Since $\mathbb{P}^\xi = \mathbb{Q}(\bullet | \xi)$ we also have $E[\frac{1}{n} \sum_{i=1}^n \psi(D_i)] = E[\psi(D)]$.

There are two major assumptions in this theorem. The first assumption says that two events that have the same probability are perturbed in the same fashion. This can be seen as a symmetry assumption. The second assumption says that events that have a small probability are only perturbed by a small amount. This can be seen as a regularity assumption.

Then, up to a one-dimensional parameter $\delta$, the variance of functions is uniquely determined. This means that using symmetry we have reduced the problem of estimating an infinite-dimensional perturbation model to a one-dimensional quantity $\delta$. Note that the statement in Theorem 2 is slightly weaker than Lemma 1, since it is only a statement about variances and not about the asymptotic distribution of empirical processes.

The distributional uncertainty model relates to other concepts in statistics such as sampling bias, correlated data, and confounding. We discuss these connections in the Appendix, Section A.3.

In practice, some researchers might object to the symmetry assumption in equation (13). It turns out that the perturbation model can be generalized. In the following section, we will give a brief outlook of how perturbation models can be used to perturb different parts of a distribution differently.

**A.2 Beyond isotropic distributional perturbations**

The discussion in Section A.1 shows that under a symmetry assumption, up to an unknown scale factor $\delta$, there exists only one type of perturbation model. However, in practice there might be a situation where one does not expect a perturbation to affect all parts of the distribution in the same way. Consider $D = (X,Y)$. For example, one might expect that the distribution of $X$ is perturbed between settings but that the measurement error is invariant. This may lead one to want to model a situation where $p(x)$ is perturbed but $p(y|x)$ is not perturbed. Under appropriate regularity conditions on $\psi$ we have

$$\mathbb{E}^\xi[\psi(X,Y)] - \mathbb{E}[\psi(X,Y)] = \mathbb{E}^\xi[\mathbb{E}[\psi(X,Y)|X]] - \mathbb{E}[\mathbb{E}[\psi(X,Y)|X]]
\overset{d}{=} \mathcal{N}(0, \delta_{\text{dist}}^2 \text{Var}_\mathbb{P}(\mathbb{E}[\psi(X,Y)|X])).$$

If $\delta_{\text{dist}}$ is known or can be estimated, this allows us to adjust variance and confidence intervals to account for uncertainty both due to sampling and distributional perturbations, similarly as in Section 3.

**A.3 Relationship to other concepts**

In this section we will see that issues that are common in data analysis (such as sampling bias, confounding, and violations of the i.i.d. assumptions) are consequences of the isotropic perturbation model. Depending on how strong the perturbations are, the issues with confounding and sampling bias are more or less severe. To be clear, the goal in this section is to show that the concept of distributional
uncertainty is connected to sampling bias and confounding, but neither of these concepts is subsumed by one of the other concepts.

In the following examples, we show that the random perturbation model implies violations of the independence assumption, sampling bias, and confounding.

**Example 2 (Violation of i.i.d. assumption).** Draw real-valued random variables $D_1 \overset{i.i.d.}{\sim} \mathbb{P}^\xi$, where $\mathbb{P}^\xi$ satisfies equation (14). Let $\sigma^2 < \infty$ denote the variance of $D_1$ under $P$, where $P$ is the marginal distribution of $(D_1, D_2, ..., D_n, \xi)$ where first $\xi$ is drawn and then $D_i \overset{i.i.d.}{\sim} \mathbb{P}^\xi$. For all $i \neq j$, and $\phi(D) \in L^2(\mathbb{P})$,

$$\text{Cov}(\phi(D_i), \phi(D_j)) = E[\phi(D_i)\phi(D_j)] - E[\phi(D_i)]E[\phi(D_j)] = E[\mathbb{E}[\phi(D)]\mathbb{E}[\phi(D)]] - E[\mathbb{E}[\phi(D)]]^2 = \delta^2\sigma^2.$$ 

Here, we used that $E[\phi(D_i)|\xi] = E[\phi(D_j)|\xi]$ and equation (14). Thus, marginally, the perturbation model induces equicorrelated data. The challenge at this point is that $\delta_{\text{dist}}$ is unknown, which means that the correlation of the covariates is unknown. For a fixed perturbation $\xi$, even if $n \rightarrow \infty$ it is impossible to distinguish between i.i.d. data drawn from $\mathbb{P}^\xi = P$ (corresponding to $\delta_{\text{dist}} = 0$) or data drawn from a distributional perturbation model with $\delta_{\text{dist}} > 0$.

**Example 3 (Sampling bias).** Let $O \in \{0,1\}$ denote the indicator whether a unit is observed. We assume that under the target population there is no sampling bias, that means $\mathbb{P}(X = \bullet|O = 1) = \mathbb{P}(X = \bullet)$. Now assume that $\mathbb{P}^\xi$ satisfies equation (14) for $D = (X,O)$. In the following, we will see that the variance of $\mathbb{P}^\xi(X = \bullet|O = 1) - \mathbb{P}(X = \bullet)$ is nonzero, i.e. the random perturbation will induce sampling bias with positive probability. For any $D$-measurable set $A$, using a Taylor expansion,

$$\mathbb{P}^\xi(X \in A|O = 1) - \mathbb{P}(X \in A) \approx \mathbb{P}(X \in A) + \frac{\mathbb{P}^\xi(O = 1, X \in A) - \mathbb{P}(O = 1, X \in A)}{\mathbb{P}(O = 1)} - \mathbb{P}(X \in A) \frac{\mathbb{P}^\xi(O = 1) - \mathbb{P}(O = 1)}{\mathbb{P}(O = 1)} - \mathbb{P}(X \in A)$$

It can be shown that this term has variance

$$\delta^2_{\text{dist}} \frac{\mathbb{P}[X \in A|(1 - \mathbb{P}[X \in A])}{\mathbb{P}[O = 1]}.$$ 

Thus, if $\mathbb{P}(X \in A) \notin \{0,1\}$, the variance of $\mathbb{P}^\xi(X \in A|O = 1) - \mathbb{P}(X \in A)$ is nonzero. Hence, if we draw an i.i.d. sample $X = (X_1, \ldots, X_n)$ from $\mathbb{P}^\xi$ and only observe units with $O = 1$, some members of the sampling population $\mathbb{P}^\xi(\bullet|O = 1)$ have lower or higher sampling probability compared to the target population $P$. In this sense, the random perturbation model induces sampling bias.

