

SAMPLE OUT-OF-SAMPLE INFERENCE BASED ON WASSERSTEIN DISTANCE

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ABSTRACT. We present a novel inference approach which we call Sample Out-of-Sample (or SOS) inference. The approach can be used widely, ranging from semi-supervised learning to stress-testing and it is fundamental in the application of data-driven Distributionally Robust Optimization (DRO). Our method enables measuring the impact of (plausible) out-of-sample scenarios on a given performance measure of interest (such as a financial loss). The methodology is inspired by Empirical Likelihood (EL), but we optimize the empirical Wasserstein distance (instead of the empirical likelihood) induced by observations. From a methodological standpoint, our analysis of the asymptotic behavior of the induced Wasserstein-distance profile function shows dramatic qualitative differences relative to EL. For instance, in contrast to EL, which typically yields chi-squared weak convergence limits, our asymptotic distributions are often not chi-squared. Also, the rates of convergence that we obtain have some dependence on the dimension in a non-trivial way but which remains controlled as the dimension increases.

Subject classifications: Non-parametric statistics; Probability; Distributionally Robust Optimization

Area of review: Stochastic Models.

1. INTRODUCTION

The goal of this paper is to introduce a novel methodology for non-parametric inference which allows incorporating the adverse impact of out-of-sample scenarios. We call the procedure Sample Out-of-Sample inference or SOS inference. Our method is general, and we discuss several applications, including Distributional Robust Optimization (DRO), semi-supervised learning and a novel stress-testing framework. We use the DRO framework in the introduction to put our contributions in perspective. We elaborate on semi-supervised learning and stress-testing applications in Section 2. A data-driven DRO problem takes the form

$$(1) \quad \min_{\theta \in \mathbb{R}^d} \max_{P \in \mathcal{U}_\delta(P_n)} E_P[l(\theta, X)],$$

where $l : \mathbb{R}^{d \times l} \rightarrow [0, \infty)$ is a cost (or loss) function, $X \in \mathbb{R}^l$ is a random element, and $\theta \in \mathbb{R}^d$ is a decision. Often, $l(\cdot, x)$ is assumed to be strictly convex and smooth (e.g. twice differentiable) and we will assume this throughout our motivating discussion. The notation $E_P(\cdot)$ denotes the expectation operator associated to the probability measure P . We use P_n to denote the empirical measure corresponding to $\{X_i\}_{i=1}^n$ i.i.d. observations which follow the distribution P_* . The set $\mathcal{U}_\delta(P_n)$ is the distributional uncertainty set. The parameter $\delta > 0$ is called the “size of the distributional uncertainty” so that the family of sets $(\mathcal{U}_\delta(P_n) : \delta \geq 0)$ is increasing (in the sense of inclusion) as a $\delta > 0$ increases and so that for $\delta = 0$, $\mathcal{U}_0(P_n) = \{P_n\}$. So, intuitively, P_n is the “center” of the distributional uncertainty region and $\delta > 0$ can be thought of as its “radius”.

Ideally, one would like to compute $\theta_* = \arg \min E_{P_*}[l(\theta, X)]$, but P_* is unknown. So, the intuition behind formulation (1) is that one is interested in choosing a decision θ , which performs well uniformly over a range of models which constitute reasonable (or plausible) variations of the data (encoded by P_n).

We are interested in variations of the empirical distribution P_n (the elements in $\mathcal{U}_\delta(P_n)$) which systematically explore the impact of *out-of-sample scenarios* in the loss function $l(\cdot)$. So, $P \in \mathcal{U}_\delta(P_n)$ should not be supported only on the underlying data set. Instead, we are interested in a framework which admits models in $P \in \mathcal{U}_\delta(P_n)$ which may be supported outside the sample $\{X_i\}_{i=1}^n$. Because of this out-of-sample exploration feature, we choose $\mathcal{U}_\delta(P_n)$ based on the Wasserstein distance of order 2, which is explained in Section 3.

Distributionally robust optimization formulations such as (1) based on the Wasserstein distances have been studied recently in a wide range of settings, especially in applications to machine learning and artificial intelligence, see for example, [39, 29, 48, 10, 17, 8, 47, 41, 18, 43, 14, 9].

All of these studies focus on the setting in which the support of the distributions inside $\mathcal{U}_\delta(P_n)$ is \mathbb{R}^d . Moreover, within the current literature, only [8] studies the optimal selection of the parameter δ by defining a natural optimization criterion. The work of [8] also shows that such criterion recovers choices which have been argued to be effective for recovery in machine learning settings for which a DRO representation can be posed.

In contrast, compared to [8], *our work is the first one that studies the statistical implications of choosing the support of the members of the distributional uncertainty $P \in \mathcal{U}_\delta(P_n)$ in a data-driven way.* One of our main contributions in this paper consists in providing a comprehensive study of an optimal data-driven choice of uncertainty size, δ , when the support of the members in $\mathcal{U}_\delta(P_n)$ is obtained from an arbitrary random sample whose size is increasing with n .

More generally, our contributions can be viewed in the lens of a novel inference framework which we call Sample-out-of-Sample inference, based on the analysis of the so-called SOS profile function for estimating equations.

In the DRO framework, we consider enriching the empirical data set $\mathcal{X}_n = \{X_i\}_{i=1}^n$ (which is assumed to be i.i.d.) by including a set of scenarios $\{Y_i\}_{i=1}^m$ (which is also assumed to be i.i.d.), with $m = \lceil \kappa n \rceil$ for some $\kappa \in [0, \infty)$. The Y_i 's and the X_i 's are not assumed share the same distribution. In order to unify the notation we write $Z_i = X_i$ for $i = 1, \dots, n$, $Z_{n+k} = Y_k$ for $k = 1, \dots, m$ and set $\mathcal{Z}_{n+m} = \{Z_j\}_{j=1}^{n+m}$. (We use \mathbf{P} to denote the probability measure supporting the infinite sequences $\{X_i\}_{i \geq 1}$ and $\{Y_i\}_{i \geq 1}$.)

In order to emphasize the difference between the analysis in [8] and our analysis here, we write $\mathcal{U}_\delta(P_n; \mathbb{R}^{l+1})$ to denote the full support case (studied in [8]) and $\mathcal{U}_\delta(P_n; \mathcal{Z}_{n+m})$ for the uncertainty set considered in our current setting.

Let us describe the optimality criterion discussed in [8] for choosing δ . Since the set $\mathcal{U}_\delta(P_n)$ is interpreted as the set of plausible variations of the data, then the set

$$(2) \quad \Lambda_\delta(P_n) = \{\theta : \theta = \arg \min E_P[l(\theta, X)] \text{ for } P \in \mathcal{U}_\delta(P_n; \mathcal{Z}_{n+m})\}$$

corresponds to the set of plausible decisions, those which are compatible with the distributional uncertainty region. Note that $\Lambda_\delta(P_n)$ is a random set which can be interpreted as a confidence region. The criterion that we utilize is the following

$$(3) \quad \min\{\delta : \mathbf{P}(\theta_* \in \Lambda_\delta(P_n)) \geq \alpha\},$$

where α is a desired confidence level.

To analyze (3) we first argue that

$$(4) \quad \{\theta_* \in \Lambda_\delta(P_n)\} = \{R_n^W(\theta_*) \leq \delta\},$$

for a suitably function, $R_n^W(\cdot)$, which we call the SOS profile function (Sample-out-of-Sample profile function). In simple words, $R_n^W(\theta_*)$ can be computed directly in terms of the shortest Wasserstein distance between P_n and the set of probability models $P \in \mathcal{U}_\delta(P_n; \mathcal{Z}_{n+m})$ for which $E_P[\nabla_{\theta} l(\theta_*, x)] = 0$.

As a consequence of (4), the optimal δ solving (3) is simply the α -quantile of $R_n^W(\theta_*)$.

In general, we can use our methodology to test the hypothesis that θ_* satisfies $E_{P_*}(h(\theta_*, x)) = 0$, simply replacing $\nabla_{\theta} l(\theta, x)$ by $h(\theta, x)$ in the definition of the SOS profile function. The hypothesis is rejected for high values of the statistics $R_n^W(\theta_*)$. Thus, it is important to compute the asymptotic distribution $R_n^W(\theta_*)$.

Our contributions are then stated at this level of generality (i.e. asymptotic analysis of $R_n^W(\theta_*)$ for the purpose of hypothesis testing). In the end, this paper involves two main contributions:

A) First, we characterize the asymptotic distribution of $R_n^W(\theta_*)$ as $n \rightarrow \infty$, see Theorems 1- 3.

We explain how to compute the asymptotic limiting distributions in Section 4.1.1.

B) Second, we discuss various extensions which, we believe, are natural to study in order to define DRO optimal transport cost functions. These include implicit DRO formulations and plug-in estimators. We illustrate the extensions in the empirical result section. For example, writing $\theta_* = (\gamma_*, v_*)$ we develop the asymptotic distribution of $R_n^W(\gamma_*, \bar{v}_n)$, where \bar{v}_n is a suitable consistent plug-in estimator for v_* as $n \rightarrow \infty$, see Corollary 2. The construction of \bar{v}_n may be based on standard empirical estimators. This extension may be used in the context of stochastic optimization with constraints, as illustrated in Section 5.

The theory that we develop in this paper parallels the main fundamental results obtained in the context of Empirical Likelihood (EL), introduced by Art Owen in [34, 32, 35]. In fact, the construction of the function $R_n^W(\cdot)$, borrows a great deal of inspiration from the Empirical Likelihood Profile function (and its extensions based on divergence criteria, rather than the likelihood function, see [35]). There are, however, several important characteristics of our framework that, we believe, add significant value to the non-parametric inference literature.

First, from a conceptual standpoint, the EL framework restricts the support of the outcomes only to the observed empirical sample and, therefore, there is no reason to expect particularly good out of sample performance of estimates based on EL. In fact, the out-of-sample problems which arise from using divergence criteria for data-driven distributional robust optimization (closely related to EL) are noted in the stochastic optimization literature, see [16]; see also [45, 3], for related work.

Second, from a methodological standpoint, the mathematical techniques needed to understand the asymptotic behavior of $R_n^W(\theta_*)$ are qualitatively different from those arising typically in the context of EL. We will show that if $l \geq 3$, then the following weak convergence limit holds (under suitable assumptions on $l(\cdot)$),

$$n^{1/2+3/(2l+2)} R_n^W(\theta_*) \Rightarrow R(\theta_*),$$

as $n \rightarrow \infty$. Note that the scaling depends on the dimension of the random vector X in a very particular way. In contrast, the Empirical Likelihood Profile function is always scaled linearly in n and the asymptotic limiting distribution is generally a chi-squared distribution with appropriate degrees of freedom and a constant scaling factor.

In our case, $R(\theta_*)$ can be explicitly characterized, depending on the dimension in a non-trivial way, but it is no longer a suitably scaled chi-squared distribution. When $l = 1$, we obtain a similar limiting distribution as in the EL case. The case $l = 2$, interestingly, requires a special analysis. In this case, the scaling remains linear in n (as in the case $l = 1$), although the limiting distribution is not exactly chi-squared, but a suitable quadratic form of a multivariate Gaussian random vector. For the case $l \geq 3$ the limiting distribution is not a quadratic transformation of a multivariate Gaussian, but a more complex (yet still explicit) polynomial function depending on the dimension. At a high level, some of the qualitative distinctions in the methodology arises because of the linear programming formulation underlying the SOS function, which will typically lead to corner solutions (i.e. basic feasible solutions in the language of linear programming). The high level intuition of

the scaling is associated with the interplay between the linear programming formulation and the coverage of a sample of size n in a space in l dimension. A high level intuition is given in more detail in Section 7.1. In contrast to the analysis of the SOS function, in the EL analysis of the profile function, the optimal solutions are amenable to a smooth perturbation analysis as $n \rightarrow \infty$ using a Taylor expansion of second (and higher) order terms. The lack of a continuously differentiable derivative (of the optimal solution as a function of θ) requires a different type of analysis relative to the approach (traced back to the classical Wilk's theorem, [46]) which lies at the core of EL analysis.

The high-level intuition developed in Section 7.1 also underscores the distinction between our development here and the analysis in [8]. In contrast to our development here, the scaling in [8] is always dimension independent. This is because the issue involving the coverage of the random scenarios in the support of the alternative distributions is not an issue that needs to be controlled. Moreover, the current setting introduces a correlation structure in the optimal transportation map, which is not present in the analysis of [8]. This is because the feasible transportation locations are now given by a random sample. To this end, we take advantage of recent sample-path martingale inequalities. The use of these inequalities is showcased in the technical Section 7.2.7 and we believe that these techniques may be applicable more broadly in non-parametric statistical analysis.

The rest of the paper is organized as follows. In Section 2 we discuss semi-supervised learning and stress testing applications which motivate the formulation in which the support of $P \in \mathcal{U}_\delta(P_n; \mathcal{Z}_{n+m})$ is data-driven. Basic definitions, including a review of the Wasserstein distance, are given in Section 3. Our main technical results are described in Section 4. We include applications of our results to settings such as stochastic optimization, risk analysis, and semi-supervised learning in Section 5. A short section including conclusions and additional discussions is given in Section 6. Finally, our technical development is given in Section 7, starting with a high level intuition of the nature of our results and scaling in Section 7.1.

2. MOTIVATING SETTINGS

2.1. Semi-supervised Learning Applications. The setting of semi-supervised learning can be used to illustrate our framework. Consider a classification problem which takes the form $\mathcal{D}_n = \{(X_i, Y_i)\}_{i=1}^n$ and $Y_i \in \{-1, 1\}$ is the i -th response variable and $X_i \in R^l$ is the i -th the predictor.

For concreteness, let us consider the logistic regression setting in which

$$P(Y_i = 1|X_i) = \frac{\exp(Y_i\beta_*^T X_i)}{1 + \exp(Y_i\beta_*^T X_i)} = 1 - P(Y_i = -1|X_i).$$

Suppose that we have access to an unlabeled data set $\{X'_i\}_{i=1}^m$ and we are interested in using this data in a meaningful way for estimating β_* . This is the semi-supervised learning setting which arises in cases in which obtaining responses or labels for every individual may be costly.

The work of [6] proposes combining both the label and unlabeled data by forming the set $\mathcal{X}_{n,m} = \mathcal{D}_n \cup (\{X'_i\}_{i=1}^m \times \{1, -1\}_{i=1}^n)$ (i.e. the original data set is enriched by considering the unlabeled data with all the possible responses recorded by the labeled data).

Then, [6] considers a Distributionally Robust Optimization (DRO) formulation for estimating β_* in which the distributional uncertainty region is defined in terms of the Wasserstein distance. The DRO formulation proposed in [6] is equivalent to the problem

$$(5) \quad \min_{\beta} \max_{\mathcal{U}_{\delta}(P_n; \mathcal{X}_{n,m}) \leq \delta} E_P[l(X, Y, \beta)],$$

which corresponds to (1).

The formulation of [6] (i.e. (5)) is of significant interest because it is a natural semi-supervised learning extension version of regularized linear regression, which is a highly popular supervised machine learning estimator (see [20]). In particular, it is shown in [8], see also [39], that replacing $\mathcal{U}_{\delta}(P_n; \mathcal{X}_{n,m})$ by $\mathcal{U}_{\delta}(P_n; \mathbb{R}^l)$ in (5) one recovers exactly regularized logistic regression and δ corresponds exactly to the regularization parameter. This connection between Wasserstein DRO and mainstream supervised learning estimators has been established for a large class of methods, including, square-root Lasso ([8]), support vector machines ([8]), group Lasso ([5]), adaptive Lasso ([9]), etc.

The methods developed in this paper provide the theoretical underpinning for the choice of the uncertainty size δ in the context of (5) which yield regularized estimators which are informed by the unlabeled data in a meaningful way.

2.2. Novel Stress-testing Framework. Consider the following stress-testing exercise. An insurance company wishes to estimate a certain expectation of interest, say $\mathbb{E}_{\mathbb{P}^*}(L(X))$, where X might represent one or several risk factors, $L(X)$ is the corresponding financial loss and $\mathbb{P}^*(\cdot)$ is the underlying probability measure which may be unknown.

The insurance company may estimate $\mathbb{E}^*(L(X))$ based on n i.i.d. (independent and identically distributed) empirical samples $X_1, \dots, X_n \in \mathbb{R}^l$. However, the regulator (or auditor) is also interested in quantifying the potential financial loss based on stress scenarios, say an i.i.d. sample $Y_1, \dots, Y_m \in \mathbb{R}^l$, where $m = \lceil \kappa n \rceil$ with $\kappa \in [0, \infty)$. It may be natural to choose $\kappa = 1$ so that the amount of information provided by the regulator and the company is balanced, but this is not necessary.

The scenarios provided by the regulator may or may not come from the same distribution as the X_i 's. In fact, typically they will come from a different distribution. The regulator's beliefs are captured by the distribution of the Y_i 's. These beliefs may, in turn, be informed by the knowledge which is accessible only by the regulator and not by the insurance company. The regulator may not necessarily question the fact that the historical data from the X_i 's follows distribution $\mathbb{P}_*(\cdot)$, but he/she might be concerned that the insurance company lacks additional information to assess the overall risk exposure better.

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On the one hand, the insurance company clearly knows well its idiosyncratic risk exposures, so the data represented by the X_n 's, arising from a model with such idiosyncratic information is meaningful and should be considered carefully. On the other hand, it is also correct that the regulator possesses additional information which should be considered in evaluating the potential impact of scenarios which may not be appropriately captured by the data of the insurance company.

So, how does one incorporate both the X_n 's and the Y_i 's in a meaningful way for the purposes of evaluating the risk of the company?

The methodology developed in this paper allows incorporating both the empirical data of the insurance company and the stress scenarios provided by the regulator a Distributionally Robust Performance Analysis (DRPA) formulation (closely related to Distributionally Robust Optimization – DRO) as we describe next.

