Complexity-Free Generalization via Distributionally Robust Optimization

Henry Lam
Department of Industrial Engineering and Operations Research, Columbia University, New York, NY 10027,
henry.lam@columbia.edu

Yibo Zeng
Department of Industrial Engineering and Operations Research, Columbia University, New York, NY 10027,
yibo.zeng@columbia.edu

Established approaches to obtain generalization bounds in data-driven optimization and machine learning mostly build on solutions from empirical risk minimization (ERM), which depend crucially on the functional complexity of the hypothesis class. In this paper, we present an alternate route to obtain these bounds on the solution from distributionally robust optimization (DRO), a recent data-driven optimization framework based on worst-case analysis and the notion of ambiguity set to capture statistical uncertainty. In contrast to the hypothesis class complexity in ERM, our DRO bounds depend on the ambiguity set geometry and its compatibility with the true loss function. Notably, when using maximum mean discrepancy as a DRO distance metric, our analysis implies, to the best of our knowledge, the first generalization bound in the literature that depends solely on the true loss function, entirely free of any complexity measures or bounds on the hypothesis class.

Key words: distributionally robust optimization, generalization bound, maximum mean discrepancy, reproducing kernel Hilbert space, hypothesis class complexity

1. Introduction

We study generalization error in the following form. Let $l : \Theta \times \mathcal{X} \rightarrow \mathbb{R}$ be a loss function over the solution space $\Theta$ and sample space $\mathcal{X} \subset \mathbb{R}^d$. Let $Z_0(\theta) = \mathbb{E}_{\xi \sim P_0}[l(\theta, \xi)]$ be the expected loss under the true distribution $P_0$ for $\xi$. This $Z_0(\theta)$ can be an objective function ranging from various operations research applications to the risk of a machine learning model. Given iid samples $\{\xi_i\}_{i=1}^n \sim P_0$, we solve a data-driven optimization problem or fit model to give solution $\theta_{\text{data}}$. The excess risk, or optimality gap of $\theta_{\text{data}}$ with respect to the oracle best solution $\theta_0^* \in \arg\min_{\theta \in \Theta} Z_0(\theta)$, is given by

$$Z_0(\theta_{\text{data}}) - Z_0(\theta_0^*)$$

(1)

This gap measures the relative performance of a data-driven solution in future test data, giving rise to a direct measurement on the generalization error. Established approaches to obtain high probability bounds for (1) have predominantly focused on empirical risk minimization (ERM), namely
using $\hat{\theta}^* \in \arg\min_{\theta \in \Theta} \{ \hat{Z}(\theta) := \mathbb{E}_{\xi \sim \hat{P}}[l(\theta, \xi)] \}$ for empirical distribution $\hat{P}$, or its regularized versions. A core determination of the quality of these bounds is the functional complexity of the model, or hypothesis class, which dictates the richness of the function class $\{l(\cdot, \cdot) : \theta \in \Theta \}$ and leads to well-known measures such as the Vapnik-Chervonenkis (VC) dimension \cite{vapnik1991}. On a high level, these complexity measures arise from the need to uniformly control the empirical error, which in turn arises from the a priori uncertainty on the decision variable $\theta$ in the optimization.

In this paper, we present an alternate route to obtain concentration bounds for \eqref{eq:1} on solutions obtained from distributionally robust optimization (DRO). The latter started as a decision-making framework for optimization under stochastic uncertainty \cite{delage2010, goh2010, wiesemann2014}, and has recently surged in popularity in machine learning, thanks to its abundant connections to regularization and variability penalty \cite{gao2017, chen2018, gotoh2018, lam2019, duchi2019, shafieezadeh-abadeh2019, kuhn2019, blanchet2019} and risk-averse interpretations \cite{ruszczynski2006, rockafellar2007}. Instead of replacing the unknown true expectation $\mathbb{E}_{\xi \sim P_0}[]$ by an empirical expectation $\mathbb{E}_{\xi \sim \hat{P}}[]$, DRO hinges on the creation of an uncertainty set or ambiguity set $\mathcal{K}$. This set lies in the space of probability distribution $P$ on $\xi$ and is calibrated from data. It obtains a solution $\bar{\theta}^*$ by minimizing the worst-case expected loss among $\mathcal{K}$

$$\bar{\theta}^* \in \arg\min_{\theta \in \Theta} \{ \bar{Z}(\theta) := \max_{P \in \mathcal{K}} \mathbb{E}_{\xi \sim P}[l(\theta, \xi)] \}. \tag{2}$$