**Example 4 (Confounding).** We consider the Neyman-Rubin model (Neyman, 1923; Rubin, 1974) where $Y(t)$ denotes the potential outcome under treatment assignment $T = t \in \{0,1\}$ and $X$ are observed covariates. The statistician observes $Y = TY(1) + (1 - T)Y(0)$. In observational studies, it is common to make the unconfoundedness assumption. Under unconfoundedness, under $P$ we have the following conditional independence:

$$\{Y(1), Y(0)\} \perp T|X.$$ 

In the following, for simplicity we assume that $X$ is discrete. If we have i.i.d. observations drawn from $P$, under a positivity assumption we can estimate $E[Y(1) - Y(0)]$ using inverse probability weighting, regression adjustment, and other methods (Hernán and Robins, 2020). In the distributional uncertainty model, we do not draw samples from $P$ but from $\mathbb{P}^\xi$, where $\mathbb{P}^\xi$ randomly deviates from $P$. We will now show that under $\mathbb{P}^\xi$, with positive probability the unconfoundedness assumption is violated.

Ignorability implies that for any function $g$

$$E[\frac{T}{\epsilon(X)} - 1]Y(t)g(X) = 0,$$
where \( e(x) = \mathbb{P}[T = 1|X = x] \). We will show that

\[
\mathbb{E}^\xi[(\frac{T}{e(X)} - 1)Y(t)g(X)] \neq 0
\]  

(15)

with positive probability. If equation (15) holds, then with positive probability under \( \mathbb{P}^\xi \)

\[
Y(t) \not\perp T|X.
\]

Let us now show that with positive probability, equation (15) holds. For simplicity, set \( g(x) = 1_{X=x} \). Choose \( x \) such that \( \mathbb{P}[X = x] \in (0, 1) \), \( e(x) \in (0, 1) \) and \( t \) such that \( \mathbb{E}[Y(t)|X = x] \neq 0 \). Then, using equation (14)

\[
\mathbb{E}^\xi[(\frac{T}{e(X)} - 1)Y(t)g(X)] - \mathbb{E}[(\frac{T}{e(X)} - 1)Y(t)g(X)]
\]

has variance

\[
\delta_{\text{dist}}^2 \mathbb{Var}_\mathbb{P} \left( (\frac{T}{e(X)} - 1)Y(t)g(X) \right).
\]

Under the stated assumptions this variance must be positive. Thus, with positive probability, equation (15) holds.

Thus, ignorability is violated with positive probability for \( \mathbb{P}^\xi \) even if it is satisfied for the unperturbed distribution \( \mathbb{P} \). Note that this model does not imply that there is confounding for a certain data set (that means, for a certain sampling distribution \( \mathbb{P}^\xi \)). This model implies that overall, across data sets, some data sets will be drawn from a distribution \( \mathbb{P}^\xi \) for which unconfoundedness is violated. The strength of the confounding is described by the (a priori unknown) parameter \( \delta_{\text{dist}} \). If we want to construct confidence intervals that cover \( \theta^0 = \mathbb{E}[Y(1) - Y(0)] \) we have to take into account both the uncertainty due to sampling and the uncertainty due to the distributional perturbation.

B Proofs

B.1 Variance calculation for equation (6)

Recall that \( D_1, \ldots, D_n \) are drawn i.i.d. from \( \mathbb{P}^\xi \), with

\[
\mathbb{P}^\xi[D = k] = \xi_k, \quad \text{for} \ k = 1, \ldots, K,
\]

where \( \xi_k \geq 0 \) are exchangeable random variables with \( \sum \xi_k = 1 \), and \( s(k) = \sum \xi_{1\leq i \leq k} \). Furthermore, let \( \bar{\psi} = \frac{1}{K} \sum_{k=1}^K \psi(k) \). Then,

\[
\mathbb{Var}_\mathbb{P}(\frac{1}{n} \sum_{i=1}^n \psi(D_i))
\]

\[=
\mathbb{Var}_\mathbb{P}(\sum_{k=1}^K \frac{s(k)}{n} \psi(k))
\]

\[=
\frac{1}{n^2} \sum_{k \neq k'} \mathbb{E}[s(k)s(k')] (\psi(k) - \bar{\psi})(\psi(k') - \bar{\psi}) + \frac{1}{n^2} \sum_k \mathbb{E}[s(k)^2] (\psi(k) - \bar{\psi})^2
\]

\[=
\frac{K}{n^2} \mathbb{E}[(s(1)^2 - s(1)s(2))] \frac{1}{K} \sum_k (\psi(k) - \bar{\psi})^2
\]

\[=
\frac{K}{n^2} \mathbb{E}[(s(1)^2 - s(1)s(2))] \mathbb{Var}_\mathbb{P}(\psi(D))
\]

\[=
\frac{K}{n^2} \mathbb{E}[(s(1)^2 - s(1)s(2)) \mathbb{Var}_\mathbb{P}(\psi(D))]
\]

\[=
\frac{K^2}{n^2(K-1)} \mathbb{Var}_\mathbb{P}(s(1)) \mathbb{Var}_\mathbb{P}(\psi(D))
\]

Here, we used repeatedly that \( \sum_k s(k) = n \).
B.2 Auxiliary results and proof of Lemma 1

Notation: We write \( \mathbb{P} \) for the target distribution and \( \mathbb{P}^\xi \) for the randomly perturbed distribution from which we draw \( n \) i.i.d. data samples \((D_i)_{i=1,...,n}\). In both examples \( \xi \) can be seen as a random variable that encodes the perturbations. The expectation of \( f(D_1,\ldots,D_n) \) over the joint distribution of \((\xi, D_1,\ldots, D_n)\) can be written as \( E_\xi[\mathbb{E}_f(D_1,\ldots,D_n)] \) where \( E_\xi \) means we take the expectation over \( \xi \) and \( \mathbb{E}_f \) means that we take the expectation over \((D_1,\ldots,D_n)\), conditionally on \( \xi \).

B.2.1 Auxiliary results

Let us first state an auxiliary lemma that will turn out helpful for proving Lemma 1.

**Lemma 4.** Let the assumptions of Lemma 1 hold. For the sequence of random variables \( \xi = (\xi(n)) \), for any bounded \( \psi(\bullet) \) we have that

\[
\mathbb{E}_\xi^\xi[\psi(D)] - \mathbb{E}[\psi(D)] \stackrel{d}{=} \mathcal{N}(0, \gamma_n^2 \text{Var}(\psi(D))) + o_p(\gamma_n)
\]

where \( \gamma_n^2 = \frac{\text{Var}(W)}{m(n)|\mathbb{E}[W]|^2} \) and where we write \( m(n) \) to make it explicit that \( m \) grows with \( n \).