Define $Z_k = X_k$ and $Z_{n+k} = Y_k$ for $k = 1, \dots, m$ (i.e. merge both the empirical samples and the stress scenarios into a set $\mathcal{Z}_{n+m} = \{Z_1, \dots, Z_{n+m}\}$). We let

$$P_n(dx) = n^{-1} \sum_{k=1}^n \delta_{\{X_k\}}(dx)$$

be the empirical distribution of the data generated by the insurance company. A natural estimate for $\mathbb{E}^*(L(X))$ based on the insurance company's data is given by

$$\mathbb{E}_{P_n}(L(X)) = n^{-1} \sum_{k=1}^n L(X_k).$$

Now, let $\mathcal{P}(\mathcal{Z}_{n+m})$ be the set of all probability distributions with support on \mathcal{Z}_{n+m} . Our DRPA approach consists in providing estimates for $\mathbb{E}_P(L(X))$ via

$$(6) \quad \theta_-(\delta), \theta_+(\delta) = \min_{P \in \mathcal{U}_\delta(P_n; \mathcal{Z}_{n,m})} , \max_{P \in \mathcal{U}_\delta(P_n; \mathcal{Z}_{n,m})} \mathbb{E}_P(L(X)).$$

We believe that the DRPA formulation (6) provides a reasonable approach for combining both the insurance company's information and the regulator's beliefs. We do not disregard the data coming from the insurance company (in fact, the empirical distribution P_n is placed at the center of the uncertainty set), but we also capture the potential impact of out-of-sample scenarios based on the regulator's beliefs.

Formulation (6) is closely related to (1) and the methodology that we present in this paper can be used to find an optimal choice for δ . In particular, an equivalent way of representing the range $[\theta_-(\delta), \theta_+(\delta)]$ is in terms of a suitably defined SOS profile function (or "SOS function"), $R_n^W(\cdot)$, as we shall see, so that

$$(7) \quad [\min\{\theta : R_n^W(\theta) \leq \delta\}, \max\{\theta : R_n^W(\theta) \leq \delta\}] = [\theta_-(\delta), \theta_+(\delta)].$$

So, the study of the function $R_n^W(\cdot)$ is key in the analysis of (6) and the selection of δ based on statistical principles, and this leads us to our contributions A)-B) described in the Introduction.

3. BASIC DEFINITIONS

Throughout our development we adopt the convention that all vectors we consider are expressed as columns, so, for example, $x^T = (x_1, \dots, x_l)$ is a row vector in \mathbb{R}^l (here we use x^T to denote the

transpose of x). Also, given a random variable $W \in \mathbb{R}^d$ so that $\mathbb{E}(W) = 0$ and $\mathbb{E}(\|W\|_2^2) < \infty$, we use $Var(W) = \mathbb{E}(WW^T)$ to denote the covariance matrix of W .

3.1. On Wasserstein Distance and Distributional Uncertainty. As we mentioned in the introduction, we utilize the Wasserstein distance of order 2 to describe the distributional uncertainty region. We consider two closed subsets of \mathbb{R}^l , namely \mathcal{X} and \mathcal{Z} . We use the notation $\mathcal{P}(\mathcal{X} \times \mathcal{Z})$ to denote all the Borel probability measures π with support on $\mathcal{X} \times \mathcal{Z}$. Any $\pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Z})$ can be thought of as the joint distribution of a pair of random vectors (X, Z) . We use the notation π_X to denote the marginal distribution of X under π ; similarly, π_Z is the marginal distribution of Z under π .

The Wasserstein distance (of order 2) between the Borel probability measures μ and ν , supported on \mathcal{X} and \mathcal{Z} , respectively, is defined as $\sqrt{D(\mu, \nu)}$, where

$$D(\mu, \nu) = \inf \left\{ \int \int \|x - z\|_2^2 \pi(dx, dz) : \pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Z}), \pi_X = \mu, \pi_Z = \nu \right\}.$$

In simple words, the square of the Wasserstein distance of order 2 (under the Euclidean metric) is defined as the minimum cost of transporting the mass encoded by μ into the mass encoded by ν ; computing the unitary-cost-per-transportation of a unit of mass from x to y as the square of the Euclidean distance between the source (x) and destination (y).

In the sequel, \mathcal{X} and \mathcal{Z} are finite cardinality sets. So, in this case, the evaluation of $D(\mu, \nu)$ is a finite dimensional linear programming problem and so, conceptually, computing $D(\mu, \nu)$ is straightforward. The Wasserstein distance is defined in great generality (for arbitrary metric spaces) as the solution of the Monge-Kantorovich problem with the cost-per-transportation defined in terms of the underlying metric. We refer the reader to [42], for more information on Wasserstein distances. Since we focus on the finite-cardinality case, it is enough with elementary notions of finite dimensional linear programming to understand the definition we use in this paper.

The distributional uncertainty set, $\mathcal{U}_\delta(P_n)$, mentioned in the Introduction to motivate our contributions can then be defined by choosing $\mathcal{X} = \mathcal{X}_n$ and $\mathcal{Z} = \mathcal{Z}_{n+m}$ and letting

$$\mathcal{U}_\delta(P_n) = \mathcal{U}_\delta(P_n; \mathcal{Z}_{n+m}) = \{P : D(P_n, P) \leq \delta\}.$$

3.2. The SOS Profile Function. To motivate the definition of the SOS Profile function, once again, we return to the DRO framework defined in the Introduction. We note from (2) that

$$\Lambda_\delta(P_n) = \{\theta : E_P[h(X, \theta)] = 0 \text{ for } P \in \mathcal{U}_\delta(P_n)\},$$

where $h(X, \theta) = \nabla_{\theta} l(X, \theta)$. So (by convexity) we have that $\theta_* \in \Lambda_\delta(P_n)$ if and only if there exists $P \in \mathcal{U}_\delta(P_n)$ such that

$$(8) \quad E_P[h(X, \theta_*)] = 0.$$

Let $R_n^W(\theta_*)$ be the smallest transportation cost (measured by $D(P_n, P)$) between P_n and any member $P \in \mathcal{P}(\mathcal{Z}_{n+m})$ for which (8). It is easy to reason that $R_n^W(\theta_*) \leq \delta$ if and only if $\theta_* \in \Lambda_\delta(P_n)$. Formally, we have the following definition for the SOS profile function $R_n^W(\theta)$, namely

$$(9) \quad R_n^W(\theta) = \min\{D(P_n, P) : E_P[h(X, \theta)] = 0\}.$$

The goal of this paper is to study the behavior of $R_n^W(\theta_*)$ under the estimating equation assumption

$$(10) \quad E_{P_*}[h(X, \theta_*)] = 0,$$

and the $\{X_i\}_{i=1}^n$ being an i.i.d. sample from P_* . We will formulate our results in terms of the estimating equation (10) for general $h(\cdot)$ (not necessarily arising from an optimization problem).

We consider this more general framework because we believe that our results may be applicable to inference settings other than DRO, for instance, the stress testing framework described earlier. In fact, we now return to such setting to explain how to use the SOS profile function in this case.

3.2.1. The SOS Profile function for stress testing setting. In the stress testing setting described earlier, we wish to select δ just as large to guarantee that $\theta_* := \mathbb{E}_{P_*}(L(X)) \in [\theta_-(\delta), \theta_+(\delta)]$ with a certain degree of confidence, which we shall denote by α .

Therefore, because of equation (7), we are interested in choosing the smallest δ so that

$$(11) \quad P\{\theta_* \in [\theta_-(\delta), \theta_+(\delta)]\} = \mathbf{P}\{R_n^W(\theta_*) \leq \delta\} = \alpha.$$

In other words, δ is chosen to be the α -quantile of the random variable

$$R_n^W(\theta_*) = \min\{D(P_n, P) : E_P[L(X) - \theta_*] = 0\}.$$

Note that this formulation is a particular case of the one introduced in (10) by letting $h(x, \theta) = L(x) - \theta$. For pedagogical reasons, we will present our results first for the SOS profile function for means first (i.e. assuming that $L(x) = x$) and later we move to more general estimating equations.

4. MAIN RESULTS

4.1. SOS Function for Means. We state the following underlying assumption throughout this subsection.

A1): Let us write $\mathcal{X}_n = \{X_1, \dots, X_n\} \subset \mathbb{R}^l$ to denote an i.i.d. sample from a continuous distribution. So, the cardinality of the set \mathcal{X}_n is n .

A2): We also consider an independent i.i.d. sample $\mathcal{Y}_m = \{Y_1, \dots, Y_m\} \subset \mathbb{R}^l$ from a continuous distribution. Throughout our discussion we shall assume that $m = [\kappa n]$ with $\kappa \in [0, \infty)$.

A3): Assume that $\mathbb{E} \|X_1\|_2^2 + \mathbb{E} \|Y_1\|_2^2 < \infty$.

A4): If $l = 1$ we assume that X_i and Y_i have positive densities $f_X(\cdot)$ and $f_Y(\cdot)$. If $l \geq 2$ we assume that X_i and Y_i have differentiable positive densities $f_X(\cdot)$ and $f_Y(\cdot)$, with bounded gradients.

Define $\mathcal{Z}_{n+m} = \{Z_1, \dots, Z_{n+m}\} = \mathcal{X}_n \cup \mathcal{Y}_m$, with $Z_k = X_k$ for $k = 1, \dots, n$, and $Z_{n+j} = Y_j$ for $j = 1, \dots, m$. For any closed set \mathcal{C} let us write $\mathcal{P}(\mathcal{C})$ to denote the set of probability measures supported on \mathcal{C} . So, in particular, a typical element $v_n \in \mathcal{P}(\mathcal{Z}_{n+m})$ takes the form

$$v_n(dz) = \sum_{k=1}^{n+m} v(k) \delta_{Z_k}(dz),$$

where $\delta_{Z_k}(dz)$ is a Dirac measure centered at Z_k . Now, we shall use $\mu_n \in \mathcal{P}(\mathcal{X}_n)$ to denote the empirical measure associated to \mathcal{X}_n , that is,

$$\mu_n(dx) = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}(dx).$$

Given any $\pi \in \mathcal{P}(\mathcal{X}_n \times \mathcal{Z}_{n+m})$ we write $\pi_X \in \mathcal{P}(\mathcal{X}_n)$ to denote the marginal distribution with respect to the first coordinate, namely $\pi_X(dx) = \int_{z \in \mathcal{Z}_{n+m}} \pi(dx, dz)$ and, likewise, we define $\pi_Z \in \mathcal{P}(\mathcal{Z}_{n+m})$ as $\pi_Z(dz) = \int_{x \in \mathcal{X}_n} \pi(dx, dz)$.

We have the following formal definition of the SOS function for estimating means.

Definition 1. The SOS function, $R_n^W(\cdot)$, to estimate $\theta_* = E(X)$ is defined as

$$(12) \quad \begin{aligned} R_n^W(\theta_*) &= \inf \left\{ \int \int \|x - z\|_2^2 \pi(dx, dz) : \right. \\ &\quad \left. \text{s.t. } \pi \in \mathcal{P}(\mathcal{X}_n \times \mathcal{Z}_{n+m}), \pi_X = \mu_n, \pi_Z = \nu_n, \int z \nu_n(dz) = \theta_* \right\}, \\ &= \inf \left\{ \int \int \|x - z\|_2^2 \pi(dx, dz) : \right. \\ &\quad \left. \text{s.t. } \pi \in \mathcal{P}(\mathcal{X}_n \times \mathcal{Z}_{n+m}), \pi_X = \mu_n, \int z \pi_Z(dz) = \theta_* \right\}. \end{aligned}$$

(Here and throughout the paper s.t. abbreviates “subject to”.)

We now state the following asymptotic distributional result for the SOS function.

Theorem 1 (SOS Profile Function Analysis for Means). *In addition to Assumptions A1)-A3), suppose that the covariance matrix of X , $\text{Var}(X)$, exists. The following asymptotic result follows*

- When $l = 1$,

$$nR_n^W(\theta_*) \Rightarrow \sigma^2 \chi_1^2$$

where $\sigma^2 = \text{Var}(X)$.

- When $l = 2$, define $\tilde{Z} \sim N(0, \text{Var}(X)) \in \mathbb{R}^l$, then

$$nR_n^W(\theta_*) \Rightarrow \rho(\tilde{Z}) \left(2 - \tilde{\eta}(\tilde{Z}) \rho(\tilde{Z})\right) \|\tilde{Z}\|_2^2$$

where $\rho := \rho(\tilde{Z})$ is the unique solution to the equation

$$\frac{1}{\rho} = \tilde{g}(\rho \tilde{Z}),$$

and $\tilde{g} : \mathbb{R}^l \rightarrow \mathbb{R}$ is a deterministic function defined as

$$\tilde{g}(x) = \mathbb{P}(\tau \leq \|x\|_2^2),$$

where τ is a random variable satisfying

$$\mathbb{P}(\tau > t) = \mathbb{E}[\exp(-(f_X(X_1) + \kappa f_Y(X_1)) \pi t)].$$

And the function $\tilde{\eta} : \mathbb{R}^l \rightarrow \mathbb{R}$ is a deterministic function given as

$$\tilde{\eta}(x) = \mathbb{E} \left[\max \left(1 - \tau / \|x\|_2^2, 0 \right) \right].$$

- When $l \geq 3$,

$$n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \Rightarrow \frac{2l+2}{l+2} \frac{\|\tilde{Z}\|_2^{1 + \frac{1}{l+1}}}{\left(\mathbb{E} \left[\frac{\pi^{l/2}}{\Gamma(l/2+1)} (f_X(X_1) + \kappa f_Y(X_1)) \right] \right)^{\frac{1}{l+1}}}$$

where $\tilde{Z} \sim N(0, \text{Var}(X)) \in \mathbb{R}^l$.

4.1.1. *Evaluating the Limiting Distribution.* In Theorem 1 and in the rest of our results, the limiting distribution depends on parameters that might be unknown. For example, take the case $l \geq 3$ in Theorem 1. We obtain that

$$(13) \quad n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \Rightarrow \frac{2l+2}{l+2} \frac{\|\tilde{Z}\|_2^{1 + \frac{1}{l+1}}}{(c_0)^{1/(l+1)}},$$

where

$$c_0 := \mathbb{E} \left[\frac{\pi^{l/2}}{\Gamma(l/2+1)} (f_X(X_1) + \kappa f_Y(X_1)) \right]$$

and $\tilde{Z} \sim N(0, \text{Var}(X))$. This situation is quite standard when developing asymptotic distributions for hypothesis testing and the remedy is to simply use any consistent plug-in estimator to estimate the unknown quantities. For instance, we can use

$$\Sigma_n = \frac{1}{n} \sum_{j=1}^n (X_j - E_{P_n}(X_j)) (X_j - E_{P_n}(X_j))^T$$

instead of $\Sigma = \text{Var}(X)$. We can also use any consistent estimator (converging on compact sets and with rapid decay at infinity) for the densities of $f_X(\cdot)$ and $f_Y(\cdot)$, say $f_X^{(n)}(\cdot)$ and $f_Y^{(n)}(\cdot)$, respectively, and estimate c_0 via

$$c_0(n) = E_{P_n} \left[\frac{\pi^{l/2}}{\Gamma(l/2+1)} \left(f_X^{(n)}(X) + \kappa f_Y^{(n)}(X_1) \right) \right],$$

which is consistent as $n \rightarrow \infty$. Because the asymptotic distribution in (13) is continuous in c_0 and Σ , it follows that estimating quantiles based on the plug-in estimators $c_0(n)$ and Σ_n in place of c_0 and Σ leads to asymptotically equivalent specifications for the asymptotic quantiles of $R_n^W(\theta_*)$.

These quantiles, in turn, can be estimated by Monte Carlo using the asymptotic limits, with the plug-in estimators in place. A completely analogous approach can be followed for the asymptotic distributions obtained in our the developments that we discuss next.

4.2. SOS Function for Estimating Equations. Throughout this subsection we assume that **A1)** and **A2)** are in force. Let us assume that $h : R^d \times R^l \rightarrow R^q$, we assume that $q \leq d$. We impose the following assumptions.

B1) Assume $\theta_* \in R^d$ satisfies

$$\mathbb{E} (h (\theta_*, X)) = 0.$$

B2) Furthermore, suppose that

$$\mathbb{E} \|h (\theta_*, X)\|_2^2 < \infty.$$

Our goal is to estimate θ_* under two reasonable SOS function formulations, which we shall discuss. These are “implicit” or “indirect” and “explicit” or “direct” formulations, we will explain their nature next.

4.2.1. Implicit SOS Formulation for Estimating Equations. The first SOS function form for estimating equations is the following, we call it Implicit SOS or Indirect SOS function because the Wasserstein distance is applied to $h (\theta, X_i)$ and $h (\theta, Z_k)$ and thus it implicitly or indirectly induces a notion of proximity among the samples.

Definition 2 (Implicit SOS Profile Function for Estimating Equations). *Let us write $\mathcal{X}_n^h (\theta_*) = \{h (\theta_*, X_i) : X_i \in \mathcal{X}_n\}$ and $\mathcal{Z}_n^h (\theta_*) = \{h (\theta_*, Z_k) : Z_k \in \mathcal{Z}_n\}$ then*

$$(14) \quad R_n^W (\theta_*) = \inf \left\{ \int \int \|h (\theta_*, x) - h (\theta_*, z)\|_2^2 \pi (dx, dz) : \right. \\ \left. s.t. \pi \in \mathcal{P} \left(\mathcal{X}_n^h (\theta_*) \times \mathcal{Z}_n^h (\theta_*) \right), \pi_X = \mu_n, \int h (\theta_*, z) \pi_Z (dz) = 0 \right\}.$$

The Implicit SOS formulation might lead to dimension reductions if l (the dimension of the ambient space of X) is large. In addition, the presence of $h (\cdot)$ in the distance evaluation allows the procedure to use the available information in a more efficient way. For instance, if $h (\theta, x) = |x| - \theta$, then the sign of x is irrelevant for the estimation problem and this will have the effect of increasing the power of the Implicit SOS function relative to the explicit counterpart.

The analysis of the Implicit SOS function follows as a direct consequence of Theorem 1; just redefine $X_i \leftarrow h(\theta_*, X_i)$, $Z_k \leftarrow h(\theta_*, Z_k)$, and apply Theorem 1 directly. Thus the proof of the next result is omitted.