The risk-averse nature of DRO is evident from the presence of an adversary that controls $P$ in \eqref{eq:2}. Moreover, if $\mathcal{K}$ is suitably chosen so that it contains the true probability with confidence (in some suitable sense) and shrinks to singleton as data size grows, then one would expect $\bar{\theta}^*$ to eventually approach the true solution, which also justifies the approach as a consistent training method. The latter can often be achieved by choosing $\mathcal{K}$ as a neighborhood ball surrounding a baseline distribution that estimates the ground truth (notably the empirical distribution), and the ball size is measured via a statistical distance.

Our main goal is to present a line of analysis to bound \eqref{eq:1} for DRO solutions that, instead of using functional complexity measures as in ERM, relies on the ambiguity set geometry and its compatibility with the true loss function. More precisely, this bound depends on two ingredients: the probability that the true distribution lies in $\mathcal{K}$ and, given that this occurs, the difference between the robust and true objective functions, namely $\bar{Z}(\cdot) - Z_0(\cdot)$, evaluated only at the true solution $\theta_0^*$. The latter property allows us to attain generalization bounds without using uniform bounds in the established ERM theory, as we demonstrate how the worst-case nature of DRO can “transfer” this
uniformity requirement into geometric requirements on only the true loss. In particular, when using the maximum mean discrepancy (MMD) \citep{gretton2012kernel} as a statistical distance in DRO, our analysis implies, to the best of our knowledge, the first generalization bound in the literature that depends solely on the true loss function $l(\theta_0^*, \cdot)$, entirely free of any functional complexity measures or bounds on the hypothesis class.

2. Related Work and Comparisons

DRO can be viewed as a generalization of (deterministic) robust optimization (RO) \citep{ben2009robust, bertsimas2011introduction}. The latter advocates the handling of unknown or uncertain parameters in optimization problems via a worst-case perspective, which often leads to minimax formulations. \citep{xu2009equivalence, xu2010equivalence} show the equivalence of ERM regularization with RO in some statistical models, and \citep{xu2012robust} further concretizes the relation of generalization with robustness.

DRO, which first appeared in \cite{scarf1958probabilistic} in the context of inventory management, applies the worst-case idea to stochastic problems where the underlying distribution is uncertain. Like in RO, it advocates a minimax approach to decision-making, but with the inner maximization resulting in the worst-case distribution over an ambiguity set $\mathcal{K}$ of plausible distributions. This idea has appeared across various disciplines like stochastic control \citep{petersen2000robust} and economics \citep{hansen2008robust, glasserman2014probabilistic}. Data-driven DRO constructs and calibrates $\mathcal{K}$ based on data when available. The construction can be roughly categorized into two approaches: 1) neighborhood ball using statistical distance, which include most commonly $\phi$-divergence \citep{ben2013robust, bavarrksan2015robust, jiang2016robust, lam2016optimal, lam2016waterstein} and Wasserstein distance \citep{esfahani2018data, blanchet2019data, gao2016certainty, chen2016distributionally}, 2) partial distributional information including moment \citep{ghaoui2003robust, delage2010distributional, goh2010distributional, wiesemann2014robust, hanasusanto2015distributionally}, distributional shape \citep{popescu2005robust, van2016distributionally, li2017distributionally, chen2020distributionally}, and marginal \citep{chen2018distributionally, doan2015distributionally, dhara2021distributionally} constraints.