**Proof.** Let \( \phi = \psi \circ h \). Without loss of generality, assume that \( \mathbb{E}[\phi(U)] = 0 \). Note that

\[
\sqrt{m}(\mathbb{E}_\xi^\xi[\phi(U)] - \mathbb{E}[\phi(U)]) = \frac{\sqrt{m} \sum_{k=1}^{m} \int_{x \in I_k} \phi(x)dx \cdot (W_k - \mathbb{E}[W])}{\sum_{k=1}^{m} W_k/m}.
\]

Let

\[
Y_{m,k} := \sqrt{m} \int_{x \in I_k} \phi(x)dx \cdot (W_k - \mathbb{E}[W]).
\]

First, note that

\[
E[Y_{m,k}] = 0
\]

for all \( k \). As the second step, we want to show that

\[
\sum_{k=1}^{m} E[Y_{m,k}^2] = \text{Var}(W) \cdot m \sum_{k=1}^{m} \left( \int_{x \in I_k} \phi(x)dx \right)^2 \rightarrow \text{Var}(W) \cdot \text{Var}_p(\phi(U)).
\]

(17)

For any \( f \in L^2([0,1]) \), define \( \Pi_m(f) \) as

\[
\Pi_m(f)(x) = \sum_{k=1}^{m} \left( m \int_{x \in I_k} f(x)dx \right) \cdot I(x \in I_k).
\]

Then, we have

\[
\left| m \sum_{k=1}^{m} \left( \int_{x \in I_k} \phi(x)dx \right)^2 - \text{Var}_p(\phi(U)) \right| = ||\phi - \Pi_m(\phi)||_2^2 \rightarrow 0.
\]

as \( m \) goes to infinity. This is because any bounded function can be approximated by a sequence of step functions of the form \( \sum_{k=1}^{m} b_k I_{I_k} \). Next we will show that for any \( \epsilon > 0 \),

\[
g_m(\epsilon) = \sum_{k=1}^{m} E[Y_{m,k}^2; |Y_{m,k}| \geq \epsilon] \rightarrow 0.
\]

(18)

This is implied by the dominated convergence theorem as

\[
\sum_{k=1}^{m} E[Y_{m,k}^2; |Y_{m,k}| \geq \epsilon] \leq \sum_{k=1}^{m} \left( \int_{x \in I_k} \phi^2(x)dx \right) E[(W_k - \mathbb{E}[W])^2I(||\phi||_\infty|W_k - \mathbb{E}[W]|/\sqrt{m} \geq \epsilon)]
\]

\[
= ||\phi||_2^2 E[(W - \mathbb{E}[W])^2I(||\phi||_\infty|W - \mathbb{E}[W]|/\sqrt{m} \geq \epsilon)] \rightarrow 0.
\]
Combining equations (16), (17), and (18), we can apply Lindeberg’s CLT. With Slutsky’s theorem, we have
\[
\sqrt{n}(\mathbb{E}^\xi[\phi(U)] - \mathbb{E}^\xi[\phi(U)]) = \frac{\sum_{k=1}^m Y_{m,k}}{\sum_{k=1}^m W_{k}/m} \overset{d}{=} \mathcal{N}(0, \text{Var}_\mathcal{P}(\phi(U))/\mathbb{E}[W]^2) + o_p(1).
\]
This completes the proof.

**Lemma 5.** Let the assumptions of Lemma 1 hold. Assume that for a sequence of random variables \(\xi = \xi(n)\) there exists a sequence \(\gamma_n\) with limit \(\delta^2 = \lim_n (1 + m\gamma_n^2) < \infty\) such that for any bounded \(\psi(\bullet)\) we have
\[
\mathbb{E}^\xi[\psi(D)] - \mathbb{E}[\psi(D)] \overset{d}{=} \mathcal{N}(0, \delta^2 \text{Var}_\mathcal{P}(\psi(D))) + o_p(\gamma_n).
\]
Then, for any bounded \(\psi(\bullet)\), it holds that
\[
\frac{1}{\sqrt{n}} \sum_{i=1}^n \psi(D^n_i) - \mathbb{E}[\psi(D)] \overset{d}{=} \mathcal{N}(0, \delta^2 \text{Var}_\mathcal{P}(\psi(D))) + o_p(1).
\]

**Proof.** In the proof, we suppress the dependence of \(\xi\) on \(n\). We want to show that for any \(x\),
\[
E_\xi \left[ \mathbb{P} \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n \psi(D^n_i) - \mathbb{E}[\psi(D)] \leq x \cdot \sqrt{\delta^2 \text{Var}_\mathcal{P}(\psi(D))} \right) \right] = \Phi(x) + o(1),
\]
where \(\Phi\) is the cdf of a standard Gaussian random variable. Let us define
\[
Y_n = x \cdot \delta \cdot \frac{\sqrt{\text{Var}_\mathcal{P}(\psi(D))}}{\sqrt{\text{Var}_\mathcal{P}(\psi(D))}} = \sqrt{n}(\mathbb{E}^\xi[\psi(D)] - \mathbb{E}[\psi(D)])/\sqrt{\text{Var}_\mathcal{P}(\psi(D))},
\]
where \(\text{Var}_\mathcal{P}(\psi(D))\) denotes the variance of \(\psi(D)\) where \(D \sim \mathbb{P}^\xi\). Then,
\[
(*) = E_\xi \left[ \mathbb{P} \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n \psi(D^n_i) - \mathbb{E}[\psi(D)] + \sqrt{n}(\mathbb{E}^\xi[\psi(D)] - \mathbb{E}[\psi(D)]) \leq x \cdot \sqrt{\delta^2 \text{Var}_\mathcal{P}(\psi(D))} \right) \right]
= E_\xi \left[ \mathbb{P} \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{\psi(D^n_i) - \mathbb{E}^\xi[\psi(D)]}{\sqrt{\text{Var}_\mathcal{P}(\psi(D))}} \leq Y_n \right) \right].
\]
We define \(g_n(y; \xi)\) as
\[
g_n(y; \xi) = \mathbb{P} \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{\psi(D^n_i) - \mathbb{E}^\xi[\psi(D)]}{\sqrt{\text{Var}_\mathcal{P}(\psi(D))}} \leq y \right).
\]
By Berry–Esseen, it holds that
\[
\sup_y \left| \mathbb{P} \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{\psi(D^n_i) - \mathbb{E}^\xi[\psi(D)]}{\sqrt{\text{Var}_\mathcal{P}(\psi(D))}} \leq y \right) - \Phi(y) \right| \leq \frac{C \mathbb{E}^\xi[\psi(D)^3]}{(\mathbb{E}^\xi[\psi(D)^2])^{3/2} \sqrt{n}},
\]
for all \(n\). Invoking equation (19) for \(\psi(D)^2\) and \(\psi(D)^3\), we have that \(\mathbb{E}^\xi[\psi(D)^3]/(\mathbb{E}^\xi[\psi(D)^2])^{3/2}\) converges in probability to \(\mathbb{E}^\xi[\psi(D)^3]/(\mathbb{E}^\xi[\psi(D)^2])^{3/2} < \infty\) as \(n \to \infty\). Then the right-hand side of the above inequality converges in probability to 0 as \(n \to \infty\), which implies that
\[
\sup_y |g_n(y; \xi) - \Phi(y)| \overset{p}{\to} 0.
\]
Using this result,
\[
(*) = E_\xi[g_n(Y_n)] = E_\xi[g_n(Y_n)] - E_\xi[\Phi(Y_n)] + E_\xi[\Phi(Y_n)]
\leq E_\xi[\sup_y |g_n(y) - \Phi(y)|] + E_\xi[\Phi(Y_n)]
= E_\xi[\Phi(Y_n)] + o(1).
\]
by the dominated convergence theorem. Using equation (19), \( Var_{\mathbb{P}}(\psi(D)) \overset{p}{\to} Var_{\mathbb{P}}(\psi(D)) \). Then, we have
\[
Y_n \overset{d}{\to} \delta x - \sqrt{\delta^2 - 1} Z,
\]
where \( Z \) is a standard Gaussian random variable. Since \( \Phi \) is bounded and continuous, by Portmanteau Lemma, we get
\[
\lim_{n \to \infty} E[\Phi(Y_n)] = E[\Phi(\delta x - \sqrt{\delta^2 - 1} Z)] = \Phi(x).
\]
This completes the proof. \( \square \)