Theorem 2 (Implicit SOS Profile Function Analysis). *Let us use denote $g_X(\cdot)$ is the density for $h(\theta_*, X_i) \in \mathbb{R}^q$ and $g_Y(\cdot)$ for the density of $h(\theta_*, Y_i) \in \mathbb{R}^q$. Then, the Wasserstein profile function defined in Equation (14) have following asymptotic results:*

- When $q = 1$,

$$nR_n^W(\theta_*) \Rightarrow \text{Var}(h(\theta_*, X_1)) \chi_1^2$$

- When $q = 2$, if $\tilde{Z} \sim N(0, \text{Var}(h(\theta_*, X))) \in \mathbb{R}^q$ then

$$nR_n^W(\theta_*) \Rightarrow \rho(\tilde{Z}) \left[2 - \eta(\tilde{Z}) \rho(\tilde{Z}) \right] \|\tilde{Z}\|_2^2,$$

where $\rho(\tilde{Z})$ is the unique solution to the equation

$$\frac{1}{\rho} = \tilde{g}(\rho\tilde{Z}),$$

and $\tilde{g} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic function defined as

$$\tilde{g}(x) = \mathbb{P}(\|x\|_2^2 \geq \tau),$$

where τ is a random variable satisfying

$$\mathbb{P}[\tau > t] = \mathbb{E}[\exp(-[g_X(h(\theta_*, X_1)) + \kappa g_Y(h(\theta_*, X_1))] \pi t)].$$

And the function $\tilde{\eta} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic continuous function given as

$$\tilde{\eta}(x) = \mathbb{E} \left[\max \left(1 - \tau / \|x\|_2^2, 0 \right) \right].$$

- When $q \geq 3$,

$$n^{1/2 + \frac{3}{2q+2}} R_n^W(\theta_*) \Rightarrow \frac{2q+2}{q+2} \frac{\|\tilde{Z}\|_2^{1 + \frac{1}{q+1}}}{\left(\mathbb{E} \left[\frac{\pi^{q/2}}{\Gamma(q/2+1)} (g_X(h(\theta_*, X_1)) + \kappa g_Y(h(\theta_*, X_1))) \right] \right)^{\frac{1}{q+1}}}$$

where $\tilde{Z} \sim N(0, \text{Var}(h(\theta_*, X))) \in \mathbb{R}^q$.

4.2.2. *Explicit SOS Formulation for Estimating Equations.* The second SOS function form we call Explicit SOS function because the Wasserstein distance is explicitly or directly applied to the samples and the scenarios.

Definition 3 (Explicit SOS Profile Function for Estimating Equations).

$$(15) \quad R_n^W(\theta_*) = \inf \left\{ \int \int \|x - z\|_2^2 \pi(dx, dz) : \right. \\ \left. s.t. \pi \in \mathcal{P}(\mathcal{X}_n \times \mathcal{Z}_{(n+m)}), \pi_X = \mu_n, \int h(\theta_*, z) \pi_Z(dz) = 0 \right\}.$$

Both the implicit and explicit SOS have their merits. We have discussed the merit of the implicit SOS formulation. For the Explicit SOS formulation, consider the stress testing application discussed in Section 2.2. The interest of an auditor or a regulator might be on the impact of scenarios on a specific performance measure of interest. One might think that the regulator applies the same stress scenarios to different insurance companies or banks, and therefore the function $h(\cdot)$ is unique to each insurance company. The regulator is interested in the impact of stress testing scenarios on the structure of the bank (modeled by $h(\cdot)$). In this setting, the Explicit SOS formulation appears more appropriate.

While the analysis of the Explicit SOS formulation is also largely based on the techniques developed for Theorem 1, it does require some additional assumptions that are not immediately clear without examining the proof of Theorem 1. In particular, in addition to **A1**), **A2**), **B1**) and **B2**), here we impose the following assumptions.

BE1) Assume that the derivative of $h(\theta_*, x)$ with respect to (w.r.t.) x , $D_x h(\theta_*, \cdot) : R^l \rightarrow R^{q \times l}$, is continuous function of x and the second derivative w.r.t. x is bounded, i.e. $\|D_x^2 h(\theta_*, \cdot)\| < \tilde{K}$ for all x .

BE2) Define $V_i = D_x h(\theta_*, X_i) \cdot D_x h(\theta_*, X_i)^T \in R^{q \times q}$ and assume that $\Upsilon = \mathbb{E}(V_i)$ is strictly positive definite.

We provide the proof of the next result in our technical Section 3.3.

Theorem 3 (Explicit SOS Profile Function Analysis). *Under assumptions A1)-A2), B1)-B2) and BE1)-BE2), we have that (15) satisfies*

- When $l = 1$,

$$nR_n^W(\theta_*) \Rightarrow \tilde{Z}^T \Upsilon^{-1} \tilde{Z}$$

where $\tilde{Z} \sim N(0, \text{Var}(h(\theta_*, X))) \in \mathbb{R}^q$.

- Assume that $l = 2$. Let $\tilde{Z} \sim N(0, \text{Var}(h(\theta_*, X))) \in \mathbb{R}^q$. It is possible to uniquely define deterministic continuous mapping, $\tilde{\zeta} : \mathbb{R}^q \rightarrow \mathbb{R}^q$, such that $\tilde{\zeta}(z)$ is defined via

$$z = -\mathbb{E} \left[V_1 I \left(\tau \leq \tilde{\zeta}^T(z) V_1 \tilde{\zeta}(z) \right) \right] \tilde{\zeta}(z),$$

where τ is independent of V_1 satisfying

$$\mathbb{P}(\tau > t) = \mathbb{E}(\exp(-[f_X(X_1) + \kappa f_Y(X_1)] \pi t)).$$

Then, we have that,

$$nR_n^W(\theta_*) \Rightarrow -2\tilde{Z}^T \tilde{\zeta}(\tilde{Z}) - \tilde{\zeta}^T(\tilde{Z}) \tilde{G}(\tilde{\zeta}(\tilde{Z})) \tilde{\zeta}(\tilde{Z}),$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}^{q \times q}$ is a deterministic continuous mapping defined as,

$$\tilde{G}(\zeta) = \mathbb{E} [V_1 \max(1 - \tau/(\zeta^T V_1 \zeta), 0)].$$

- Suppose that $l \geq 3$. It is possible to uniquely define deterministic continuous mapping $\tilde{\zeta} : \mathbb{R}^q \rightarrow \mathbb{R}^q$, such that

$$z = -\mathbb{E} \left[\frac{\pi^{l/2} (f_X(X_1) + \kappa f_Y(X_1))}{\Gamma(l/2 + 1)} V_1 \cdot \left(\tilde{\zeta}^T(z) V_1 \tilde{\zeta}(z) \right)^l \right] \tilde{\zeta}(z),$$

(note that V_1 is a function of X_1 , so these are correlated). Moreover,

$$n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \Rightarrow -2\tilde{Z}^T \tilde{\zeta}(\tilde{Z}) - \frac{2}{l+2} \tilde{G}(\tilde{Z}),$$

where $\tilde{Z} \sim N(0, \text{Var}(h(\theta_*, X))) \in \mathbb{R}^q$ and $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic continuous function defined as,

$$\tilde{G}(\zeta) = \mathbb{E} \left[\frac{\pi^{l/2}}{\Gamma(l/2 + 1)} (f_X(X_1) + \kappa f_Y(X_1)) (\zeta^T V_1 \zeta)^{l/2+1} \right].$$

We should observe that unlike the implicit formulation, the rate of convergence will only depend on the dimension of data $X_i \in \mathbb{R}^l$, but the shape of asymptotic distribution is determined by the estimating functions $h(\theta_*, X_i) \in \mathbb{R}^q$.

4.3. Plug-in Estimators for SOS Functions. In many situations, for example in the context of stochastic optimization, we are interested in a specific parameter $\theta_* = (\gamma_*, \nu_*) \in R^{d+p}$ such that $\mathbb{E}[h(\gamma_*, \nu_*, X)] = 0$, where $\nu_* \in R^p$ is the nuisance parameter (for example Lagrange multipliers in the setting of constrained optimization).

We shall discuss a method that allows us to deal with the nuisance parameter using a plug-in estimator, while taking advantage of the SOS framework for the estimation of γ_* . After we state our assumptions we will provide the results in this section and the proofs, which follow closely those of Theorems 3 and 2 will be given in Section 7.

Throughout this subsection, let us suppose that $h(\gamma, \nu, x) \in \mathbb{R}^q$. In addition, we impose the following assumptions.

C1) Given γ_* there is a unique $\nu_* \in R^p$ such that

$$(16) \quad \mathbb{E}[h(\gamma_*, \nu, X)] = 0$$

and, given ν_* , we also assume that γ_* satisfies

$$(17) \quad \mathbb{E}[h(\gamma, \nu_*, X)] = 0.$$

C2) We have access to a suitable estimator v_n such that the sequence

$$\left\{ n^{1/2} (v_n - \nu_*) \right\}_{n=1}^{\infty} \text{ is tight,}$$

and

$$\frac{1}{\sqrt{n}} \sum_{i=1}^n h(\gamma_*, v_n, X_i) \Rightarrow \tilde{Z}',$$

for some random variable \tilde{Z}' , as $n \rightarrow \infty$.

C3) Assume that $h(\gamma, \cdot, x)$ is continuously differentiable a.e. (almost everywhere with respect to the Lebesgue measure) in some neighborhood \mathcal{V} around ν_* .

C4) Suppose that there is a function $M(\cdot) : R^l \rightarrow (0, \infty)$ satisfying that

$$\begin{aligned} \|h(\gamma_*, \nu, x)\|_2^2 &\leq M(x) \text{ for a.e. } \nu \in \mathcal{V}, \\ \|D_\nu h(\gamma_*, \nu, x)\|_2^2 &\leq M(x) \text{ for a.e. } \nu \in \mathcal{V}, \end{aligned}$$

and $E(M(X_1)) < \infty$.

4.3.1. **Plug-in Estimators for Implicit SOS Functions.** We are interested in studying the plug-in implicit SOS function (or implicit pseudo-SOS profile function) given by

$$(18) \quad R_n^W(\gamma_*) = \inf \left\{ \int \int \|h(\gamma_*, v_n, x) - h(\gamma_*, v_n, z)\|_2^2 \pi(dx, dz) : \right. \\ \left. \text{s.t. } \pi \in \mathcal{P} \left(\mathcal{X}_n^h(\gamma_*, v_n) \times \mathcal{Z}_{n+m}^h(\gamma_*, v_n) \right), \pi_X = \mu_n, \int h(\gamma_*, v_n, z) \pi_Z(dz) = 0 \right\},$$

where,

$$\mathcal{X}_n^h(\gamma_*, v_n) = \{h(\gamma_*, v_n, x) : x \in \mathcal{X}_n\}, \quad \mathcal{Z}_{n+m}^h(\gamma_*, v_n) = \{h(\gamma_*, v_n, z) : z \in \mathcal{Z}_{(n+m)}\}.$$

We typically will use (16) to find a plug-in estimator v_n . Under suitable assumptions on the consistency and convergence rate of the plug-in estimator we have an asymptotic result for (18), as we indicate next.

Corollary 1 (Plug-in for Implicit SOS Formulation). *Assuming **A1**)-**A2**), and **C1**)-**C4**) hold. Moreover, suppose denote $g_X(\cdot)$ as the density for $h(\gamma_*, v_*, X_i) \in \mathbb{R}^q$ and $g_Y(\cdot)$ for the density of $h(\gamma_*, v_*, Y_i) \in \mathbb{R}^q$. We notice $\tilde{Z}' \in \mathbb{R}^q$ is defined in C2). We obtain that (18) has following asymptotic behavior*

- When $q = 1$,

$$nR_n^W(\gamma_*) \Rightarrow \left(\tilde{Z}'\right)^2.$$

- When $q = 2$,

$$nR_n^W(\gamma_*) \Rightarrow \rho\left(\tilde{Z}'\right) \left[2 - \tilde{\eta}\left(\tilde{Z}'\right) \rho\left(\tilde{Z}'\right)\right] \left\|\tilde{Z}'\right\|_2^2$$

where $\rho\left(\tilde{Z}\right)$ is the unique solution to the equation

$$\frac{1}{\rho} = \tilde{g}\left(\rho\tilde{Z}\right),$$

and $\tilde{g} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic continuous function defined as

$$\tilde{g}(x) = \mathbb{P}\left(\|x\|_2^2 \geq \tau\right).$$

The function $\tilde{\eta} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic continuous function defined as

$$\tilde{\eta}(x) = \mathbb{E}\left[\max\left(1 - \tau/\|x\|_2^2, 0\right)\right].$$

Moreover, \tilde{Z}' is defined in assumption C2) and τ satisfies

$$\mathbb{P}[\tau > t] = \mathbb{E}[\exp(-[g_X(h(\gamma_*, \nu_*, X_1)) + \kappa g_Y(h(\gamma_*, \nu_*, X_1))] \pi t)].$$

- When $q \geq 3$,

$$n^{1/2 + \frac{3}{2q+2}} R_n^W(\gamma_*) \Rightarrow \frac{2q+2}{q+2} \frac{\|\tilde{Z}'\|_2^{1 + \frac{1}{q+1}}}{\left(\mathbb{E}\left[\frac{\pi^{q/2}}{\Gamma(q/2+1)} (g_X(h(\gamma_*, \nu_*, X_1)) + \kappa g_Y(h(\gamma_*, \nu_*, X_1)))\right]\right)^{\frac{1}{q+1}}}.$$

4.3.2. Plug-in Estimators for Explicit SOS Functions. We can also analyze plug-in estimators for Explicit SOS profile functions. We now define the explicit plug-in (or pseudo) SOS function based on (15) as simply plugging-in the nuisance parameter:

$$(19) \quad R_n^W(\gamma_*) = \inf \left\{ \int \int \|x - z\|_2^2 \pi(dx, dz) : \right. \\ \left. \text{s.t. } \pi \in \mathcal{P}\left(\mathcal{X}_n^h(\gamma_*, \nu_n) \times \mathcal{Z}_{n+m}^h(\gamma_*, \nu_n)\right), \pi_X = \mu_n, \int h(\gamma_*, \nu_n, z) \pi_Z(dz) = 0 \right\}.$$

In addition to **C1)** to **C4)** introduced at the beginning of this subsection, we shall impose the following additional assumptions:

C5) Define $\bar{V}_i(\nu_*) = D_x h(\gamma_*, \nu_*, X_i) \cdot D_x h(\gamma_*, \nu_*, X_i)^T$ and assume that $\bar{\Upsilon} = E(\bar{V}_i)$ is strictly positive definite.

C6) The function $M(\cdot)$ from condition **C4)** also satisfies

$$\|D_x h(\gamma_*, \nu, x)\|_2^2 \leq M(x) \text{ for a.e. } \nu \in \mathcal{V}. \\ \|D_\nu D_x h(\gamma_*, \nu, x)\|_2^2 \leq M(x) \text{ for a.e. } \nu \in \mathcal{V}.$$

C7) The second derivative w.r.t. x exist and bounded, i.e. $\|D_x^2 h(\gamma_*, \nu, x)\| < \tilde{K}$ for a.e. $\nu \in \mathcal{V}$ and all x .

Corollary 2 (Plug-in for Explicit SOS Formulation). $X_i \in \mathbb{R}^l$, $h(\gamma, \nu, x) \in \mathbb{R}^q$. Assume that A1)-A2) and C1)-C7) hold. We notice \tilde{Z}' is defined in C2). Then, the SOS profile function defined in Equation (19) has the following asymptotic properties.

- When $l = 1$,

$$nR_n^W(\gamma_*) \Rightarrow \tilde{Z}'^T \bar{\Upsilon}^{-1} \tilde{Z}'.$$

- Suppose that $l = 2$. It is possible to uniquely define deterministic continuous mapping $\tilde{\zeta} : \mathbb{R}^q \rightarrow \mathbb{R}^q$, such that

$$z = -\mathbb{E} \left[\bar{V}_1 I \left(\tau \leq \tilde{\zeta}^T(z) \bar{V}_1 \tilde{\zeta}(z) \right) \right] \tilde{\zeta}(z),$$

where τ is independent of \bar{V}_1 and it satisfies

$$\mathbb{P}(\tau > t) = \mathbb{E}(\exp(-[f_X(X_1) + \kappa f_Y(X_1)] \pi t)).$$

Furthermore,

$$nR_n^W(\theta_*) \Rightarrow -2\tilde{\zeta}^T(\tilde{Z}') \tilde{Z}' - \tilde{\zeta}^T(\tilde{Z}') \tilde{G}(\tilde{\zeta}(\tilde{Z}')) \tilde{\zeta}(\tilde{Z}'),$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}^{q \times q}$ is a deterministic continuous mapping defined as,

$$\tilde{G}(\zeta) = \mathbb{E}[\bar{V}_1 \max(1 - \tau/(\zeta^T \bar{V}_1 \zeta), 0)].$$

- Assume that $l \geq 3$. A deterministic and continuous mapping $\tilde{\zeta} : \mathbb{R}^q \rightarrow \mathbb{R}^q$ can be defined uniquely so that

$$z = -\mathbb{E} \left[\frac{\pi^{l/2} (f_X(X_1) + \kappa f_Y(X_1))}{\Gamma(l/2 + 1)} \bar{V}_1 \left(\tilde{\zeta}^T(z) \bar{V}_1 \tilde{\zeta}(z) \right)^l \right] \tilde{\zeta}(z)$$

(note that \bar{V}_1 is a function of X_1). Moreover,

$$n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \Rightarrow -2\tilde{\zeta}^T(\tilde{Z}') \tilde{Z}' - \frac{2}{l+2} \tilde{G}(\tilde{\zeta}(\tilde{Z}')),$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic continuous function defined as,

$$\tilde{G}(\zeta) = \mathbb{E} \left[\frac{\pi^{l/2}}{\Gamma(l/2 + 1)} (f_X(X_1) + \kappa f_Y(X_1)) (\zeta^T \bar{V}_1 \zeta)^{l/2+1} \right].$$

5. APPLICATION TO STOCHASTIC OPTIMIZATION AND STRESS TESTING

We will provide an application of the SOS inference framework to quantify model uncertainty in the context of stochastic programming. Motivating applications include the evaluation of Conditional Value at Risk (C-VaR) and semi-supervised learning settings, as we shall discuss in the examples below.