The former approach has the advantage that the ambiguity set or the attained robust objective value consistently approaches the truth \citep{ben2013robust, bertsimas2018distributionally}. The second approach, on the other hand, provides flexibility on decision-maker when limited data is available which proves useful on a range of operational or risk-related settings \citep{zhang2016distributionally, lam2017distributionally, zhao2017distributionally}.

The first approach above, namely statistical-distance-based DRO, has gained momentum especially in statistics and machine learning in recent years. We categorize its connection with statistical performance into three lines, and position our results in this paper within each of them.
2.1. Absolute Bounds on Expected Loss

The classical approach to obtain guarantees for data-driven DRO is to interpret the ambiguity set $K$ as a nonparametric confidence region, namely that $\mathbb{P}[P_0 \in K] \geq 1 - \delta$ for small $\delta \in (0, 1)$. In this case, the confidence guarantee on the set can be translated into a confidence bound on the true expected loss function evaluated at the DRO solution $\tilde{\theta}^*$ in the form

$$\mathbb{P}[Z_0(\tilde{\theta}^*) \leq \bar{Z}(\tilde{\theta}^*)] \geq 1 - \delta$$

via a direct use of the worst-case definition of $\bar{Z}$. This implication is very general, with $K$ taking possibly any geometry (e.g., Delage and Ye 2010, Ben-Tal et al. 2013, Bertsimas et al. 2018, Esfahani and Kuhn 2018). A main concern on results in the form (3) is that the bound could be loose (i.e., a large $\bar{Z}(\tilde{\theta}^*)$). This, in some sense, is unsurprising as the analysis only requires a confidence guarantee on the set $K$, with no usage of other more specific properties, which is also the reason why the bound (3) is general. When $K$ is suitably chosen, a series of work has shown that the bound (3) can achieve tightness in some well-defined sense. Van Parys et al. (2020), Sutter et al. (2020) show that when $K$ is a Kullback-Leibler divergence ball, $\bar{Z}(\tilde{\theta}^*)$ in (3) is the minimal among all possible data-driven formulations that satisfy a given exponential decay rate on the confidence. Lam (2019), Gupta (2019), Duchi et al. (2021) show that for divergence-based $K$, $\bar{Z}(\theta)$ matches the confidence bound obtained from the standard central limit theorem (CLT) by deducing that it is approximately $\bar{Z}(\theta)$ plus a standard deviation term (see more related discussion momentarily).

Our result leverages part of the above “confidence translation” argument, but carefully twisted to obtain excess risk bounds for (1). We caution that (3) is a result on the validity of the estimated objective value $\bar{Z}(\tilde{\theta}^*)$ in bounding the true objective value $Z_0(\tilde{\theta}^*)$. The excess risk (1), on the other hand, measures the generalization performance of a solution in comparison with the oracle best. The latter is arguably more intricate as it involves the unknown true optimal solution $\theta^*$ and, as we will see, (3) provides an intermediate building block in our analysis of (1).

2.2. Variability Regularization

In a series of work Lam (2016, 2018), Gotoh et al. (2018), Duchi and Namkoong (2019), Duchi et al. (2021), it is shown that DRO using divergence-based ball, i.e., $K = \{P \in \mathcal{P} : D(P, \hat{P}) \leq \eta\}$ for some threshold $\eta > 0$ and $D$ a $\phi$-divergence (e.g., Kullback-Leibler, $\chi^2$-distance), satisfies a Taylor-type expansion

$$\bar{Z}(\theta) = \hat{Z}(\theta) + C_1(\theta) \sqrt{\eta} + C_2(\theta) \eta + \cdots$$