### B.2.2 Proof of Lemma 1

Now let us show that the Lemma 1 holds.

**Proof.** Without loss of generality for notational simplicity we restrict ourselves to the case \( l = 1 \), i.e. \( \psi : D \to \mathbb{R} \). As before we write \( \phi(D) = \psi \circ h(U) \). For any \( \psi \in L^2(\mathbb{P}) \) and for any \( \epsilon > 0 \), there exits a bounded function \( \psi^B \) such that \( E[\psi(D)] = E[\psi^B(D)] \) and \( ||\psi - \psi^B||_{L^2} < \epsilon \). Note that
\[
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\psi(D_i^n) - E[\psi(D)]) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\psi(D_i^n) - \psi^B(D_i)) \tag{a}
\]
\[
+ \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\psi^B(D_i^n) - E[\psi^B(D)]) \tag{b}
\]
Without loss of generality, let’s assume that \( E[\psi(D)] = 0 \). Note that
\[
(a) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( (\psi - \psi^B)(D_i^n) - E[\xi(\psi - \psi^B)(D)] \right) + \frac{\sqrt{n}E[\xi](\psi - \psi^B)^2(D)}{\sqrt{n}} \tag{a.1}
\]
\[
(b) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \psi(D_i^n) - E[\psi(D)] \right) \tag{a.2}
\]
The marginal variance of (a.1) is
\[
E[Var(\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\psi - \psi^B)(D_i^n) - E[\xi((\psi - \psi^B)(D)]) | \xi)] \leq E[\xi((\psi - \psi^B)^2(D))]
\]
\[
= E[(\psi - \psi^B)^2(D)].
\]
Therefore, we can write (a.1) = \( \epsilon \cdot s_n \) with \( E[s_n] = 0 \) and \( Var(s_n) \leq 1 \). Recall that we write \( \phi(D) = \psi \circ h(U) \). Note that for any \( \phi \in L^2([0,1]) \) such that \( E[\phi(U)] = 0 \),
\[
\sqrt{m}(E[\phi(U)]) = \frac{\sqrt{m} \sum_{k=1}^{m} \int_{x \in I_k} \phi(x) dx \cdot (W_k - E[W])}{\sum_{k=1}^{m} W_k/m}.
\]
The denominator converges in probability to \( E[W] \). The numerator has mean 0 and its variance is
\[
Var(W) \sum_{k=1}^{m} m \left( \int_{x \in I_k} \phi(x) dx \right)^2 \leq Var(W) \sum_{k=1}^{m} \int_{x \in I_k} \phi^2(x) dx
\]
\[
= Var(W)E[\phi^2(U)]
\]
where the first inequality holds by Jensen’s inequality with \( m \int_{x \in I_k} dx = 1 \). Therefore, using the argument above with \( \phi = (\psi - \psi^B) \circ h \), we get that
\[
(a.2) = \frac{\epsilon \cdot s'_n}{E[W] + o_p(1)}.
\]
with \( E[s'_n] = 0 \) and \( Var(s'_n) \leq Var(W) \). Combining the results, we have \( (a) = O_p(\epsilon) \). Moreover, with Lemma 4 and Lemma 5, we have that
\[
(b) \overset{d}{=} \mathcal{N}(0, \delta^2 Var_{\mathbb{P}}(\psi^B(D))) + o_p(1)
\]
\[
\overset{d}{=} \mathcal{N}(0, \delta^2 Var_{\mathbb{P}}(\psi(D))) + s''_n + o_p(1).
\]
where \( \delta^2 = 1 + r \text{Var}(W)/E[W]^2 \) and \( s''_n \sim N(0, \text{Var}(\psi(D) - \psi^B(D))) = O_p(\epsilon) \). Note that results hold for arbitrary \( \epsilon > 0 \). Therefore, for any \( \psi \in L^2(\mathbb{P}) \),
\[
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D^*_i) - \mathbb{E}[\psi(D)] \overset{d}{\rightarrow} N(0, \delta^2 \text{Var}_p(\psi(D))) + o_p(1).
\]

\[\square\]

### B.3 Examples of variance inflation induced by non-i.i.d. sampling

**Non-i.i.d. sampling.** In the following examples we discuss how Assumption 1 with \( \delta \neq 1 \) arises in non-standard sampling settings. For simplicity, we start with an artificial example: sampling with replacement from an unknown subpopulation.