We are interested in the value function of a stochastic programming problem formulation via

$$(20) \quad \begin{aligned} C_* &= \min_{\theta} \mathbb{E}[m(\theta, X)] \\ &s.t. \mathbb{E}[\phi(\theta, X)] \leq 0. \end{aligned}$$

We assume that the objective function $\psi(\theta) = \mathbb{E}[m(\theta, X)]$ is a convex function in θ ; while the constraints $\mathbb{E}[\phi(\theta, X)] \leq 0$ specify a convex region in θ ; for example we shall assume that $\phi(\cdot, x)$ is a convex function for any x .

Following [10], the goal is to estimate the optimal value function using the SOS formulation and we will apply a plug-in estimator for θ_* (which is treated as a nuisance parameter). Subsequently, when introducing the Lagrangian relaxation of (20) we will be able to also introduce a plug-in estimator for the associated Lagrange multiplier. Therefore, for simplicity, we shall focus on the unconstrained minimization problem $C_* = \min_{\theta} \{\mathbb{E}[m(\theta, X)]\}$.

The authors in [24, 25] provide a discussion for some potential approaches to derive nonparametric confidence interval (including Empirical Likelihood, a Bayesian approach, Bootstrap and the Delta method). In [24, 25] it is argued that the Empirical Likelihood method tends to have superior finite sample performance, and [7] provides an optimal (in certain sense) specification for the Empirical Likelihood approach. More importantly, in [7] an approach combining Empirical Likelihood and a plug-in estimator for the optimizer is introduced, which avoids solving a non-convex optimization problem introduced in the discussion of [24].

Our goal in this section is to derive a plug-in estimator based on the SOS inference approach introduced in Section 4. The approach that we introduce next is the analog of the plug-in strategy discussed in [7] in order to find a robustified confidence interval for C_* .

The following corollary plays the key role in specifying confidence interval for C_* . The result is a direct extension of Corollary 1 and Corollary 2, provided the following assumptions are in place.

D1): Assume $\psi(\cdot)$ is convex differentiable in θ and there is a unique optimizer θ_* .

D2): Assume that $\psi(\cdot)$ is strongly convex at θ_* , that is, for every θ there exist $\delta > 0$, such that

$$M(\theta) \geq M(\theta_*) + \delta \|\theta - \theta_*\|_2^2.$$

Corollary 3. *Let us consider stochastic programming problem $C_* = \min_{\theta} M(\theta) = \min_{\theta} \mathbb{E}[m(\theta, X)]$.*

Assume that D1)-D2) hold. We consider the estimating equations to be the derivative condition and

value function condition

$$\mathbb{E}[m(\theta_*, X) - C_*] = 0, \text{ and } \mathbb{E}[D_{\theta}m(\theta_*, X)] = 0.$$

For simplicity, let us denote $h(\theta_*, C_*, x) = \left(m(\theta_*, x) - C_*, D_{\theta}m(\theta_*, X)^T\right)^T$. We are interested in C_* only and consider a sample average approximation (SAA) estimator for θ_* to be $\hat{\theta}_{SAA}$. For $h(\cdot, C_*, x)$ we assume C1)-C7) hold. Let us denote $U \sim N(0, \text{Var}(m(\theta_*, X))) \in \mathbb{R}$ and $U(0) = (U, \vec{0})^T \in \mathbb{R}^{d+1}$. Recall the implicit and explicit formulations for general estimating equation SOS function defined in Definition 2 and Definition 3, we have the following asymptotic results.

For the implicit SOS formulation, we have

- When $d = 1$ (estimating equation dimension is $d + 1 = 2$)

$$nR_n^W(C_*) \Rightarrow \rho(U) [2 - \tilde{\eta}(U) \rho(U)] U^2,$$

where $\rho(U)$ is the unique solution to

$$\frac{1}{\rho} = \tilde{g}(\rho U),$$

and $\tilde{g} : \mathbb{R} \rightarrow \mathbb{R}$ is a deterministic continuous function defined as

$$\tilde{g}(x) = \mathbb{P}[x^2 \geq \tau].$$

$\tilde{\eta}(x)$ is also a deterministic function, defined as

$$\tilde{\eta}(x) = \mathbb{E}[\max(1 - \tau/x^2, 0)],$$

and τ satisfies

$$\mathbb{P}[\tau > t] = E(\exp(-g(h(\theta_*, C_*, X_1)) \pi t)).$$

- When $d \geq 2$,

$$n^{1/2 + \frac{3}{2d+4}} R_n^W(C_*) \Rightarrow \frac{2d+4}{d+3} \frac{\|U\|^{1 + \frac{1}{d+2}}}{\mathbb{E}\left[\frac{\pi^{(d+1)/2}}{\Gamma((d+3)/2)} g_X(h(\theta_*, C_*, X_1))\right]^{\frac{1}{d+2}}}.$$

For the explicit formulation, we have following asymptotic results (we use $\zeta_{[1]}$ denote first element of vector ζ)

- When $l = 1$,

$$nR_n^W(C_*) \Rightarrow v_{1,1}U^2,$$

where $v_{1,1}$ is the $(1, 1)$ element of matrix Υ^{-1} .

- Suppose that $l = 2$. It is possible to uniquely define deterministic continuous mapping $\tilde{\zeta} : \mathbb{R}^q \rightarrow \mathbb{R}^q$, such that

$$z = -\mathbb{E} \left[\bar{V}_1 I \left(\tau \leq \tilde{\zeta}^T(z) \bar{V}_1 \tilde{\zeta}(z) \right) \right] \tilde{\zeta}(z),$$

where τ is independent of U satisfying

$$\mathbb{P}(\tau > t) = \mathbb{E}(\exp(-[f_X(X_1) + \kappa f_Y(X_1)]\pi t)).$$

Furthermore,

$$nR_n^W(\theta_*) \Rightarrow -2U\tilde{\zeta}_{[1]} - \tilde{\zeta}^T(U(0))\tilde{G}(\tilde{\zeta})\tilde{\zeta}(U(0)),$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}^{q \times q}$ is a deterministic continuous mapping defined as

$$\tilde{G}(\zeta) = \mathbb{E} \left[\bar{V}_1 \max \left(1 - \frac{\tau}{\zeta^T \bar{V}_1 \zeta}, 0 \right) \right],$$

and U is independent with \bar{V}_1 and τ .

- Assume that $l \geq 3$. A continuous function $\tilde{\zeta} : \mathbb{R}^q \rightarrow \mathbb{R}^q$ can be defined uniquely so that

$$z = -\mathbb{E} \left[\frac{\pi^{l/2} (f_X(X_1) + \kappa f_Y(X_1))}{\Gamma(l/2 + 1)} \bar{V}_1 \left(\tilde{\zeta}^T(z) \bar{V}_1 \tilde{\zeta}(z) \right)^l \right] \tilde{\zeta}(z)$$

(note that \bar{V}_1 is a function of X_1). Moreover,

$$n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \Rightarrow -2U\tilde{\zeta}_{[1]} - \frac{2}{l+2} \tilde{G}(\tilde{\zeta}(U(0))),$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic function given as

$$\tilde{G}(\zeta) = \mathbb{E} \left[\frac{\pi^{l/2}}{\Gamma(l/2 + 1)} f_X(X_1) (\zeta^T \bar{V}_1 \zeta)^{l/2+1} \right],$$

and U and X_1 are independent.

As indicated earlier, the corollary is a special case of Corollary 1 and Corollary 2, so the proof is omitted. The estimating equations correspond to the first order optimality condition (i.e. the first derivative equal to zero), condition and the corresponding optimal value equation. We use sample average approximation estimator as the underlying plug-in estimator.

We notice that for sample average approximation, under assumptions D1)-D2), it has been shown in [38, 40] that the optimizer $\hat{\theta}_{SAA}$ and the optimal value function $\frac{1}{n} \sum_{i=1}^n m(\hat{\theta}_{SAA}, X_i)$ satisfy

$$\begin{aligned}\hat{\theta}_{SAA} - \theta_* &= O(1/n^{1/2}) \\ \frac{1}{n} \sum_{i=1}^n \nabla_{\theta} m(\hat{\theta}_{SAA}, X_i) &= 0, \\ \frac{1}{\sqrt{n}} \sum_{i=1}^n (m(\hat{\theta}_{SAA}, X_i) - C_*) &\Rightarrow N(0, \text{Var}(m(\theta_*, X))).\end{aligned}$$

So, Corollary 2 and Corollary 1 apply.

Similar as the derivation in [7] in the setting of Empirical Likelihood, for the plug-in estimator derived from sample average approximation, if we denote $n^{1/2+3/(2d+4)} R_n^{W(\text{implicit})}(C_*) \Rightarrow R_0^{(\text{implicit})}$ and $n^{1/2+3/(2l+2)} R_n^{W(\text{explicit})}(C_*) \Rightarrow R_0^{(\text{explicit})}$, we can specify a robust 95% confidence interval for C_* under both explicit and implicit formulation by:

$$\text{CI}^{(\cdot)}(C_*) = \left\{ C \in \mathbb{R} \mid n^{\alpha} R_n^{W^{(\cdot)}}(C) \leq R_0^{(\cdot)}(95\%) \right\}$$

where α depends on the formulation and dimension as in Corollary 3 and $R_0^{(\cdot)}(95\%)$ is the upper 95% quantile for $R_0^{(\text{explicit})}$ (or $R_0^{(\text{implicit})}$). The upper/lower bound of confidence interval ($C_{up}^{(\cdot)}/C_{lo}^{(\cdot)}$) can be found by solving the linear programming problem

$$\begin{aligned}C_{up}^{(\cdot)}/C_{lo}^{(\cdot)} &= \max_{\pi(i,j)} / \min_{\pi(i,j)} \left\{ \sum_{i,j=1}^n \pi(i,j) m(\hat{\theta}_{SAA}, X_i) \right. \\ &\quad \left. \text{s.t. } \pi(i,j) \geq 0 \sum_{j=1}^n \pi(i,j) = 1/n; \sum_{i,j=1}^n \pi(i,j) \|X_i - X_j\|_2^2 \leq R_0^{(\cdot)}(95\%) \right\}.\end{aligned}$$

Next, we are going to provide a numerical example in quantifying C-VaR using the methodology we developed above.

Example 1 (Quantify the uncertainty of Conditional Value at Risk (C-VaR)). *In this example we would like to consider find a SOS based 95% confidence interval for conditional value at risk with 90% level. The conditional value at risk with α -level is given as solving the stochastic programming problem:*

$$C\text{-VaR}(\alpha) = \inf_{\theta} \left\{ \theta + \frac{1}{1-\alpha} \mathbb{E} \left[\left(\sum_{k=1}^l X^{(k)} - \theta \right)^+ \right] \right\}.$$

We shall test our method using simulated data under different distributional assumptions. We a sample i.i.d. observations $\{X_i\}_{i=1}^n \subset \mathbb{R}^l$. We will apply the SOS inference procedure to provide a non-parametric confidence interval for C-VaR(90%). In order to verify the coverage probability we use data simulated from normal distribution and Laplace (double exponential) distributions. We consider the case $l = 4$. For the normal distribution setting we assume $X_i \sim N(0, I_{4 \times 4})$, while for Laplace distribution we consider for each $k = 1, \dots, 4$, $X_i^k \sim \text{Laplace}(0, 1)$ and all of these random variables are independent. For these two cases, we can calculate the solution in closed form; for the normal setting the optimizer is $\theta^ = 2.5632$ and optimal value function is $C\text{-VaR}(0.9) = 3.510$; for Laplace setting the optimizer is $\theta^* = 3.497$ with optimal value function equal to $C\text{-VaR}(0.9) = 5.066$. As for this example, we have three approaches in which our SOS procedure can be applied: 1) implicit SOS formulation (ISOS); 2) explicit SOS formulation assuming data being of dimension l (ESOS-O), i.e. $X_i = (X_i^{(1)}, \dots, X_i^{(l)})^T \in \mathbb{R}^l$; 3) explicit formulation assuming data being of dimension 1 (ESOS-C), i.e. $X_i = X_i^{(1)} + \dots + X_i^{(l)} \in \mathbb{R}$. We compare our methods with empirical likelihood method (EL) in [7], nonparametric bootstrap method (BT), and CLT based Delta method (CLT) discussed in Theorem 5.7 [40]. We consider four settings $n = 20, 50, 100$ and 500. For each setting, we repeat the experiment $N = 1000$ times, and note down the empirical coverage probability, mean of upper and lower bounds, and the mean and standard deviation of the interval width for each method. The results are summarized in Table 1 for Normal distribution and Table 2 for Laplace distribution below.*

We can observe that, the three SOS-based approaches tend to have better coverage probabilities in all cases for both distributions comparing to EL, bootstrap and the Delta method. Especially for small sample situations ($n = 10, 20$) EL and all of the SOS-based approaches appear to perform better than everything else. It is discussed in [24] that EL has better finite sample performance compared to the Delta method and bootstrap. We can also notice that all empirical SOS methods tend to have smaller variance compared to others, especially for relatively large sample sizes ($n = 100, 500$).

Between the three SOS methods, we can see that explicit formulations work better comparing to implicit, which follows our discussion after Definition 3. For the two explicit-formulation methods, since we know the data affects the objective function in the form $X_i^{(1)} + \dots + X_i^{(l)}$, we would expect better performance if we combine the data in a single dimension. The numerical results validate our intuition.

n	Method	Coverage Probability	Mean Lower Bound	Mean Upper Bound	Mean Interval Length	S.D. of Length
20	ESOS-C	79.8%	2.59	4.68	2.09	0.79
	ESOS-O	73.4%	2.55	4.65	2.10	1.21
	ISOS	70.8%	2.34	4.87	2.53	0.82
	EL	71.7%	2.61	5.18	2.57	1.92
	BT	55.6%	1.76	3.88	2.12	1.23
	CLT	71.8%	2.01	4.52	2.51	1.87
50	ESOS-C	93.3%	2.67	4.57	1.90	0.30
	ESOS-O	91.0%	2.63	4.54	1.91	0.57
	ISOS	87.3%	2.70	4.75	2.05	0.56
	EL	89.2%	2.81	4.78	1.96	0.83
	BT	82.7%	2.30	4.25	1.95	0.77
	CLT	86.6%	2.47	4.44	1.97	0.78
100	ESOS-C	92.8%	2.84	4.20	1.36	0.08
	ESOS-O	92.4%	2.80	4.22	1.42	0.23
	ISOS	91.3%	2.89	4.32	1.53	0.25
	EL	91.4%	2.94	4.46	1.52	0.43
	BT	90.1%	2.67	4.16	1.49	0.41
	CLT	90.4%	2.75	4.17	1.42	0.39
500	ESOS-C	95.3%	3.16	3.85	0.69	0.01
	ESOS-O	94.9%	3.14	3.77	0.63	0.05
	ISOS	91.2%	3.19	3.88	0.79	0.03
	EL	93.9%	3.20	3.93	0.73	0.08
	BT	94.2%	3.16	3.84	0.68	0.07
	CLT	94.7%	3.17	3.84	0.67	0.08

TABLE 1. $\alpha = 0.9$ —**Conditional Value at Risk with Gaussian Data.** The data X is simulated from 4-dim standard Gaussian distribution, while each dimension is independent. We consider sample size $n = 20, 50, 100$, and 500 . We repeat the experiments $N = 1000$ times and record the coverage probability for the confidence interval (CI), the average upper and lower bound for CI, also the average length and standard deviation for CI. ESOS-C is the explicit formulation of SOS with combined data, ESOS-O stands for explicit-SOS with original data, ISOS is the implicit SOS, EL stands for empirical likelihood, BT is short for nonparametric bootstrap, and CLT is the asymptotic CI method.

Example 2 (Semi-supervised Learning). We consider the DRO formulation for Semi-Supervised Learning (SSL) as suggested in [6]. We formulate the data-driven DRO problem and compare the results for choosing the distributional uncertainty size with the above asymptotic results of SOS function as suggested in Corollary 3. We consider the minibone data set from UCI machine learning data base [4]. We consider logistic regression as our baseline model and form SSL-DRO formulation. For each iteration, we randomly split the data into labeled training set with size $n = 30$, unlabeled training set with size $N - n = 5000$, and testing set with size $n = 125034$. We compare the choice of the uncertainty size using 5-fold cross-validation and SoS asymptotic results. We also include the

n	Method	Coverage Probability	Mean Lower Bound	Mean Upper Bound	Mean Interval Length	S.D. of Length
20	ESOS-C	78.2%	3.57	6.89	3.32	1.10
	ESOS-O	73.8%	3.48	7.10	3.62	1.91
	ISOS	73.1%	3.87	7.55	3.68	1.16
	EL	72.3%	3.56	8.00	4.44	3.30
	BT	58.1%	2.40	6.01	3.61	2.40
	CLT	70.5%	2.53	6.90	4.37	3.24
50	ESOS-C	89.4%	3.78	6.64	2.86	0.42
	ESOS-O	89.3%	3.69	6.78	3.09	0.89
	ISOS	80.1%	4.21	7.17	2.96	0.63
	EL	86.2%	3.89	7.43	3.53	1.66
	BT	80.5%	3.15	6.58	3.43	1.54
	CLT	83.6%	3.29	6.64	3.35	1.54
100	ESOS-C	91.9%	3.93	6.22	2.29	0.14
	ESOS-O	90.8%	3.88	6.30	2.42	0.43
	ISOS	86.6%	4.30	6.78	2.44	0.36
	EL	89.9%	4.10	6.66	2.56	0.86
	BT	86.2%	3.71	6.16	2.45	0.81
	CLT	87.6%	3.76	6.17	2.41	0.79
500	ESOS-C	94.7%	4.53	5.62	1.09	0.06
	ESOS-O	94.3%	4.46	5.59	1.13	0.08
	ISOS	92.1%	4.43	5.61	1.17	0.13
	EL	94.0%	4.53	5.78	1.25	0.18
	BT	92.2%	4.46	5.58	1.12	0.16
	CLT	93.1%	4.45	5.48	1.13	0.15

TABLE 2. $\alpha = 0.9$ —**Conditional Value at Risk with Laplace Data.** The data X is simulated from 4-dim standard Laplace distribution, while each dimension is independent. We consider sample size $n = 20, 50, 100,$ and 500 . We repeat the experiments $N = 1000$ times and record the coverage probability for the confidence interval (CI), the average upper and lower bound for CI, also the average length and standard deviation for CI. ESOS-C is the explicit formulation of SOS with combined data, ESOS-O stands for explicit-SOS with original data, ISOS is the implicit SOS, EL stands for empirical likelihood, BT is short for nonparametric bootstrap, and CLT is the asymptotic CI method.

results for logistic regression and regularized logistic regression as reference. We report the average training error and testing error as log-exponential loss and testing accuracy as accurate classification rate. The mean and standard deviation of the training error, testing error, and testing accuracy are evaluated via 500 independent experiments. The details are included in Table 3.

	Training Error	Testing Error	Testing Accuracy
Logistic Regression	0 ± 0	18.2 ± 10.0	$.678 \pm .059$
LRL1 with CV	$.401 \pm .167$	$.910 \pm .131$	$.717 \pm .041$
DRO-SSL with CV	$.287 \pm .047$	$.609 \pm .054$	$.710 \pm .032$
DRO-SSL with SoS	$.304 \pm .045$	$.682 \pm .048$	$.709 \pm .028$

TABLE 3. Numerical Results for Semi-supervised Learning.

6. CONCLUSIONS AND DISCUSSION

This paper introduces a methodology inspired by Empirical Likelihood, but in which the likelihood ratio function is replaced by a Wasserstein distance. The method that we propose is motivated by

the problem of systematically finding estimators which are incorporate out-of-sample performance in their design. s

In turn, as a motivation for the need of finding these types of estimators we discussed applications to stress testing and semi-supervised learning, which have been discussed in the body of this paper. a Another way in which we can justify our framework is as an approximation approach to solving the problem

$$\min_{\theta \in R^l} \max_{P \in \mathcal{U}_\delta(P_n; \mathbb{R}^d)} E_P[l(X, \theta)].$$

It turns out that in great generality (see [16])

$$\max_{P \in \mathcal{U}_\delta(P_n; \mathbb{R}^d)} E_P[l(X, \theta)] = \min_{\lambda \geq 0} \{\lambda \delta + E_{P_n}[f(X, \theta; \lambda)]\},$$

where $f(x, \theta; \lambda)$ is defined as the solution of an optimization problem involving a parameter $y \in \mathbb{R}^d$ which we refer to as the “inner optimization problem”. The inner optimization problem is typically not convex and therefore it is challenging to solve. There are cases in which the inner optimization problem can be solved in closed form, however, and many of those cases have been documented in the literature in [16]. Our results can be used to suitably calibrate an alternative formulation which may be more tractable given that $y \in \mathbb{R}^d$ is replaced by $y \in \mathcal{Z}_{n,m}$.

There are a number of structural properties in our procedure that are worth investigating and which we plan to explore in future work. For instance, the choice of a particular Wasserstein’s metric, we believe it deserves substantial analysis. In this paper we have chosen the L_2 Wasserstein metric to illustrate our results. The methodology that we propose can be extended to cover other Wasserstein metrics, so on the technical side our work provides the foundations for such extensions. However, it is the impact of such selection what appears to also bring about interesting connections; this already is made evident from our work [8] in which we see that the connections that we mentioned earlier in this discussion (to LASSO and SVM) are made after carefully choosing a natural Wasserstein metric.

In addition, given the parallel philosophy underpinning the method that we proposed (based on Empirical Likelihood), the results on this paper open up a significant amount of research opportunities which are parallel to the substantial literature produced in the area of Empirical Likelihood during the last three decades. We mention, in particular, applications to regression problems (see

[33, 12, 44, 49, 13, 30, 26, 21, 27, 15, 45, 50]), econometrics (see [31, 11, 23, 1, 19, 22]), and additional recent work on stochastic optimization (see [24, 25, 7]). The methodology we propose could be extended to the above applications by simply replacing the Empirical Likelihood function by the SOS function and by applying asymptotic theorems developed in this paper (or natural extensions).

7. METHODOLOGICAL DEVELOPMENT

We shall analyze the limiting distribution of the SOS profile function for means first. In order to gain some intuition let us perform some basic manipulations. First, without loss of generality we assume $\theta_* = 0$, otherwise, we can let $\tilde{X}_i = X_i - \theta_*$ and apply the analysis to the \tilde{X}_i 's.

7.1. The Dual Problem and High-Level Understanding of Results.

The Dual Problem. Let us revisit the definition of (12) and write it as a linear programming problem,

$$(21) \quad R_n^W(\theta_*) = \min_{\pi(i,j) \geq 0} \sum_{i=1}^n \sum_{j=1}^{m+n} \pi(i,j) \|X_i - Z_j\|_2^2$$

$$\text{s.t.} \quad \begin{cases} \sum_{j=1}^{m+n} \pi(i,j) = 1/n, \text{ for all } i \\ \sum_{j=1}^{m+n} (\sum_{i=1}^n \pi(i,j)) Z_j = 0 \end{cases}.$$

We know with probability 1 when $n \rightarrow \infty$, $\bar{0}$ is in the convex hull of Z_j , thus the original linear programming problem is feasible for all n large enough with probability one. Applying the strong duality theorem for linear programming problem, see for example, [28], we can write (21) in the dual formulation as

$$R_n^W(\theta_*) = \max_{\lambda, \tilde{\gamma}_i} \left\{ -\frac{1}{n} \sum_{i=1}^n \tilde{\gamma}_i \right\}$$

$$\text{s.t.} \quad \tilde{\gamma}_i + \|X_i - Z_j\|_2^2 - \lambda^T Z_j \geq 0 \text{ for all } i, j.$$

Let us define $\gamma_i = \tilde{\gamma}_i - \lambda^T Z_i$. By the constraint in the above optimization problem, if we take $i = j$, we have $\tilde{\gamma}_i \geq \lambda^T Z_i$, which is equivalent to $\gamma_i \geq 0$. Then, we can write the optimization problem in γ_i 's as

$$R_n^W(\theta_*) = \max_{\lambda, \gamma_i \geq 0} \left\{ -\lambda^T \bar{X}_n - \frac{1}{n} \sum_{i=1}^n \gamma_i \right\}$$

$$\text{s.t.} \quad -\lambda^T X_i - \gamma_i \leq -\lambda^T Z_j + \|X_i - Z_j\|_2^2, \text{ for all } i, j.$$

We can further simplify the constraints by minimizing over j , while keeping i fixed, therefore arriving to the simplified dual formulation

$$(22) \quad R_n^W(\theta_*) = \max_{\lambda, \gamma_i \geq 0} \left\{ -\lambda^T \bar{X}_n - \frac{1}{n} \sum_{i=1}^n \gamma_i \right\}$$

$$\text{s.t. } -\lambda^T X_i - \gamma_i \leq \inf_j \left\{ -\lambda^T Z_j + \|X_i - Z_j\|_2^2 \right\}, \text{ for all } i.$$

High-Level Intuitive Analysis. At this point we can perform a high-level analysis which can help us guide our intuition about our result. First, consider an approximation performed by freeing the Z_j in the constraints of (22), in this portion the reader can appreciate that the assumption that X_j has a density yields

$$(23) \quad \inf_j \left\{ \|Z_j - (X_i + \lambda/2)\|_2^2 \right\} = \epsilon_n(i),$$

where error $\epsilon_n(i)$ is small as $n \rightarrow \infty$ and it will be discussed momentarily. Equation (23) is equivalent to

$$\inf_j \left\{ -\lambda^T Z_j + \|X_i - Z_j\|_2^2 \right\} = -\lambda^T X_i - \|\lambda\|_2^2 / 4 + \epsilon_n(i).$$

Hence, the i -th constraint in (22) takes the form

$$-\lambda^T X_i - \gamma_i \leq -\lambda^T X_i - \|\lambda\|_2^2 / 4 + \epsilon_n(i),$$

and thus (22) can ultimately be written as

$$(24) \quad R_n^W(\theta_*) = - \min_{\lambda, \gamma_i \geq 0} \left\{ \lambda^T \bar{X}_n + \frac{1}{n} \sum_{i=1}^n \gamma_i \right\}$$

$$\text{s.t. } \gamma_i \geq (1 - \epsilon_n(i)) \|\lambda\|_2^2 / 4 \text{ for all } i.$$

Now, observe that if Z_j was free, then the optimal choice in (23) would be $a_*(i) = X_i + \lambda/2$.

Consider the case $l = 1$, in this case it is not difficult to convince ourselves (because of the existence of a density) that $\epsilon_n(i) = O_p(1/n)$ as $n \rightarrow \infty$ (basically with a probability which is bounded away from zero there will be a point in the sample $\{Z_1, \dots, Z_{m+n}\} \setminus X_i$ which is within $O_p(1/n)$ distance of $a_*(i)$). Then it is intuitive to expect the approximation

$$R_n^W(\theta_*) = - \min_{\lambda} \left\{ \lambda^T \bar{X}_n + (1 + O_p(1/n)) \lambda^2 / 4 \right\},$$

which formally yields an optimal selection

$$\lambda_* = -\frac{\bar{X}_n}{(1/2 + O_p(1/n))} = -2\bar{X}_n + O_p\left(1/n^{3/2}\right),$$

and therefore we expect, due to the Central Limit Theorem (CLT), that

$$(25) \quad nR_n^W(\theta_*) = n\bar{X}_n^2 + nO_p\left(1/n^{3/2}\right) \Rightarrow Var(X) \chi_1^2,$$

as $n \rightarrow \infty$. This analysis will be made rigorous in the next subsection.

Let us continue our discussion in order to elucidate why the rate of convergence in the asymptotic distribution of $R_n^W(\theta_*)$ depends on the dimension. Such dependence arises due to the presence of the error term $\epsilon_n(i)$. Note that in dimension $l = 2$, we expect $\epsilon_n(i) = O_p(1/n^{1/2})$; this time, with positive probability (uniformly as $n \rightarrow \infty$) we must have that a point in the sample $\{Z_1, \dots, Z_{m+n}\} \setminus X_i$ is within $O_p(1/n^{1/2})$ distance of $a_*(i)$ (because the probability that X_i lies inside a ball of size $1/n^{1/2}$ around a point a is of order $O(1/n^{1/2})$). Therefore, in the case $l = 2$ we formally have $\lambda_*(n) = -\bar{X}_n + O_p(n^{-1/2})$, but we know from the CLT that $\bar{X}_n = O_p(n^{-1/2})$ so this time contribution of $\epsilon_i(n)$ is non-negligible.

Similarly, when $l \geq 3$ this simple analysis allows us to conclude that the contribution of $\epsilon_i(n) = O(n^{-1/l})$ will actually dominate the behavior of $\lambda_*(n)$ and this explains why the rate of convergence depends on the dimension of the vector X_i , namely, l . The specific rate depends on a delicate analysis of the error being $\epsilon_i(n)$ which is performed in the next sub-section. A key technical device introduced in our proof technique is a Poisson point process which approximates the number of points in $\{Z_1, \dots, Z_{m+n}\} \setminus X_i$ which are within a distance of size $O(n^{-1/l})$ from the free optimizer $a_*(i)$ arising in (23).

The introduction of this point process, which in turn is required to analyze $\epsilon_i(n)$, makes the proof of our result substantially different from the standard approach used in the theory of Empirical Likelihood (see [34, 32, 36]), which builds on [46].

7.2. Proof of Theorem 1. The proof of Theorem 1 is divided in several steps which we will carefully record so that we can build from these steps in order to prove the remaining results in the paper.

7.2.1. Step 1 (Dual Formulation and Lower Bound): Using the same transformations introduced in (21) we can obtain the dual formulation of the SOS profile function (12), which is a natural adaptation of (22), namely

$$R_n^W(\theta_*) = \max_{\lambda, \gamma_i \geq 0} \left\{ -\lambda \bar{X}_n - \frac{1}{n} \sum_{i=1}^n \gamma_i \right\}$$

s.t. $-\lambda^T X_i - \gamma_i \leq \inf_j \left\{ -\lambda^T Z_j + \|X_i - Z_j\|_2^2 \right\}$, for all i .

Observe that the following lower bound applies by optimizing over $a \in R^l$ instead of $a = Z_j \in \mathcal{Z}_n$, therefore obtaining the lower bound

$$\begin{aligned} \inf_j \left\{ -\lambda^T Z_j + \|X_i - Z_j\|_2^2 \right\} &\geq \inf_a \left\{ -\lambda^T a + \|X_i - a\|_2^2 \right\} \\ &= -\lambda^T X_i - \|\lambda\|_2^2 / 4, \end{aligned}$$

with the optimizer $a_*(X_i, \lambda) = X_i + \lambda/2$.

7.2.2. Step 2 (Auxiliary Poisson Point Processes): Then, for each i let us define a point process,

$$N_n^{(i)}(t, \lambda) = \# \left\{ Z_j : \|Z_j - a_*(X_i, \lambda)\|_2^2 \leq t^{2/l}/n^{2/l}, Z_j \neq X_i \right\},$$

(recall that $Z_j \in R^l$). Observe that, actually, we have

$$N_n^{(i)}(t, \lambda) = N_n^{(i)}(t, \lambda, 1) + N_n^{(i)}(t, \lambda, 2),$$

where

$$\begin{aligned} N_n^{(i)}(t, \lambda, 1) &= \# \left\{ X_j : \|X_j - a_*(X_i, \lambda)\|_2^2 \leq t^{2/l}/n^{2/l}, X_j \neq X_i \right\}, \\ N_n^{(i)}(t, \lambda, 2) &= \# \left\{ Y_j : \|Y_j - a_*(X_i, \lambda)\|_2^2 \leq t^{2/l}/n^{2/l} \right\}. \end{aligned}$$

For any X_j with $j \neq i$, conditional on X_i , due to the assumption of density and the formula for the volume of l -dimensional ball ([37]), we have,

$$\begin{aligned} &\mathbb{P} \left[\|X_j - a_*(X_i, \lambda)\|_2^2 \leq t^{2/l}/n^{2/l} \mid X_i \right] \\ &= f_X(a_*(X_i, \lambda)) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \frac{t}{n} + o_p(t/n) = f_X(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \frac{t}{n} + o_p(t/n). \end{aligned}$$

Similarly,

$$\mathbb{P} \left[\|Y_j - a_*(X_i, \lambda)\|_2^2 \leq t^{2/l}/n^{2/l} \mid X_i \right] = f_Y(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \frac{t}{n} + o_p(t/n).$$

Since we have i.i.d. structure for the data points, thus we know, $N_n^{(i)}(t, \lambda, 1)$ and $N_n^{(i)}(t, \lambda, 2)$ conditional on X_i follow binomial distributions,

$$\begin{aligned} N_n^{(i)}(t, \lambda, 1) \mid X_i &\sim \text{Bin} \left(f_X(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(d/2 + 1)} \frac{t}{n} + o_p(t/n), n - 1 \right), \\ N_n^{(i)}(t, \lambda, 2) \mid X_i &\sim \text{Bin} \left(f_Y(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \frac{t}{n} + o_p(t/n), [\kappa n] \right), \\ N_n^{(i)}(t, \lambda) &= N_n^{(i)}(t, \lambda, 1) + N_n^{(i)}(t, \lambda, 2). \end{aligned}$$

Moreover, we have as $n \rightarrow \infty$,

$$f_X(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \frac{t}{n} \times (n - 1) \rightarrow f_X(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} t.$$

Thus, by Poisson approximation to the binomial distribution, we have the weak convergence result

$$N_n^{(i)}(\cdot, \lambda, 1) \mid X_i \Rightarrow \text{Poisson} \left(f_X(X_i + \lambda/2) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \cdot \right),$$

in $D[0, \infty)$.

So we have that $N_n^{(i)}(\cdot, \lambda, 1)$, conditional on X_i , is asymptotically a time homogeneous Poisson process with rate $f_X(X_i + \lambda/2) \pi^{d/2}/\Gamma(d/2 + 1)$. Similar considerations apply to $N_n^{(i)}(\cdot, \lambda, 2) \mid X_i$ which yield that

$$N_n^{(i)}(\cdot, \lambda) \mid X_i \Rightarrow \text{Poi}(\Lambda(X_i, \lambda) \cdot),$$

where

$$\Lambda(X_i, \lambda) = [f_X(X_i + \lambda/2) + \kappa f_Y(X_i + \lambda/2)] \frac{\pi^{l/2}}{\Gamma(l/2 + 1)}.$$

Let us write $T_i(n)$ to denote the first arrival time of $N_n^{(i)}(\cdot, \lambda)$, that is,

$$T_i(n) = \inf \left\{ t \geq 0 : N_n^{(i)}(t, \lambda) \geq 1 \right\}$$

Then, we can specify the survival function for $T_i(n)$ to be:

$$(26) \quad \mathbb{P}[T_i(n) > t \mid X_i] = \mathbb{P}\left[N_n^{(i)}(t, \lambda) = 0 \mid X_i\right] = \exp(-\Lambda(X_i, \lambda)t) \left(1 + O\left(1/n^{1/l}\right)\right),$$

uniformly on t over compact sets. The error rate $O(1/n^{1/l})$ is obtained by a simple Taylor expansion of the exponential function applied to the middle term in the previous string of equalities. Motivated by the form in the right hand side of (26) we define $\tau_i(X_i)$ to be a random variable such that

$$\mathbb{P}[\tau_i(X_i) > t \mid X_i] = \exp(-\Lambda(X_i, \lambda)t),$$

and we drop the dependence on X_i and the subindex i when we refer to the unconditional version of $\tau_i(X_i)$, namely

$$\mathbb{P}[\tau > t] = \mathbb{E}[\exp(-\Lambda(X_1, \lambda)t)].$$

We finish Step 2 with the statement of two technical lemmas. The first provides a rate of convergence for the Glivenko-Cantelli theorem associated to the sequence $\{T_i(n)\}_{i=1}^n$.