**Example 5** (Sampling with replacement from an unknown subpopulation). Assume that \( D'_1, \ldots, D'_m \) drawn i.i.d. from \( \mathbb{P} \). Set \( \xi = (D'_1, \ldots, D'_m) \). We define the randomly perturbed distribution \( \mathbb{P}^\xi \) as the empirical measure
\[
\mathbb{P}^\xi(D \in \bullet) = \frac{1}{m} \sum_{i=1}^{m} 1_{D'_i \in \bullet}.
\]
Let \( n \rightarrow \infty \) and assume that \( m(n) \) is a sequence of integers such that \( \frac{n}{m(n)} \) converges to some limit \( r \in (0, \infty) \). Conditionally on \( \xi \), let \( (D_1^n, \ldots, D_n^n) \) be i.i.d. draws from \( \mathbb{P}^\xi \). Then equation (7) holds for any \( \psi(\bullet) \) with finite second moment with
\[
\delta^2 = 1 + r.
\]

**Proof.** Suppose that \( D'_1, \ldots, D'_m \) are drawn from \( \mathbb{P} \) for some sequence \( m = m(n) \). Let \( \mathbb{P}^\xi \) denote the empirical measure of \( D'_1, \ldots, D'_m \). Then by the CLT, for any \( \psi(\bullet) \) with finite second moment,
\[
\mathbb{E}^\xi[\psi(D)] - \mathbb{E}[\psi(D)] = \frac{1}{m} \sum_{i=1}^{m} \psi(D'_i) - \mathbb{E}[\psi(D)]
\]
\[
\overset{d}{\rightarrow} N(0, \gamma_n^2 \text{Var}_p(\psi(D))) + o_p(\gamma_n)
\]
where \( \gamma_n^2 = 1/m(n) \). By applying Lemma 5 and following the proof of Lemma 1, for any \( \psi(\bullet) \) with finite second moment, we get
\[
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D_i^n) - \mathbb{E}[\psi(D)] \overset{d}{\rightarrow} N(0, \delta^2 \text{Var}_p(\psi(D))) + o_p(1)
\]
where \( \delta^2 = 1 + r \).

**Sampling with replacement from a finite population might seem a bit artificial.** The next example shows that a similar conclusion holds if we sample clusters, where units in a single cluster are highly correlated, and units between clusters are independent. If the cluster structure is known, one can use clustered standard errors. However, in general the dependence structure might be unknown.

**Example 6** (Sampling clusters with unobserved membership). Here, we consider a setting where some observations are associated, but where the overall dependence structure is unknown. This is similar to the previous setting, but there are no ties in the data set. Consider \( \mathbb{P} \) a probability distribution with positive density over a compact subset of \( \mathbb{R}^p \). Draw i.i.d. observations \( D'_1, \ldots, D'_m \) from \( \mathbb{P} \). Set \( \xi = (D'_1, \ldots, D'_m) \). Conditionally on \( \xi \), let \( (D_1^n, \ldots, D_n^n) \) be i.i.d. draws from \( \mathbb{P}^\xi \), where
\[
\mathbb{P}^\xi(D \in \bullet) = \frac{1}{m} \sum_{i=1}^{m} \mathbb{P}(D \in \bullet || D'_i - D \|_2 \leq \epsilon_n),
\]
where \( \epsilon_n > 0 \) is a deterministic sequence with \( \epsilon_n = o(1/\sqrt{n}) \). Furthermore, let \( n \rightarrow \infty \) and assume that \( m = m(n) \) is a sequence of integers such that \( \frac{n}{m(n)} \) converges to some limit \( r \in (0, \infty) \). Then, equation (7) holds for any bounded Lipschitz continuous \( \psi(\bullet) \) with
\[
\delta^2 = 1 + r.
\]
Proof. Using Lipschitz continuity and \( \epsilon_n = o(1/\sqrt{n}) \), we have

\[
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D'_i) - \mathbb{E}[\psi(D)] \triangleq \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D''_i) - \mathbb{E}[\psi(D)] + o_p(1),
\]

where the \( D' \) are drawn with replacement from \( D'_1, \ldots, D'_m \). We can now invoke Example 5. \( \square \)

### B.4 Proof of Proposition 1

Proof. Note that

\[
\text{Var}_p(\phi^k(D)) = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\phi}^k(D_i) - \phi^k(D_i) \right)^2(\text{i}) + \frac{2}{n} \sum_{i=1}^{n} \left( \hat{\phi}^k(D_i) - \phi^k(D_i) \right) \left( \phi^k(D_i) - \frac{1}{n} \sum_{i=1}^{n} \phi^k(D_i) \right) \left( \phi^k(D_i) - \frac{1}{n} \sum_{i=1}^{n} \phi^k(D_i) \right)(\text{ii}) + \frac{1}{n} \sum_{i=1}^{n} \left( \phi^k(D_i) - \frac{1}{n} \sum_{i=1}^{n} \phi^k(D_i) \right)^2(\text{iii}).
\]

As the \( \phi^k \) has finite fourth moments, we can use Lemma 1 to obtain (iii) = \( \text{Var}_p(\phi^k(D)) + o_p(1) \). Then by Cauchy-Schwartz inequality and Jensen’s inequality,

\[
(\text{i}) \leq \frac{2}{n} \sum_{i=1}^{n} \left( \hat{\phi}^k(D_i) - \phi^k(D_i) \right)^2 + 2 \left( \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\phi}^k(D_i) - \phi^k(D_i) \right) \right)^2 \leq \frac{4}{n} \sum_{i=1}^{n} \left( \hat{\phi}^k(D_i) - \phi^k(D_i) \right)^2.
\]

Since our influence function estimators are consistent, (i) = \( o_p(1) \). Then again by Cauchy-Schwartz inequality, (ii) = \( o_p(1) \). Combining results, we get

\[
\text{Var}_p(\phi^k(D)) = \text{Var}_p(\phi^k(D)) + o_p(1).
\]

This completes the proof. \( \square \)

### B.5 Proof of Theorem 1

Proof. By Assumption 1, 2 and Lemma 1,

\[
\left( \sqrt{n} (\hat{\theta}^1 - \theta^0) \vdot \vdot \vdot \sqrt{n} (\hat{\theta}^K - \theta^0) \right) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \phi^1(D_i) \vdot \vdot \vdot \phi^K(D_i) \right) + o_p(1) \triangleq \delta Z + o_p(1)
\]

where \( Z = (Z_1, \ldots, Z_K)^T \sim \mathcal{N}(0, \text{diag}(\text{Var}(\phi^1), \ldots, \text{Var}(\phi^K))) \). As \( n \to \infty \), using that \( \sum \alpha_k = 1 \) and \( \alpha_k = \alpha_k + o_p(1) \),

\[
\sqrt{n} (\hat{\theta}^w - \theta^0) = \sqrt{n} \sum_{k=1}^{K} \alpha_k (\hat{\theta}^k - \theta^0) + o_p(1) \triangleq \delta \sum_{k=1}^{K} \alpha_k Z_k + o_p(1) \triangleq \delta \mathcal{N}(0, \alpha) + o_p(1), \quad (20)
\]
where \( \alpha = \frac{1}{\text{Var}(\phi_k(D))} \). By a similar calculation, we have that

\[
n\hat{\sigma}_{\text{bet}}^2 = \delta^2 \sum_{k=1}^{K} \alpha_k (Z_k - \sum_{j=1}^{K} \alpha_j Z_j)^2 + o_p(1).
\]