Lemma 1. *For any $T \in (0, \infty)$ (deterministic) and $\alpha \in (0, 2]$, we have that*

$$\overline{\lim}_{n \rightarrow \infty} \mathbb{E} \left(\sup_{t \in [0, T]} \left| \frac{1}{n^{1/2}} \sum_{i=1}^n (I(T_i(n) \leq t) - \mathbb{P}[T_i(n) \leq t]) \right| \right) < \infty,$$

and

$$\overline{\lim}_{n \rightarrow \infty} \mathbb{E} \left(\sup_{t \in [0, T]} \left| \frac{1}{n^{1/2}} \sum_{i=1}^n (\max(t^2 - T_i(n)^\alpha, 0) - \mathbb{E}[\max(t^2 - T_i(n)^\alpha, 0)]) \right| \right) < \infty.$$

The second technical lemma deals with local properties of the distribution of $T_i(n)$. The proofs of both of these technical results are given at the end of the proof of Theorem 1, in Section 7.2.7.

Lemma 2. *For $X_i \in \mathbb{R}^l$ and any finite t , we have the Poisson approximation to binomial as:*

$$\mathbb{P}[T_i(n) \leq t] - \mathbb{P}[\tau \leq t] = O(t^{1+1/l}/n^{1/l}),$$

and

$$\mathbb{P}[T_i(n) \leq t] - \mathbb{P}[\tau \leq t] = \mathbb{P}[\tau > t] O(1/n^l).$$

7.2.3. **Step 3 (Closest Point and SOS Function Simplification):** Note that the i -th constraint, namely,

$$-\gamma_i \leq \lambda^T X_i + \inf_j \left\{ -\lambda^T Z_j + \|X_i - Z_j\|_2^2 \right\},$$

can be written as

$$\begin{aligned} -\gamma_i &\leq \inf_j \left\{ -\lambda^T (Z_j - X_i) + \|X_i - Z_j\|_2^2 \right\} \\ &= -\|\lambda\|_2^2 / 4 + \inf_j \left\{ \|Z_j - (\lambda/2 + X_i)\|_2^2 \right\} \\ &= -\|\lambda\|_2^2 / 4 + T_i^{2/l}(n) / n^{2/l}. \end{aligned}$$

However, since $\gamma_i \geq 0$ we must have that

$$-\gamma_i \leq -\|\lambda\|_2^2 / 4 + \min \left(T_i^{2/l}(n) / n^{2/l}, \|\lambda\|_2^2 / 4 \right).$$

Therefore, the SOS profile function takes the form

$$R_n^W(\theta_*) = \max_{\lambda} \left\{ -\lambda^T \bar{X}_n - \|\lambda\|_2^2 / 4 + \frac{1}{n} \sum_{i=1}^n \min \left(\frac{T_i^{2/l}(n)}{n^{2/l}}, \|\lambda\|_2^2 / 4 \right) \right\}.$$

To simplify the notation, let us redefine $\lambda \leftarrow 2\lambda$ then we have that the simplified SOS profile function becomes:

$$(27) \quad R_n^W(\theta_*) = \max_{\lambda} \left\{ -2\lambda^T \bar{X}_n - \frac{1}{n} \sum_{i=1}^n \max \left(\|\lambda\|_2^2 - \frac{T_i^{2/l}(n)}{n^{2/l}}, 0 \right) \right\}.$$

7.2.4. **Step 4 (Case $l = 1$):** When $l = 1$, let's denote $\sqrt{n}\bar{X}_n = Z_n$ and $\sqrt{n}\lambda = \zeta$, where by CLT we can show $Z_n \Rightarrow \tilde{Z} \sim N(0, \sigma^2)$, where when $l = 1$ we have $\sigma^2 = \Sigma$. Then, as $n \rightarrow \infty$, we have:

$$\begin{aligned} nR_n^W(\theta_*) &= \max_{\zeta} \left\{ -2\zeta Z_n - \frac{1}{n} \sum_{i=1}^n \max(\zeta^2 - T_i^2(n) n^{-1}, 0) \right\} \\ &= \max_{\zeta} \left\{ -2\zeta Z_n - \mathbb{E} [\max(\zeta^2 - T_i^2(n) n^{-1}, 0)] \right\} + o_p(1) \end{aligned}$$

The second equation follows the estimate in (Lemma 1). We know the objective function as a function of ζ is a strictly convex function. Since as $\zeta = b|Z_n|$ with $b \rightarrow \pm\infty$ implies that the objective function will tend to $-\infty$, we conclude that the sequence of global optimizers is compact and each optimizer (i.e. for each n) could be characterized by the first order optimality condition almost surely. To make the analysis more clear, let us denote the expectation in the maximization

problem to be $g(\zeta, n)$, as a function of ζ , i.e.

$$G(\zeta, n) = \mathbb{E} [\max(\zeta^2 - T_i^2(n) n^{-1}, 0)],$$

which is a deterministic function of ζ and for any n it is convex. Moreover, the derivative of $G(\zeta, n)$ is,

$$g(\zeta, n) = \nabla_{\zeta} G(\zeta, n) = 2\zeta \mathbb{P}(T_i(n) \leq n\zeta^2).$$

We need to notice that while taking the derivative we require exchanging the derivative and expectation, this can be done true hereby the Dominated Convergence Theorem since

$$\delta^{-1} \left| \max\left((\zeta + \delta)^2 - T_i^2(n) n^{-1}, 0\right) - \max\left(\zeta^2 - T_i^2(n) n^{-1}, 0\right) \right| \leq 2|\zeta|,$$

for all $\delta > 0$. We can take the derivative with respect to ζ in $-2\zeta Z_n - G(\zeta, n)$ and set it to zero, as $n \rightarrow \infty$ we obtain

$$Z_n = -\zeta P(T_i(n) \leq n\zeta^2) = -\zeta P(\tau \leq n\zeta^2) + o_p(1) = -\zeta + o_p(1).$$

This estimate follows the second result of Lemma 2. Therefore, the optimizer ζ_n^* , satisfies $\zeta_n^* = -Z_n + o_p(1)$, as $n \rightarrow \infty$. Then, we plug it into the objective function to obtain that the scaled SOS profile function satisfies

$$nR_n^W(\theta_*) = 2Z_n^2 - G(Z_n, n) + o_p(1) \text{ as } n \rightarrow \infty.$$

We should notice $G(Z_n, n)$ is a function defined via expectation and evaluated at Z_n , thus it is a random variable depends on Z_n . By definition and $E[|X|] = \int_0^\infty \mathbb{P}[|X| \geq t] dt$, we know as $n \rightarrow \infty$,

$$\begin{aligned} G(\zeta, n) &= \int_0^{\zeta^2} \mathbb{P}[T_i^2(n) \leq n(\zeta^2 - t)] dt \\ &= \int_0^{\zeta^2} \mathbb{P}[\tau^2(n) \leq n(\zeta^2 - t)] dt + o(1) \\ &= \int_0^{\zeta^2} 1 dt + o(1) = \zeta^2 + o(1), \end{aligned}$$

where the second equality is derived from the second argument of Lemma 2. Then for the SOS profile function, it becomes,

$$nR_n^W(\theta_*) = 2Z_n^2 - Z_n^2 + o_p(1) = Z_n^2 + o_p(1) \text{ as } n \rightarrow \infty.$$

Applying the continuous mapping theorem and the Central Limit Theorem for Z_n , we have

$$nR_n^W(\theta_*) \Rightarrow \sigma^2 \chi_1^2.$$

7.2.5. **Step 5 (Case $l = 2$):** Once again we introduce the substitution $\zeta = \sqrt{n}\lambda$ and $\sqrt{n}\bar{X}_n = Z_n$ into (27). Then, scaling the profile function by n , as $n \rightarrow \infty$ we have

$$\begin{aligned} nR_n^W(\theta_*) &= \max_{\zeta} \left\{ -2\zeta^T Z_n - \frac{1}{n} \sum_{i=1}^n \max \left(\|\zeta\|_2^2 - T_i(n), 0 \right) \right\} \\ (28) \quad &= \max_{\zeta} \left\{ -2\zeta^T Z_n - \mathbb{E} \left[\max \left(\|\zeta\|_2^2 - T_i(n), 0 \right) \right] \right\} + o_p(1), \end{aligned}$$

where the previous estimate follows by applying Lemma 1 (the error is obtained by localizing ζ on a compact set, which is valid because the sequence of global optimizers is easily seen to be tight). The objective function is strictly convex as a function of ζ and we know when $\|\zeta\|_2 \rightarrow \infty$ the objective function tends to $-\infty$, thus each global maximizer (for each n) can be characterized by the first order optimality condition almost surely. Similar as Case $l = 1$, let us denote

$$G(\zeta, n) = \mathbb{E} \left[\max \left(\|\zeta\|_2^2 - T_i(n), 0 \right) \right].$$

It is a continuous differentiable and convex function in ζ and with derivative equals

$$g(\zeta, n) = \nabla_{\zeta} G(\zeta, n) = 2\zeta \mathbb{P} \left[\|\zeta\|_2^2 \geq T_i(n) \right] = 2\zeta \mathbb{P} \left[\|\zeta\|_2^2 \geq \tau \right] + o(1) \text{ as } n \rightarrow \infty,$$

where the first equality requires applying the Dominated Convergence Theorem, as in the case $l = 1$ and the second estimate follows the first argument in Lemma 2. Combining the above estimation, we have the first order optimality condition becomes

$$(29) \quad Z_n = -\zeta \mathbb{P} \left[\|\zeta\|_2^2 \geq \tau \right] + o_p(1) = -\zeta \tilde{g}(\zeta) + o_p(1) \text{ as } n \rightarrow \infty,$$

where $\tilde{g}(\zeta) = \mathbb{P} \left[\|\zeta\|_2^2 \geq \tau \right]$ is a deterministic function of ζ . Using equation (29), we conclude that the optimizer ζ_n^* , satisfies $\zeta_n^* = -\rho Z_n + o_p(1)$, for some ρ . In turn, plugging in this representation

into equation (29), as $n \rightarrow \infty$ we have

$$\|\zeta_n^*\|_2 \tilde{g}(\zeta_n^*) + o_p(1) = \|Z_n\|_2.$$

Sending $n \rightarrow \infty$, we conclude that ρ is the unique solution to

$$(30) \quad \frac{1}{\rho} = \tilde{g}(\rho \tilde{Z}).$$

Since the objective function is strictly convex and the above equation is derived from first order optimality condition, we know the solution exists and is unique (alternatively we can use the continuity and monotonicity of left and right hand side of (30), to argue the existence and uniqueness).

Let us plug in the optimizer back to the objective function and we can see the scaled SOS profile function becomes

$$nR_n^W(\theta_*) = 2\rho \left(\|\tilde{Z}\|_2^2 \right) \|Z_n\|_2^2 - G(\zeta_n^*, n) + o_p(1).$$

For a positive random variable Y , we have: $\mathbb{E}[Y] = \int_0^\infty \mathbb{P}[Y \geq t] dt$. Therefore, for ζ in a compact set, as $n \rightarrow \infty$ we have the following estimate

$$\begin{aligned} G(\zeta, n) &= \int_0^{\|\zeta\|_2^2} \mathbb{P}[\|\zeta\|_2^2 - T_i(n) \geq t] dt \\ &= \int_0^{\|\zeta\|_2^2} \mathbb{P}[\|\zeta\|_2^2 - \tau \geq t] dt + o(1) \\ &= \|\zeta\|_2^2 \int_0^1 \mathbb{P}[1 - \tau/\|\zeta\|_2^2 \geq s] ds + o(1) \\ &= \|\zeta\|_2^2 \mathbb{E} \left[\max \left(1 - \tau/\|\zeta\|_2^2, 0 \right) \right] + o(1) \\ &= \|\zeta\|_2^2 \tilde{\eta}(\zeta) + o(1), \end{aligned}$$

where we define $\tilde{\eta}(\zeta) = \mathbb{E} \left[\max \left(1 - \tau/\|\zeta\|_2^2, 0 \right) \right]$ is a deterministic continuous function of ζ . The second equation follows the first result of Lemma 2. Finally combine $G(\zeta, n)$ and the first term, using the CLT and continuous mapping theorem, where we denote $Z_n \Rightarrow \tilde{Z} \sim N(0, \text{Var}(X))$, as $n \rightarrow \infty$ we have:

$$\begin{aligned} nR_n^W(\theta_*) &= 2\rho \left(\tilde{Z} \right) \|Z_n\|_2^2 - \rho \left(\tilde{Z} \right)^2 \tilde{\eta}(Z_n) \|Z_n\|_2^2 + o_p(1) \\ &\Rightarrow 2\rho \left(\tilde{Z} \right) \|\tilde{Z}\|_2^2 - \rho \left(\tilde{Z} \right)^2 \tilde{\eta}(\tilde{Z}) \|\tilde{Z}\|_2^2. \end{aligned}$$

7.2.6. **Step 6 (Case $l \geq 3$):** For simplicity, let us write $\sqrt{n}\bar{X}_n = Z_n$ and $n^{\frac{3}{2l+2}}\lambda = \zeta$, then as $n \rightarrow \infty$ we have

$$\begin{aligned} & n^{1/2+\frac{3}{2l+2}}R_n^W(\theta_*) \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} \frac{1}{n} \sum_{i=1}^n \max \left(\left\| \frac{\zeta}{n^{(\frac{3}{2l+2}-\frac{1}{l})}} \right\|_2^2 - T_i^{2/l}(n), 0 \right) \right\} \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} \mathbb{E} \left[\max \left(\left\| \frac{\zeta}{n^{(\frac{3}{2l+2}-\frac{1}{l})}} \right\|_2^2 - T_1^{2/l}(n), 0 \right) \right] \right\} + o_p(1). \end{aligned}$$

The estimate in the previous display is due to an application of Lemma 1. Similar as for the lower dimensional case, let us denote

$$G(\zeta, n) = n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} \mathbb{E} \left[\max \left(\left\| \frac{\zeta}{n^{(\frac{3}{2l+2}-\frac{1}{l})}} \right\|_2^2 - T_1^{2/l}(n), 0 \right) \right],$$

being a deterministic function continuous and differentiable as a function of ζ . As we discussed for the case $l = 2$ case, the objective function is strictly convex in ζ , the global optimizers are not only tight, but each optimizer is also characterized by first order optimality conditions almost surely. We can apply the Dominated Convergence Theorem, as we discussed for $l = 1$ and the gradient of $G(\zeta, n)$ has the following estimate as $n \rightarrow \infty$,

$$\begin{aligned} g(\zeta, n) &= \nabla_{\zeta} G(\zeta, n) = 2n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} \zeta \mathbb{P} \left[T_i(n) \leq \left\| \zeta n^{-(\frac{3}{2l+2}-\frac{1}{l})} \right\|_2^l \right] \\ &= 2n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} \zeta \mathbb{P} \left[\tau \leq \left\| \zeta n^{-(\frac{3}{2l+2}-\frac{1}{l})} \right\|_2^l \right] + o(1). \end{aligned}$$

The second equality estimate is considering ζ within a compact set and the derivation follows the first argument in Lemma 2. Then the first order optimality condition for the SOS profile function becomes,

$$Z_n = -n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} \zeta \mathbb{P} \left[\tau \leq \left\| \zeta n^{-(\frac{3}{2l+2}-\frac{1}{l})} \right\|_2^l \right] + o(1) \text{ as } n \rightarrow \infty.$$

For notation simplicity, let us define

$$\kappa_n = \zeta n^{-(\frac{3}{2l+2}-\frac{1}{l})}.$$

We can observe for ζ in a compact set, $\left\| \zeta n^{-(\frac{3}{2l+2}-\frac{1}{l})} \right\|_2^l = \|\kappa_n\|_2^l \rightarrow 0$, as $n \rightarrow \infty$, then we can write

$$\begin{aligned} \mathbb{P} \left[\tau \leq \|\kappa_n\|_2^l \right] &= 1 - \mathbb{P} \left[\tau > \|\kappa_n\|_2^l \right] = 1 - \mathbb{E} \left[\mathbb{P} \left[\tau > \|\kappa_n\|_2^l \mid X_1 \right] \right] \\ &= \mathbb{E} \left[1 - \exp \left(- \frac{\pi^{l/2} (f_X(X_1 + \kappa_n) + f_Y(X_1 + \kappa_n))}{\Gamma(l/2 + 1)} \|\kappa_n\|_2^l \right) \right] \\ &= \mathbb{E} \left[\frac{\pi^{l/2}}{\Gamma(l/2 + 1)} [f_X(X_1) + f_Y(X_1)] \|\kappa_n\|_2^l \right] + o_p \left(n^{-(\frac{3l}{2l+2}-1)} \right) \\ &= C \|\kappa_n\|_2^l + o_p \left(n^{-(\frac{3l}{2l+2}-1)} \right), \end{aligned}$$

where we denote

$$C = \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \mathbb{E} [f_X(X_1) + f_Y(X_1)].$$

Plug it back into the optimizer, and as $n \rightarrow \infty$ we have:

$$Z_n = -C n^{(1/2-\frac{3}{2l+2})} n^{-(\frac{3l}{2l+2}+1)} \zeta \|\zeta\|_2^l + o_p(1) = -C \zeta \|\zeta\|_2^l + o_p(1).$$

We know that within the objective function, the second term is only based on the L_2 norm of ζ , thus to maximize the objective function we will asymptotically select $\zeta_n^* = -c_* Z_n (1 + o(1))$, where $c_* > 0$ is suitably chosen, thus, we conclude that the optimizer takes the form,

$$\zeta_n^* = -Z_n \|Z_n\|_2^{(\frac{1}{l+1}-1)} / C^{\frac{1}{l+1}} + o_p(1).$$

Plugging-in the optimizer back into the objective function, as $n \rightarrow \infty$ we have:

$$n^{1/2+\frac{3}{2l+2}} R_n^W(\theta_*) = -2\zeta_n^{*T} Z_n - G(\zeta_n^*, n) + o_p(1).$$

Let us focus on the analysis of $G(\zeta, n)$ in a compact set. By definition, we can notice that inside the previous expectation there is a positive random variable bounded by $\left\| \frac{\zeta}{n^{(\frac{3}{2l+2}-\frac{1}{l})}} \right\|_2^2 = \|\kappa_n\|_2^2$,

thus as $n \rightarrow \infty$ we have the following estimate for the expectation as.

$$\begin{aligned}
 & \mathbb{E} \left[\max \left(\|\kappa_n\|_2^2 - T_1^{2/l}(n), 0 \right) \right] = \mathbb{E} \left[\mathbb{E} \left[\max \left(\|\kappa_n\|_2^2 - T_1^{2/l}(n), 0 \right) \mid X_1 \right] \right] \\
 & = \mathbb{E} \left[\int_0^{\|\kappa_n\|_2^2} \mathbb{P} \left[T_1(n) \leq (\kappa_n - t)^{l/2} \mid X_1 \right] dt \right] \\
 & = \mathbb{E} \left[\int_0^{\|\kappa_n\|_2^2} \mathbb{P} \left[\tau \leq \left(\|\kappa_n\|_2^2 - t \right)^{l/2} \mid X_1 \right] + O \left(1/n^{-1/2+1/l} \right) dt \right] \\
 & = \mathbb{E} \left[\int_0^{\|\kappa_n\|_2^2} \left(1 - \exp \left(- \frac{\pi^{l/2} \left(f_X \left(X_1 + \frac{\zeta}{n^{\frac{3}{2l+2}}} \right) + f_Y \left(X_1 + \frac{\zeta}{n^{\frac{3}{2l+2}}} \right) \right)}{\Gamma(l/2 + 1)} \left(\|\kappa_n\|_2^2 - t \right)^{l/2} \right) \right) dt \right] \\
 & \quad + O \left(1/n^{-1/2+3/l-\frac{6}{2l+2}} \right) \\
 & = C \frac{2}{l+2} \left\| \frac{\zeta}{n^{\left(\frac{3}{2l+2}-\frac{1}{l}\right)}} \right\|^{l+2} + O \left(1/n^{-1/2+3/l-\frac{6}{2l+2}} \right)
 \end{aligned}$$

The estimate in third equation follows by applying the first argument in Lemma 2. The final equality estimate is due to $\|\kappa_n\|_2^2 = \left\| \zeta n^{-\left(\frac{3}{2l+2}-\frac{1}{l}\right)} \right\|_2^2 \rightarrow 0$ as $n \rightarrow \infty$. Then, owing to the previous results, as $n \rightarrow \infty$ we have estimate for $G(\zeta, n)$ as

$$\begin{aligned}
 G(\zeta, n) & = -\frac{2C}{l+2} n^{(1/2+\frac{3}{2l+2}-\frac{2}{l})} n^{(-\frac{3l+6}{2l+2}+\frac{l+2}{l})} \|\zeta\|_2^{l+2} + o(1) \\
 & = -\frac{2C}{l+2} \|\zeta\|_2^{l+2} + o(1).
 \end{aligned}$$

Finally, we can know that, as $n \rightarrow \infty$, by the CLT we have $Z_n \Rightarrow \tilde{Z}$, then using continuous mapping theorem, we have that the scaled SOS profile function has the asymptotic distribution given by

$$\begin{aligned}
 & n^{1/2+\frac{5}{4l+2}} R_n^W(\theta_*) \\
 & = 2 \|Z_n\|_2^2 \frac{\|Z_n\|_2^{\left(\frac{1}{l+1}-1\right)}}{C^{\frac{1}{l+1}}} - \frac{2}{l+2} \frac{\|Z_n\|_2^{1+\frac{1}{l+1}}}{C^{\frac{1}{l+1}}} + o_p(1) \\
 & = \frac{2l+2}{l+2} \frac{\|Z_n\|_2^{1+\frac{1}{l+1}}}{C^{\frac{1}{l+1}}} + o_p(1) \Rightarrow \frac{2l+2}{l+2} \frac{\|\tilde{Z}\|_2^{1+\frac{1}{l+1}}}{C^{\frac{1}{l+1}}}.
 \end{aligned}$$

7.2.7. Proofs of Technical Lemmas in Step 2 .

Proof of Lemma 1. We shall introduce some notation which will be convenient throughout our development. Define for $t \geq 0$,

$$\begin{aligned} F_n(t) &= P(T_i(n) \leq t), \\ D_i(t) &= I(T_i(n) \leq t), \quad \bar{D}_i(t) = I(T_i(n) \leq t) - F_n(t), \\ \bar{F}_n(t) &= 1 + n^{-1/2} \sum_{i=1}^n \bar{D}_i(t). \end{aligned}$$

Therefore, we are interested in studying

$$\bar{F}_n(t) - 1 = \frac{1}{n^{1/2}} \sum_{i=1}^n (I(T_i(n) \leq t) - F_n(t)).$$

We will start by studying

$$\mathbb{E}[\sup\{\bar{F}_n(t) : t \in [0, T]\}].$$

First, we define

$$h_n(t) = \frac{\bar{F}_n(t_-)}{\left(\bar{F}_n^*(t_-)^2 + [\bar{F}_n](t_-)\right)^{1/2}},$$

where, for a given function $\{g(t) : t \in [0, T]\}$, we define

$$\begin{aligned} g^*(t) &= \sup\{g(s) : s \in [0, t]\}, \\ [g](t) &= \int_0^t (dg(s))^2. \end{aligned}$$

In addition, $[g](t)$ is defined as the quadratic variational process, i.e.,

$$[g](t) = \lim_{n \rightarrow \infty} \sum_{i=1}^n \left[g\left(\frac{i \times t}{n}\right) - g\left(\frac{(i-1) \times t}{n}\right) \right]^2.$$

In particular,

$$[\bar{F}_n](t) = \frac{1}{n} \sum_{i=1}^n I(T_i(n) \leq t).$$

We observe that $\bar{F}_n^*(t) \geq 1$, therefore $h_n(t)$ is well defined; moreover, note that

$$h_n(t)^2 \leq 1.$$

We invoke Theorem 1.2 of [2] and conclude that

$$\sup_{0 \leq t \leq T} \bar{F}_n(t) \leq 6\sqrt{[\bar{F}_n](T)} + 2 \int_0^T h_n(t) d\bar{F}_n(t).$$

Now we analyze the integral in the right hand side of the previous display. Observe that

$$\begin{aligned} \mathbb{E} \left(\int_0^T h_n(t) d\bar{F}_n(t) \right) &= \frac{1}{n^{1/2}} \sum_{i=1}^n \mathbb{E} \left(\int_0^T h_n(t) d\bar{D}_i(t) \right) \\ (31) \qquad \qquad \qquad &= n^{1/2} \mathbb{E} \left(\int_0^T h_n(t) d\bar{D}_1(t) \right). \end{aligned}$$

Let us write

$${}_1\bar{F}_n(t) = \bar{F}_n(t) - \bar{D}_1(t)/n^{1/2},$$

that is, we simply remove the last term in the sum defining $\bar{F}_n(t)$. We have that

$$h_n(t) = \frac{{}_1\bar{F}_n(t_-) + \bar{D}_1(t_-)/n^{1/2}}{\left(\bar{F}_n^*(t_-)^2 + [{}_1\bar{F}_n](t_-) + [D_1](t_-)/n\right)^{1/2}},$$

moreover,

$$|{}_1\bar{F}_n^*(t) - \bar{F}_n^*(t)| \leq 1/n^{1/2}.$$

We then can write

$$\begin{aligned} (32) \qquad h_n(t) &= \frac{{}_1\bar{F}_n(t_-) + \bar{D}_1(t_-)/n^{1/2}}{\left(\bar{F}_n^*(t_-)^2 + [{}_1\bar{F}_n](t_-) + [D_1](t_-)/n\right)^{1/2}} \\ &= \frac{{}_1\bar{F}_n(t_-)}{\left({}_1\bar{F}_n^*(t_-)^2 + [{}_1\bar{F}_n](t_-)\right)^{1/2}} \left(1 + \frac{L_n(t_-)}{n^{1/2}}\right), \end{aligned}$$

where we can select a deterministic constant $c \in (0, \infty)$ such that $|L_n(t)| \leq c$ for $j = 0$ and 1 assuming $n \geq 4$ (this constrain in n is imposed so that a Taylor expansion for the function $1/(1-x)$ can be developed for $x \in (0, 1)$). We now insert (32) into (31) and conclude that if we define

$$\bar{h}_n(t) = \frac{{}_1\bar{F}_n(t_-)}{\left({}_1\bar{F}_n^*(t_-)^2 + [{}_1\bar{F}_n](t_-)\right)^{1/2}},$$

it suffices to verify that

$$n^{1/2} \mathbb{E} \left(\int_0^T \bar{h}_n(t) d\bar{D}_1(t) \right) < \infty.$$

Define $\tilde{h}_n(t)$ to be a copy of $\bar{h}_n(t)$, independent of X_1 and $T_1(n)$. In particular, $\tilde{h}_n(t)$ is constructed by using all of the X_j 's except for X_1 , which might be replaced by an independent copy, X'_1 , of X_1 . Observe that the number of processes $\{\bar{D}_i(t) : t \leq T\}$ that depend on $T_1(n)$ and X_1 is smaller than $N_n(T, \lambda, 1)$. Therefore, similarly as we obtained from the analysis leading to the definition of $\bar{h}_n(\cdot)$, we have that a random variable $\bar{L}_{N_n(T, \lambda, 1)}$ can be defined so that $|\bar{L}_{N_n(T, \lambda, 1)}| \leq c(1 + N_n(T, \lambda, 1))$ for some (deterministic) $c > 0$ and $n \geq 4$ and satisfying

$$\begin{aligned} & \mathbb{E} \left(\int_0^T \bar{h}_n(t) d\bar{D}_1(t) \right) \\ &= \mathbb{E} \left(\bar{h}_n(T_1(n)) I(T_1(n) \leq T) \right) - \mathbb{E} \left(\tilde{h}_n(T_1(n)) I(T_1(n) \leq T) \right) \\ &= \mathbb{E} \left(\tilde{h}_n(T_1(n)) I(T_1(n) \leq T) \right) - \mathbb{E} \left(\tilde{h}_n(\tau_i(X_i)) I(\tau_i(X_i) \leq T) \right) \\ &+ \mathbb{E} \left(\bar{L}_{N_n(T, \lambda, 1)} / n^{1/2} \right) \\ &= \mathbb{E} \left(\bar{L}_{N_n(T, \lambda, 1)} / n^{1/2} \right). \end{aligned}$$

We have that

$$\left| \mathbb{E} \left(\bar{L}_{N_n(T, \lambda, 1)} / n^{1/2} \right) \right| \leq |\mathbb{E}(c(1 + N_n(T, \lambda, 1)))| / n^{1/2} = O(1/n^{1/2}).$$

Consequently, we conclude that

$$n^{1/2} \mathbb{E} \left(\int_0^T \bar{h}_n(t) d\bar{D}_1(t) \right) = O(1),$$

as $n \rightarrow \infty$, as required. Thus we proved that the first part of the lemma holds. For the second part, we observe that

$$\begin{aligned} & \overline{\lim}_{n \rightarrow \infty} \mathbb{E} \left(\sup_{t \in [0, T]} \left| \frac{1}{n^{1/2}} \sum_{i=1}^n (\max(t^2 - T_i(n)^\alpha, 0) - \mathbb{E}[\max(t^2 - T_i(n)^\alpha, 0)]) \right| \right) \\ &= \overline{\lim}_{n \rightarrow \infty} \mathbb{E} \left(\sup_{t \in [0, T]} \left| \int_0^t \frac{1}{n^{1/2}} \sum_{i=1}^n (2s I(T_i^\alpha(n) \leq s^2) - 2s \mathbb{P}[T_i^\alpha(n) \leq s^2]) ds \right| \right) \\ &\leq \overline{\lim}_{n \rightarrow \infty} \int_0^T \mathbb{E} \left(\sup_{t \in [0, T]} \left| \frac{1}{n^{1/2}} \sum_{i=1}^n (2t I(T_i^\alpha(n) \leq t^2) - 2t \mathbb{P}[T_i^\alpha(n) \leq t^2]) \right| \right) dt \\ &\leq 2T^2 \overline{\lim}_{n \rightarrow \infty} \mathbb{E} \left(\sup_{t \in [0, T]} \left| \frac{1}{n^{1/2}} \sum_{i=1}^n (I(T_i(n) \leq t) - \mathbb{P}[T_i(n) \leq t]) \right| \right) < \infty. \end{aligned}$$

Hence, applying the result for the first part of the lemma, we conclude the second part as well. \square

Proof of Lemma 2.

$$\begin{aligned} \mathbb{P}[T_i(n) \leq t] &= \mathbb{P}\left(\text{Bin}\left(\mathbb{P}\left(\|X_i - a(X_i, \lambda)\|_2 \leq t^{1/l}/n^{1/l}\right), n-1\right) \geq 1\right) \\ &= 1 - \left(1 - \mathbb{P}\left(\|X_i - a(X_i, \lambda)\|_2 \leq t^{1/l}/n^{1/l}\right)\right)^n. \end{aligned}$$

Then, as $n \rightarrow \infty$ and $t \rightarrow 0^+$

$$\mathbb{P}\left(\|X_j - a(X_i, \lambda)\|_2 \leq t^{1/l}/n^{1/l}\right) = c_0 t/n + c_1 t/n \cdot t^{1/l}/n^{1/l} + o\left(t^{1+1/l}/n^{1+1/l}\right).$$

Therefore by the Poisson approximation to the Binomial distribution we know:

$$\begin{aligned} \mathbb{P}[T_i(n) \leq t] &= 1 - \exp(-c_0 t) + O\left(t^{1+1/l}/n^{1/l}\right), \\ \mathbb{P}[\tau \leq t] &= 1 - \exp(-c_0 t). \end{aligned}$$

Thus we proved the first claim:

$$\mathbb{P}[T_i(n) \leq t] - \mathbb{P}[\tau \leq t] = O\left(t^{1+1/l}/n^{1/l}\right).$$

The second claim follows the definition of τ and equation (26), where as $n \rightarrow \infty$ we have

$$\begin{aligned} \mathbb{P}[T_i(n) \leq t] - \mathbb{P}[\tau \leq t] &= \mathbb{P}[T_i(n) > t] - \mathbb{P}[\tau > t] \\ &= \mathbb{E}[\exp(-\Lambda(\lambda, X_1))] \left(1 + O\left(1/n^l\right)\right) - \mathbb{E}[\exp(-\Lambda(\lambda, X_1))] \\ &= \mathbb{P}[\tau > t] O\left(1/n^l\right). \end{aligned}$$

□

7.3. Proofs of Additional Theorems. In this subsection, we are going to provide the proofs of the remaining theorems and corollaries (Theorem 2, Theorem 3, Corollary 1 and Corollary 2). We are going to follow closely the proof of Theorem 1 and discuss the differences inside each of its steps.

7.3.1. Proofs of SOS Theorems for General Estimation. We will first prove the corresponding theorems for general estimating equations. As we discussed before, Theorem 2 is the direct generalization of Theorem 1 and we are going to only discuss the proof of Theorem 3 in this part.

Proof of Theorem 3. Let us first denote $\bar{h}_n(\theta) = \frac{1}{n} \sum_{i=1}^n h(\theta, X_i)$. The analogue of **Step 1**, namely, the dual formulation takes the form

$$R_n^W(\theta_*) = \max_{\lambda} \left\{ -\lambda^T \bar{h}_n(\theta_*) - \frac{1}{n} \sum_{i=1}^n \max_j \left\{ \lambda^T h(\theta_*, Z_j) - \lambda^T h(\theta_*, X_i) - \|X_i - Z_j\|_2^2 \right\}^+ \right\}.$$

Step 2 and 3 are given as follows, for $l = 1$ and $l = 2$, let us denote $\sqrt{n} \bar{h}_n(\theta_*) = Z_n$ and $\sqrt{n} \lambda = 2\zeta$, we can scale the SOS profile function by n , arriving to

$$nR_n^W(\theta_*) = \max_{\zeta} \left\{ -2\zeta^T Z_n - \frac{1}{n} \sum_{i=1}^n n \max_j \left\{ 2 \frac{\zeta^T}{\sqrt{n}} h(\theta_*, Z_j) - 2 \frac{\zeta^T}{\sqrt{n}} h(\theta_*, X_i) - \|X_i - Z_j\|_2^2 \right\}^+ \right\}.$$

For each i , let us consider the maximization problem

$$(33) \quad \max_j \left\{ 2 \frac{\zeta^T}{\sqrt{n}} h(\theta_*, Z_j) - 2 \frac{\zeta^T}{\sqrt{n}} h(\theta_*, X_i) - \|X_i - Z_j\|_2^2 \right\}.$$

Similar as Step 1 of the proof for Theorem 1, we would like to solve the maximization problem (33) by first minimizing over z (as a free variable), instead of over j and then quantify the gap. Observe that the uniform bound $\|D_x^2 h(\theta_*, \cdot)\| < \tilde{K}$ stated in BE1) implies that for all n large enough (in particular, $n^{1/2} > 2\tilde{K} \|\zeta\|$) implies that

$$(34) \quad \max_z \left\{ 2 \frac{\zeta^T}{\sqrt{n}} h(\theta_*, z) - 2 \frac{\zeta^T}{\sqrt{n}} h(\theta_*, X_i) - \|X_i - z\|_2^2 \right\},$$

has an optimizer in the interior. Therefore, by the differentiability assumption stated in BE1) we know that any global minimizer, $\bar{a}_*(X_i, \zeta)$, of the problem (34) satisfies

$$(35) \quad \begin{aligned} \bar{a}_*(X_i, \zeta) &= X_i + D_x h(\theta_*, \bar{a}_*(X_i, \zeta))^T \cdot \frac{\zeta}{n^{1/2}} \\ &= X_i + D_x h(\theta_*, X_i)^T \cdot \frac{\zeta}{n^{1/2}} + O\left(\frac{\|\zeta\|_2^2}{n} \|D_x h(\theta_*, \bar{a}_*(X_i, \zeta))\|_2\right). \end{aligned}$$

Moreover, owing to BE1), we obtain that

$$(36) \quad \|D_x h(\theta_*, \bar{a}_*(X_i, \zeta)) - D_x h(\theta_*, X_i)\|_2 \leq \tilde{K} \frac{\|\zeta\|_2}{n^{1/2}}.$$

Consequently, if we define

$$a_*(X_i, \zeta) = X_i + D_x h(\theta_*, X_i)^T \cdot \frac{\zeta}{n^{1/2}},$$

we obtain due to (35) and (36) that

$$\|a_*(X_i, \zeta) - \bar{a}_*(X_i, \zeta)\|_2 = O\left(\frac{\|\zeta\|_2^2}{n} \left(\|D_x h(\theta_*, X_i)\|_2 + \frac{\|\zeta\|_2}{n^{1/2}}\right)\right).$$