Thus,

\[
n\hat{\sigma}_{\text{bet}}^2 \overset{d}{=} \delta^2 \alpha L_K + o_p(1), \tag{21}
\]

where

\[
L_K = \frac{1}{\alpha} \sum_{k=1}^{K} \alpha_k (Z_k - \sum_{j=1}^{K} \alpha_j Z_j)^2.
\]

We will now show that

\[
L_K \sim \chi^2(K-1) \perp \frac{1}{\sqrt{\alpha}} \sum_{j=1}^{K} \alpha_j Z_j \sim \mathcal{N}(0, 1). \tag{22}
\]

First, note that

\[
L_K = \sum_{k=1}^{K} \left( Z_k \frac{\sqrt{\alpha_k}}{\sqrt{\alpha}} - \frac{\sqrt{\alpha_k}}{\sqrt{\alpha}} \sum_{j=1}^{K} \alpha_j Z_j \right)^2.
\]

With this definition,

\[
L_K = \sum_{k=1}^{K} \left( \frac{\sqrt{\alpha_k}}{\sqrt{\alpha}} Z_k - \frac{\sqrt{\alpha_k}}{\sqrt{\alpha}} \sum_{j=1}^{K} \alpha_j Z_j \right)^2
\]

\[
= \sum_{k=1}^{K} \left( \frac{\sqrt{\alpha_k}}{\sqrt{\alpha}} Z_k - \sum_{j=1}^{K} \sqrt{\alpha_j} \frac{\sqrt{\alpha_k}}{\sqrt{\alpha}} Z_j \right)^2
\]

\[
= \sum_{k=1}^{K} (Z_k - w_k \sum_{j=1}^{K} w_j Z_j)^2
\]

where \( Z_k := Z_k \sqrt{\alpha_k}/\sqrt{\alpha} = Z_k / \sqrt{\text{Var}(\phi_k)} \) are i.i.d. standard normal and \( w_k := \sqrt{\alpha_k} \). Please note that \( \sum_k w_k^2 = 1 \). Thus, we can write this equation

\[
L_K = \| \tilde{Z} - w (w \cdot \tilde{Z}) \|^2 = \| (\text{Id} - \Pi) \tilde{Z} \|^2_2,
\]

where \( \Pi \) projects on the one-dimensional subspace spanned by \( w \). Let \( b_1, \ldots, b_{K-1} \) be an orthonormal basis of the span of \( \Pi \). Then, by rotational invariance of the \( \ell_2 \) norm,

\[
L_K = \| (\text{Id} - \Pi) \tilde{Z} \|^2_2 = \sum_{k=1}^{K-1} (b_k \cdot \tilde{Z})^2.
\]

Furthermore, since the \( b_k \) are orthogonal to each other \( b_k \cdot \tilde{Z} \) are independent standard Gaussians. Thus, \( L_K \) follows a \( \chi^2(K-1) \) distribution. Furthermore, since the \( b_k \) are orthogonal to \( w \), \( L_K \) is independent of

\[
\sum_{k=1}^{K} w_k \tilde{Z}_k.
\]

Furthermore, by definition

\[
\frac{1}{\sqrt{\alpha}} \sum_{k=1}^{K} \alpha_k Z_k = \sum_{k=1}^{K} w_k \tilde{Z}_k \sim \mathcal{N}(0, 1)
\]
and thus $L_K$ is independent of $\frac{1}{\sqrt{\alpha}} \sum_{k=1}^{K} \alpha_k Z_k$. Therefore, (22) holds. Using (22) with (21) and (20), we get

$$
\frac{\hat{\delta}^W - \theta_0}{\sigma_{\text{bet}}/\sqrt{K-1}} = \frac{d}{\sqrt{\alpha \delta \sqrt{L_K}/(K-1)}} + o_P(1) = \frac{\sum_{k=1}^{K} \alpha_k Z_k}{\sqrt{L_K}/(K-1)} = T_{K-1} + o_P(1).
$$

where $T_{K-1}$ is a t-distributed random variable with $K-1$ degrees of freedom. This completes the proof. \qed

### B.6 Proof of Theorem 2

**Proof.** In this proof, if not specified otherwise, all variances and covariances are meant with respect to $\mathbb{Q}$, that is marginally over both the variation in $D$ and $\xi$. We will directly work with $U = h(D)$. Define

$$f(x) = \text{Var}(\mathbb{P}(U \in [0, x]))$$

Let $A$ and $B$ be two disjoint subsets of $[0, 1]$. Define $a = \mathbb{P}(U \in A)$ and $b = \mathbb{P}(U \in B)$. Then,

$$f(a + b) = \text{Var}(\mathbb{P}(U \in A \cup B))$$

$$= \text{Var}(\mathbb{P}(U \in A)) + \text{Var}(\mathbb{P}(U \in B)) + 2\text{Cov}(\mathbb{P}(U \in A), \mathbb{P}(U \in B))$$

$$= f(a) + f(b) + 2\text{Cov}(\mathbb{P}(U \in A), \mathbb{P}(U \in B))$$

Thus, for any two disjoint sets $A$ and $B$,

$$\text{Cov}(\mathbb{P}(U \in A), \mathbb{P}(U \in B)) = \frac{f(a + b) - f(a) - f(b)}{2}$$

Define

$$g(a, b) = \frac{f(a + b) - f(a) - f(b)}{2}.$$  \hspace{1cm} (23)

Let us first show that $f$ is continuous. Let $a_n \to a$, $a_n \geq a$. Then,

$$f(a_n) - f(a) = f(a) + 2g(a_n - a, a) + f(a_n) - f(a) = 2g(a_n - a, a) + f(a_n - a).$$

By Cauchy-Schwartz,

$$g(a_n - a, a) \leq \sqrt{f(a_n - a)f(a)}.$$  

By assumption, $f(a_n - a) \to 0$. Thus, $f(a_n) \to f(a)$. The case $a_n \to a$, $a_n \leq a$ can be treated analogously. Thus, $f(\bullet)$ and $g(\bullet, \bullet)$ are continuous.

Partition the probability space into disjoint $D$-measurable events $A_i$, $i = 1, \ldots, n$ with $\mathbb{P}(U \in A_i) = 1/n$. Then,

$$0 = \text{Var}(\mathbb{P}(\cup A_i) - \mathbb{P}(\cup A_i)) = nf(1/n) + n(n - 1)g(1/n, 1/n)$$

Thus,

$$g(1/n, 1/n) = -1/(n-1)f(1/n)$$  \hspace{1cm} (24)

We will now show that $f(x) = x(1 - x)\delta^2_{\text{dist}}$ for $x = 1/2^k$, where $\delta^2_{\text{dist}} = 4f(1/2)$. This will show that up to the constant $\delta^2_{\text{dist}} = 4f(1/2)$, $f$ and $g$ are uniquely defined. First, we will show this equality for $x = 1/4$.

$$f(1/2) = f(1/4) + f(1/4) + 2g(1/4, 1/4) = 2f(1/4) - 2/3f(1/4)$$

Thus,

$$f(1/4) = 4/3f(1/4)$$

Rearranging,

$$f(1/4) = 1/4(1 - 1/4)4f(1/2) = x(1 - x)\delta^2_{\text{dist}}$$

for $x = 1/4$. Induction step: Assume that

$$f(x) = x(1 - x)\delta^2_{\text{dist}}$$

for $x = 1/4$. Induction step: Assume that
for $x = 1/2^k$. Now we want to show that
\[
f(x/2) = x/2(1 - x/2)\delta_{\text{dist}}^2
\]
To this end, using (23) and (24),
\[
f(x) = f(x/2) + f(x/2) - 2/(2/x - 1)f(x/2)
\]
Thus,
\[
f(x) = (2 - 2x/(2 - x))f(x/2) = (4 - 2x - 2x)/(2 - x)f(x/2) = (4 - 4x)/(2 - x)f(x/2).
\]
By induction assumption,
\[
f(x/2) = (2 - x)/(4 - 4x)x(1 - x)\delta_{\text{dist}}^2 = x/2(1 - x/2)\delta_{\text{dist}}^2.
\]
Thus, by induction for all $x = 1/2^k$,
\[
f(x) = x(1 - x)\delta_{\text{dist}}^2.
\]
Now we want to show that for any $k$ and $j \leq 2^k$ and $x = j/2^k$,
\[
f(x) = x(1 - x)\delta_{\text{dist}}^2.
\]
For any $k$ and $j$ with $1 \leq j \leq 2^k$, using the definition of $f$ and (24),
\[
f(j/2^k, j'/2^k) = jf(1/2^k) - j(j - 1)/(2^k - 1)f(1/2^k) = (2^k - 1)/(2^k - 1)jf(1/2^k)
\]
\[
= (j^2 - j^2)/(2^k - 1)1/2^k(1 - 1/2^k)\delta_{\text{dist}}^2 = (j^2 - j^2)1/2^k1/2^k\delta_{\text{dist}}^2
\]
Thus, for all $k$ and $j \leq 2^k$, and $x = j/2^k$,
\[
f(x) = x(1 - x)\delta_{\text{dist}}^2.
\]
Using continuity of $f$, for all $x \in [0, 1]$,
\[
f(x) = x(1 - x)\delta_{\text{dist}}^2.
\]
We will now derive an explicit formula for $g$. For any $k$ and $j, j'$ with $j + j' \leq 2^k$,
\[
g(j/2^k, j'/2^k) = jj'g(1/2^k, 1/2^k) = -jj'/2^k - 1)f(1/2^k) = -jj'/2^k - 1)f(1/2^k)
\]
\[
= -jj'1/2^k1/2^k\delta_{\text{dist}}^2 = -j^2/j^2\delta_{\text{dist}}^2.
\]
By continuity, for all $x \geq 0, y \geq 0$ with $x + y \leq 1$,
\[
g(x, y) = -xy\delta_{\text{dist}}^2.
\]
Now assume that for some $D$-measurable disjoint sets $A_i$ and some constants $y_i$,
\[
\psi(D) = \sum 1_{A_i} y_i
\]
Then,
\[
\text{Var}(\mathbb{E}[\psi(D)] - \mathbb{E}[\psi(D)]) = \sum_i y_i^2 f(\mathbb{P}(A_i)) + \sum_{i \neq j} y_i y_j g(\mathbb{P}(A_i), \mathbb{P}(A_j))
\]
To simplify, let’s write $p_i = \mathbb{P}(A_i)$. Using explicit formulas for $f$ and $g$,
\[
\text{Var}(\mathbb{E}[\psi(D)] - \mathbb{E}[\psi(D)]) = \sum_i \delta_{\text{dist}}^2 p_i (1 - p_i) - \sum_{i \neq j} \delta_{\text{dist}}^2 y_i y_j p_i p_j
\]
(25)
On the other hand,
\[
\delta_{\text{dist}}^2 \text{Var}_\mathbb{P}(\psi(D)) = \delta_{\text{dist}}^2 (\sum_i p_i (1 - p_i) y_i^2 + \sum_{i \neq j} \text{Cov}(1_{A_i}, 1_{A_j}) y_i y_j)
\]
As the sets are disjoint, $\text{Cov}(1_{A_i}, 1_{A_j}) = -p_i p_j$. Thus,
\[
\delta_{\text{dist}}^2 \text{Var}_\mathbb{P}(\psi(D)) = \delta_{\text{dist}}^2 (\sum_i p_i (1 - p_i) y_i^2 + \sum_{i \neq j} -p_i p_j y_i y_j)
\]
(26)
Combining equation (25) with equation (26),
\[
\text{Var}(\mathbb{E}[\psi(D)] - \mathbb{E}[\psi(D)]) = \delta_{\text{dist}}^2 \text{Var}_\mathbb{P}(\psi(D)).
\]
By measure-theoretic induction, this result is extended to any $\psi(D) \in L^2(\mathbb{P})$. 
\[\square\]
B.7 Asymptotic behaviour of $M$-estimators

B.7.1 Proof of Lemma 2

Proof. The proof proceeds as in van der Vaart (2000) with $m_{\theta} = -L(\theta, D)$ and $P_n$ denoting the empirical measure of $D^\theta_1, \ldots, D^\theta_n$ and $d(\cdot, \cdot)$ the $\ell_2$ norm in $\mathbb{R}^d$. The only difference is in the step where van der Vaart (2000) uses the law of large numbers to show that with probability going to 1, we have

$$\frac{1}{n} \sum_{i=1}^{n} m_{U_{\hat{\theta}}}(D^\theta_i) = E[m_{U_{\hat{\theta}}}(D)] + o_p(1)$$

for all $j = 1, \ldots, p$. Since the data is not i.i.d. we cannot use the classical law of large numbers to get this step. Instead, we apply Lemma 1 to get

$$\frac{1}{n} \sum_{i=1}^{n} m_{U_{\hat{\theta}}}(D^\theta_i) = E[m_{U_{\hat{\theta}}}(D)] + o_p(1).$$