Then, after performing a Taylor expansion and applying inequality (36) we obtain that

$$\begin{aligned} & 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, X_i) - 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, \bar{a}_*(X_i, \zeta)) + \|X_i - \bar{a}_*(X_i, \zeta)\|_2^2 \\ &= 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, X_i) - 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, a_*(X_i, \zeta)) + \|X_i - a_*(X_i, \zeta)\|_2^2 \\ &+ O\left(\frac{\|\zeta\|_2^3}{n^{3/2}}\right) + O\left(\frac{\|D_x h(\theta_*, X_i)\|_2^2 \|\zeta\|_2^3}{n^{3/2}}\right). \end{aligned}$$

In turn, a direct calculation gives that, as $n \rightarrow \infty$

$$\begin{aligned} -\frac{\zeta^T V_i \zeta}{n} &= 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, X_i) - 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, a_*(X_i, \zeta)) + \|X_i - a_*(X_i, \zeta)\|_2^2 \\ &+ O\left(\frac{\|D_x h(\theta_*, X_i)\|_2^2 \|\zeta\|_2^3}{n^{3/2}}\right). \end{aligned}$$

Similarly as in Step 2 of the proof of Theorem 1 we can define the point process $N^{(i)}(t, \zeta)$ and $T_i(n)$. We know the gap between freeing the variable z and restricting the maximization over the Z_j 's (i.e. the difference between (34) and (33)) is

$$\begin{aligned} & \max_j \left\{ \frac{1}{n} \zeta^T V_i \zeta - \left(2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, Z_j) - 2\frac{\zeta^T}{\sqrt{n}}h(\theta_*, X_i) - \|X_i - Z_j\|_2^2 \right) \right\} \\ &+ O\left(\frac{\|D_x h(\theta_*, X_i)\|_2^2 \|\zeta\|_2^3}{n^{3/2}}\right). \end{aligned}$$

By the definition of $T_i(n)$, we can write the profile function for $l = 1$ as

$$\begin{aligned} & nR_n^W(\theta_*) \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - \frac{1}{n} \sum_{i=1}^n \max \left(\zeta^T V_i \zeta - \frac{T_i^2(n)}{n} + O\left(\frac{\|D_x h(\theta_*, X_i)\|_2^2 \|\zeta\|_2^3}{n^{1/2}}\right), 0 \right) \right\}. \end{aligned}$$

Note that the sequence of global optimizers is tight as $n \rightarrow \infty$ because $\mathbb{E}(V_i)$ is assumed to be strictly positive definite with probability one. In turn, from the previous expression we obtain, following a similar derivation as in the proof of Theorem 1 (invoking Lemma 1) and using the fact

that ζ can be restricted to compact sets, that as $n \rightarrow \infty$

$$nR_n^W(\theta_*) = \max_{\zeta} \left\{ -2\zeta^T Z_n - \mathbb{E} \left[\max \left(\zeta^T V_1 \zeta - \frac{T_1^2(n)}{n} \right) \right] \right\} + o_p(1).$$

Then, for $l = 2$, as $n \rightarrow \infty$ we have estimate for the profile function as

$$nR_n^W(\theta_*) = \max_{\zeta} \left\{ -2\zeta^T Z_n - \mathbb{E} \left[\max \left(\zeta^T V_1 \zeta - T_1^2(n) \right) \right] \right\} + o_p(1).$$

When $l \geq 3$, let us denote $\sqrt{n}\bar{h}_n(\theta_*) = Z_n$ and $n^{\frac{3}{2l+2}}\lambda = 2\zeta$, we can scale profile function by $n^{\frac{1}{2} + \frac{3}{2l+2}}$ and write it as

$$\begin{aligned} & n^{\frac{1}{2} + \frac{3}{2l+2}} R_n^W(\theta_*) \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - \frac{1}{n} \sum_{i=1}^n n^{\frac{1}{2} + \frac{3}{2l+2}} \max_j \left\{ 2 \frac{\zeta^T}{n^{2l+2}} h(\theta_*, Z_j) - 2 \frac{\zeta^T}{n^{2l+2}} h(\theta_*, X_i) - \|X_i - Z_j\|_2^2 \right\}^+ \right\}. \end{aligned}$$

By applying same derivation as for $l = 1$ and 2 above, we can define a point process $N^{(i)}(t, \zeta)$ and $T_i(n)$ as in the proof of Theorem 1. As $n \rightarrow \infty$, we have the estimate for profile function becomes

$$\begin{aligned} & n^{\frac{1}{2} + \frac{3}{2l+2}} R_n^W(\theta_*) \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - n^{\frac{1}{2} + \frac{3}{2l+2} - \frac{2}{l}} \frac{1}{n} \sum_{i=1}^n \max \left(n^{-(\frac{6}{2l+2} - \frac{2}{l})} \zeta^T V_i \zeta - T_i^{2/l}(n), 0 \right) \right\} + o_p(1) \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - n^{\frac{1}{2} + \frac{3}{2l+2} - \frac{2}{l}} \mathbb{E} \left[\max \left(n^{-(\frac{6}{2l+2} - \frac{2}{l})} \zeta^T V_1 \zeta - T_1^{2/l}(n), 0 \right) \right] \right\} + o_p(1). \end{aligned}$$

The final estimation follows as in the proof for Theorem 1 (i.e. applying Lemma 1).

In **Step 4** for $l = 1$, as $n \rightarrow \infty$ the objective function is

$$nR_n^W(\theta_*) = \max_{\zeta} \left\{ -2\zeta^T Z_n(\theta_*) - \mathbb{E} \left[\max \left(\zeta^T V_1 \zeta - \frac{T_1^2(n)}{n}, 0 \right) \right] \right\} + o_p(1).$$

Let us denote $G : \mathbb{R}^l \rightarrow \mathbb{R}$ to be a deterministic continuous function, defined as

$$G(\zeta, n) = \mathbb{E} \left[\max \left(\zeta^T V_1 \zeta - \frac{T_1^2(n)}{n}, 0 \right) \right].$$

We know $\Upsilon = \mathbb{E}[V_1]$ is symmetric strictly positive definite matrix, then the objective function is strictly convex and differentiable in ζ . Thus the (unique) global maximizer is characterized by the first order optimality condition almost surely. We take derivative w.r.t. ζ and set it to be 0,

applying the same estimation in the original proof the first order optimality condition becomes

$$(37) \quad Z_n = -\Upsilon\zeta + o_p(1) \text{ as } n \rightarrow \infty.$$

Since Υ is invertible, for any n we can solve optimal $\zeta_n^* = -\Upsilon^{-1}Z_n + o_p(1)$. Plugging ζ_n^* in the objective function, as $n \rightarrow \infty$ we have

$$nR_n^W(\theta_*) = 2Z_n^T\Upsilon^{-1}Z_n - G(-\Upsilon^{-1}Z_n, n) + o_p(1).$$

As $n \rightarrow \infty$, we can apply the same estimation in the proof of Theorem 1, it becomes

$$nR_n^W(\theta_*) \Rightarrow \tilde{Z}^T\Upsilon^{-1}\tilde{Z}.$$

Thus we proof the claim for $l = 1$.

In **Step 5** for $l = 2$, as $n \rightarrow \infty$ the objective function has estimate

$$nR_n^W(\theta_*) = \max_{\zeta} \left\{ -2\zeta^T Z_n(\theta_*) - \mathbb{E} \left[\max(\zeta^T V_1 \zeta - T_1(n), 0) \right] \right\} + o_p(1).$$

Still, we denote $G(\zeta, n)$ to be a deterministic function given as,

$$G(\zeta, n) = \mathbb{E} \left[\max(\zeta^T V_1 \zeta - T_1(n), 0) \right].$$

Same as discussed in for $l = 1$, the objective function is strictly convex and differentiable in ζ , thus the (unique) global maximizer could be characterized via first order optimality condition almost surely. We take derivative w.r.t. ζ and set it to be 0, applying same estimation in the proof of Theorem 1 the first order optimality condition becomes

$$(38) \quad Z_n = -\mathbb{E} \left[V_1 1_{(\tau \leq \zeta^T V_1 \zeta)} \right] \zeta + o_p(1) \text{ as } n \rightarrow \infty.$$

We know the objective function is strictly convex differentiable, then for fixed Z_n there is a unique ζ_n^* that satisfies the first order optimality condition (38). We plug in the optimizer and the objective function becomes

$$nR_n^W(\theta_*) = -2Z_n^T\zeta_n^* - G(\zeta_n^*, n) + o_p(1) \text{ as } n \rightarrow \infty.$$

As $n \rightarrow \infty$, we can apply the same estimation in the proof of Theorem 1, we have

$$nR_n^W(\theta_*) \Rightarrow -2\tilde{Z}^T \tilde{\zeta} - \tilde{\zeta}^T \tilde{G}(\tilde{\zeta}) \tilde{\zeta},$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}^q \times \mathbb{R}^q$ is a deterministic continuous mapping defined as,

$$\tilde{G}(\zeta) = \mathbb{E} [V_1 \max(1 - \tau/(\zeta^T V_1 \zeta), 0)],$$

and $\tilde{\zeta} := \tilde{\zeta}(\tilde{Z})$ is the unique solution to

$$\tilde{Z} = -\zeta \mathbb{E} [V_1 1_{(\tau \leq \zeta^T V_1 \zeta)}].$$

Then we proved the claim for $l = 2$.

Finally, in **Step 6** for $l \geq 3$, as $n \rightarrow \infty$ the objective function is

$$\begin{aligned} & n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \\ &= \max_{\zeta} \left\{ -2\zeta^T Z_n - n^{(1/2 + \frac{3}{2l+2} - \frac{2}{l})} \mathbb{E} \left[\max \left(n^{-(\frac{6}{2l+2} - \frac{2}{l})} \zeta^T V_1 \zeta - T_1^{2/l}(n), 0 \right) \right] \right\} + o_p(1). \end{aligned}$$

We denote $G(\zeta, n)$ to be a deterministic function defined as,

$$G(\zeta, n) = n^{(1/2 + \frac{3}{2l+2} - \frac{2}{l})} \mathbb{E} \left[\max \left(n^{-(\frac{6}{2l+2} - \frac{2}{l})} \zeta^T V_1 \zeta - T_1^{2/l}(n), 0 \right) \right].$$

Follows the same discussion above for $l = 1$ and 2, we know the objective function is strictly convex differentiable in ζ and the global maximizer is characterized by first order optimality condition almost surely. We take derivative of the objective function w.r.t. ζ and set it to be 0. We apply the same technique as in the proof of Theorem 1, the first order optimality condition becomes

$$(39) \quad Z_n = -\mathbb{E} \left[V_1 \frac{\pi^{l/2} (f_X(X_1) + \kappa f_Y(X_1))}{\Gamma(l/2 + 1)} V_1 (\zeta^T V_1 \zeta)^l \right] \zeta + o_p(1). \text{ as } n \rightarrow \infty$$

The objective condition is strictly convex differentiable and for fixed Z_n there is a unique ζ_n^* satisfying the first optimality condition (39). We plug ζ_n^* into the objective function and it becomes

$$n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) = -2Z_n^T \zeta_n^* - G(\zeta_n^*, n) + o_p(1) \text{ as } n \rightarrow \infty.$$

As $n \rightarrow \infty$, we can apply same estimate in the proof of Theorem 1, we have

$$n^{1/2 + \frac{3}{2l+2}} R_n^W(\theta_*) \Rightarrow -2\tilde{Z}^T \tilde{\zeta} - \frac{2}{l+2} \tilde{G}(\tilde{\zeta}),$$

where $\tilde{G} : \mathbb{R}^q \rightarrow \mathbb{R}$ is a deterministic continuous function given as,

$$\tilde{G}(\zeta) = \mathbb{E} \left[\frac{\pi^{l/2} (f_X(X_1) + \kappa f_Y(X_1))}{\Gamma(l/2 + 1)} (\zeta^T V_1 \zeta)^{l/2+1} \right],$$

and $\tilde{\zeta} := \tilde{\zeta}(\tilde{Z})$ is the unique solution to

$$\tilde{Z} = -\mathbb{E} \left[V_1 \frac{\pi^{l/2} (f_X(X_1) + \kappa f_Y(X_1))}{\Gamma(l/2 + 1)} V_1 (\zeta^T V_1 \zeta)^l \right] \zeta.$$

We proved the claim for $l \geq 3$ and finish the proof for Theorem 3. \square

7.3.2. Proofs of SOS Theorems for General Estimation with Plug-In. The proofs of the plug-in version of SOS theorems for general estimation equation also mainly follows the proof of Theorem 1, we are going to discuss the different steps here.

Proof of Corollary 1. For implicit formulation, as we discussed for Theorem 2, we can redefine $X_i \leftarrow h(\gamma_*, \nu_n, X_i)$, $Z_k \leftarrow h(\gamma_*, \nu_n, Z_k)$, $X_i(*) \leftarrow h(\gamma_*, \nu_*, X_i)$ and $Z_k(*) \leftarrow h(\gamma_*, \nu_*, X_i)$. Then the proof for the implicit formulation with plug-in goes as follows.

In **Step 1**, the dual formulation is similar given as

$$\begin{aligned} R_n^W(\gamma_*) &= \max_{\lambda, \gamma_i \geq 0} \left\{ -\lambda \bar{X}_n - \frac{1}{n} \sum_{i=1}^n \gamma_i \right\} \\ \text{s.t. } & -\gamma_i \leq \min_j \left\{ \lambda^T X_i - \lambda^T Z_j + \|X_i - Z_j\|_2^2 \right\}, \text{ for all } i. \end{aligned}$$

We can apply first order Taylor expansion to $h(\gamma_*, \nu_n, X_i)$ w.r.t. ν , then we have

$$h(\gamma_*, \nu_n, X_i) = h(\gamma_*, \nu_*, X_i) + O_p \left(\frac{\|D_\nu h(\gamma_*, \bar{\nu}_n, X_i)\|}{n^{1/2}} \right),$$

where $\bar{\nu}_n$ is a point between ν_n and ν_* . By our change of notation for X_i , $X_i(*)$, Z_k and $Z_k(*)$ and the above Taylor expansion, we can observe

$$Z_k = Z_k(*) + \epsilon_n(Z_k),$$

where $\epsilon_n(Z_k) = O_p(\|D_\nu h(\gamma_*, \bar{\nu}_n, Z_k)\|/n^{1/2})$.

In **Step 2** we can define a point process $N_n^{(i)}(t, \lambda)$ and $T_i(n)$ as in the proof of Theorem 1, but the rate becomes

$$\Lambda(X_i, \lambda) = [f_X(X_i + \lambda/2 + \epsilon_n(X_i)) + \kappa f_Y(X_i + \lambda/2 + \epsilon_n(X_i))] \frac{\pi^{l/2}}{\Gamma(l/2 + 1)}.$$

As $n \rightarrow \infty$, same as in the proof of Theorem 1 and Theorem 3 we can argue $\lambda \rightarrow 0$. Then we can define τ same as in the proof of Theorem 1 and has the with same distribution

$$\mathbb{P}[\tau \geq t] = \mathbb{E} \left[\exp \left(- (f_X(X_1) + \kappa f_Y(X_1)) \frac{\pi^{l/2}}{\Gamma(l/2 + 1)} \right) \right].$$

Then the rest of the proof in **Step 3, 4, 5 and 6** stay the same as that of Theorem 1, but replacing the CLT for Z_n by the asymptotic distribution given in C2). \square

Proof of Corollary 2. For explicit formulation, the proof follows more closely the proof of Theorem 3 and we are discussing the differences as follows.

In **Step 1**, the dual formulation takes the form

$$\begin{aligned} R_n^W(\theta_*) \\ = \max_{\lambda} \left\{ -\lambda^T \bar{h}_n(\gamma_*, \nu_n) - \frac{1}{n} \sum_{i=1}^n \max_j \left\{ \lambda^T h(\gamma_*, \nu_n, Z_j) - \lambda^T h(\gamma_*, \nu_n, X_i) - \|X_i - Z_j\|_2^2 \right\}^+ \right\}. \end{aligned}$$

Step 2 and 3 Follows the same as for the proof of Theorem 3 however we need to notice that difference is the definition of $\bar{a}_*(X_i, \zeta)$, for $l = 1$ and 2 we have

$$\begin{aligned} (40) \quad \bar{a}_*(X_i, \zeta) &= X_i + D_x h(\gamma_*, \nu_n, \bar{a}_*(X_i, \zeta)) \cdot \frac{\zeta}{n^{1/2}} \\ &= X_i + D_x h(\gamma_*, \nu_n, X_i) \cdot \frac{\zeta}{n^{1/2}} + O \left(\frac{\|\zeta\|_2^2}{n} \|D_x h(\gamma_*, \nu_n, \bar{a}_*(X_i, \zeta))\|_2 \right) \\ &= X_i + D_x h(\gamma_*, \nu_*, X_i) \cdot \frac{\zeta}{n^{1/2}} + O \left(\frac{\|\zeta\|_2^2}{n} \|D_x h(\gamma_*, \nu_n, \bar{a}_*(X_i, \zeta))\|_2 \right) \\ (41) \quad &+ O \left(\frac{\|\zeta\|_2}{n^{1/2}} \|\nu_n - \nu_*\|_2 \|D_x h(\gamma_*, \nu_n, \bar{a}_*(X_i, \zeta))\|_2 \|D_\nu D_x h(\gamma_*, \bar{\nu}_n, \bar{a}_*(X_i, \zeta))\|_2 \right), \end{aligned}$$

where $\bar{\nu}_n$ is a point between ν_n and ν_* . By assumption C5)-C7) we can notice the rest of step 2 and 3 stay the same as in the proof of Theorem 3. In **Step 4, 5 and 6** we use $Z_n = \frac{1}{n^{1/2}} \sum_{i=1}^n h(\gamma_*, \nu_n, X_i) \Rightarrow \tilde{Z}'$ given in C2). \square

ACKNOWLEDGMENT. Support from NSF through Awards 1436700, 1820942, 1838576 is gratefully acknowledged. The authors are also grateful to Karthyek Murthy and Henry Lam for helpful discussions.

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