B.7.2 Proof of Lemma 3

Proof. The proof follows van der Vaart (2000), Theorem 5.41, with $\Psi_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} \partial_{\theta} L(\theta, D^\theta_i)$ and $\Psi_n = \frac{1}{n} \sum_{i=1}^{n} \partial_{\theta}^2 L(\theta, D^\theta_i)$. There are only three steps where the arguments are slightly different. First, we cannot justify the bound

$$\hat{\Psi}_n(\hat{\theta}_n) = O_P(1)$$

via the law of large numbers since the data is not i.i.d. Instead, we can use Lemma 1 for $\psi(D) = h(D)$ to get

$$\|\hat{\Psi}_n(\hat{\theta}_n)\| \leq \frac{1}{n} \sum_{i=1}^{n} h(D^\theta_i) = O_P(1).$$

Analogously, we cannot apply the law of large numbers to $\hat{\Psi}_n(\theta^0) = \frac{1}{n} \sum_{i=1}^{n} \partial_{\theta}^2 L(\theta^0, D^\theta_i)$. Instead, we use Lemma 1 with $\psi(D) = \partial_{\theta}^2 L(\theta^0, D)$ to get

$$\frac{1}{n} \sum_{i=1}^{n} \partial_{\theta}^2 L(\theta^0, D^\theta_i) = E[\partial_{\theta}^2 L(\theta^0, D)] + o_P(1).$$

Similarly, we show that $\Psi_n(\theta^0) = \frac{1}{n} \sum_{i=1}^{n} \partial_{\theta} L(\theta^0, D^\theta_i) = O_P(1/\sqrt{n})$. The rest of the proof proceeds as in van der Vaart (2000), Theorem 5.41. \qed

C Robust calibrated inference

In some cases, the data analyst may trust one of the estimators $\hat{\theta}^k$ more than others. For example, the data analyst may be convinced that $\hat{\theta}^1 = \theta^0$ but may not be sure whether $\hat{\theta}^k = \theta^0$ for $k \geq 2$. In this case, the data analyst may report the confidence interval for $\theta^0$ using $\hat{\theta}^1$ instead of $\hat{\theta}^W$ with $\delta$ estimated by looking at the between-estimator variance of the remaining $K-1$ estimators. Now we present how to build asymptotic valid confidence intervals in such cases.

Theorem 3. (Asymptotic validity of calibrated confidence interval). Suppose Assumption 1 holds for $k = 1, \ldots, K$ and the influence functions $\phi^1(D), \ldots, \phi^K(D)$ are uncorrelated. Suppose $\theta^1 = \theta^0$ but $\theta^k$ may not be $\theta^0$ for $k \geq 2$. Furthermore assume that we have consistent estimates of the variances of influence functions such that $\text{Var}_0(\phi^k(D)) = \text{Var}_0(\phi^0(D)) + o_p(1)$ for $k = 1, \ldots, K$. Let $\hat{\theta}^W = \sum_{k=2}^{K} \hat{\alpha}_k \hat{\theta}^k$ be the inverse-variance weighted estimator of $K-1$ estimators where the weights are

$$\hat{\alpha}_k = \frac{1}{\text{Var}_0(\phi^k(D))} \frac{1}{\sum_{j=2}^{K} \text{Var}_0(\phi^j(D))}.$$
Let $\hat{\sigma}_{\text{bet}}$ be the weighted between-estimator variance of $K - 1$ estimators defined as

$$
\hat{\sigma}_{\text{bet}}^2 = \sum_{k=2}^{K} \hat{\alpha}_k (\hat{\theta}^k - \bar{\theta}^W)^2.
$$

Then for any $\alpha \in (0, 1)$, it holds that as $n \to \infty$,

$$
\lim \inf_{n \to \infty} P \left( \theta^0 \in \left[ \hat{\theta}^1 \pm t_{K-2,1-\alpha/2} \cdot \sqrt{\frac{\sum_{j=2}^{K} \text{Var}_P(\phi^j(D)) \hat{\sigma}_{\text{bet}}}{\text{Var}_P(\phi^1(D)) \sqrt{K-2}}} \right] \right) \geq 1 - \alpha,
$$

where $t_{K-2,1-\alpha/2}$ is the $1 - \alpha/2$ quantile of the $t$ distribution with $K - 2$ degrees of freedom. To be clear, here we marginalize over both the randomness due to sampling and the randomness due to the distributional perturbation.

The resulting confidence intervals are expected to be conservative. Firstly, we lose one degree of freedom of the $t$-distribution. Secondly, we get an overcoverage if $\theta^k \neq \theta^0$ for $k \geq 2$.

**Proof.** If $\theta^k \neq \theta^0$ for some $k \geq 2$, then by asymptotic linearity $\hat{\sigma}_{\text{bet}}^2$ converges to some $\tau^2 > 0$. As in the proof of Theorem 1, we get $\hat{\theta}^1 - \theta^0 = N(0, \delta^2 \text{Var}(\phi^1)/n) + o_P(1/\sqrt{n})$. Since the variance estimates are consistent,

$$
P \left( \theta^0 \in \left[ \hat{\theta}^1 \pm t_{K-2,1-\alpha/2} \cdot \sqrt{\frac{\sum_{j=2}^{K} \text{Var}_P(\phi^j(D)) \hat{\sigma}_{\text{bet}}}{\text{Var}_P(\phi^1(D)) \sqrt{K-2}}} \right] \right) \to 1.
$$

Now let us consider the case $\theta^0 = \theta^1 = \ldots = \theta^K$. From the proof of Theorem 1, we know that

$$
\frac{\sqrt{n}(\hat{\theta}^1 - \theta^0)}{\sqrt{\text{Var}_P(\phi^1(D))}} \overset{d}{=} \delta Z + o_P(1)
$$

where $Z \sim N(0, 1)$. Moreover,

$$
n \hat{\sigma}_{\text{bet}}^2 \overset{d}{=} \delta^2 \frac{1}{\sum_{j=2}^{K} \text{Var}_P(\phi^j(D))} \cdot L_{K-1} + o_P(1),
$$

where $L_{K-1}$ follows the chi-square distribution with $K - 2$ degrees of freedom. Note that $Z$ and $L_{K-1}$ are independent. Then, we get

$$
\frac{\hat{\theta}^1 - \theta^0}{\hat{\sigma}_{\text{bet}} \sqrt{\sum_{j=2}^{K} \frac{1}{\text{Var}_P(\phi^j(D))}/\sqrt{K-2}}} \overset{d}{=} \frac{Z}{\sqrt{L_{K-1}/(K-2)}} + o_P(1).
$$

Thus, we get

$$
P \left( \frac{Z}{\sqrt{L_{K-1}/(K-2)}} \leq x \right) = P(t_{K-2} \leq x)
$$

where $t_{K-2}$ is a $t$-distributed random variable with $K - 2$ degrees of freedom. This completes the proof. \qed