where $C_1(\theta)$ is the standard deviation of the loss function, $\sqrt{\text{Var}_0[l(\theta, \xi)]}$, multiplied by a constant that depends on $\phi$. Similarly, if $D$ is the Wasserstein distance and $\eta$ is of order $1/n$, (4) holds with $C_1(\theta)$ being the gradient norm or the Lipschitz norm (Blanchet et al.
Furthermore, Staub and Jegelka (2019), which is perhaps closest to our work, studies MMD as the DRO statistical distance and derives a high-probability bound for $\bar{Z}(\theta)$ similar to the RHS of (4), with $C_1(\theta)$ being the reproducing kernel Hilbert space (RKHS) norm of $l(\theta, \cdot)$. Results of the form (4) can be used to show that $\bar{Z}(\theta)$, upon choosing $\eta$ properly (of order $1/n$), gives a confidence bound on $Z_0(\theta)$ (Lam 2019, Duchi et al. 2021). Moreover, this result can be viewed as a duality of the empirical likelihood theory (Lam and Zhou 2017, Blanchet et al. 2019a, Duchi et al. 2021, Blanchet and Kang 2021).

In connecting (4) to the solution performance, there are three implications. First, the robust objective function $\bar{Z}(\theta)$ can be interpreted as approximately a mean-variance optimization, and Gotoh et al. (2018, 2021) prove that, thanks to this approximation, the DRO solution can lower the variance of the attained loss which compensates for its under-performance in the expected loss, thus overall leading to a desirable risk profile. Gotoh et al. (2018, 2021) have taken a viewpoint that the variance of the attained loss is important in the generalization. On the other hand, when the expected loss, i.e., the true objective function $Z_0(\theta)$, is the sole consideration, the approximation (4) is used in two ways. One way is to obtain bounds in the form

$$Z_0(\hat{\theta}^*) \leq \min_{\theta \in \Theta} \left\{ Z_0(\theta) + \frac{C_1(\theta)}{\sqrt{n}} \right\} + O(1/n)$$

thus showing that DRO performs optimally, up to $O(1/n)$ error, on the variance-regularized objective function (Duchi and Namkoong 2019). From this, Duchi and Namkoong (2019) deduces that under special situations where there exists $\theta$ with both small risk $Z_0(\theta)$ and variance $\text{Var}_0[l(\theta, \xi)]$, (5) can be translated into a small excess risk bound of order $1/n$. Moreover, such an order also desirably appears for DRO in some non-smooth problems where ERM could bear $1/\sqrt{n}$. The second way is to use DRO as a mathematical route to obtain uniform bounds in the form

$$Z_0(\theta) \leq \bar{Z}(\theta) + \frac{C_1(\theta)}{\sqrt{n}} + O(1/n), \quad \forall \theta \in \Theta,$$

which is useful for proving the generalization of ERM. In particular, we can translate (6) into a high probability bound for $Z_0(\hat{\theta}^*) - Z_0(\theta^*)$ of order $1/\sqrt{n}$. This use is studied in, e.g., Gao (2020) in the case of Wasserstein and Staub and Jegelka (2019) in the case of MMD.

Despite these rich results, both (5) and (6), and their derived bounds on the excess risk (1), still contain functional complexity measures of the hypothesis class manifested in the choice of the ball size $\eta$ or coefficient $C_1(\theta)$. Our main message in this paper is that this dependence can be completely removed, when using the solution of a suitably constructed DRO. Note that this is different from localized results for ERM, e.g., local Rademacher complexities (Bartlett et al. 2005). Although the latter establishes better generalization bounds by mitigating some dependence on the hypothesis class, local dependence still exists and cannot be removed.
2.3. Risk Aversion

It is known that any coherent risk measure (e.g., conditional value-at-risk) \cite{Ruszczynski2006, Rockafellar2007} of a random variable (in our case $l(\theta, \xi)$) is equivalent to the robust objective value $\bar{Z}(\theta)$ with a particular $K$. Thus, DRO is equivalent to a risk measure minimization, which in turn explains its benefit in controlling tail performances. In machine learning, this rationale has been adopted to enhance performance on minority subpopulations and in safety or fairness-critical systems \cite{Duchi2018, Hashimoto2018, Duchi2020}. A related application is adversarial training \cite{Goodfellow2015} in deep learning, in which RO or DRO is used to improve test performances on perturbed input data and adversarial examples \cite{Goodfellow2015, Madry2018, Sinha2018}. DRO has also been used to tackle distributional shifts in transfer learning \cite{Sagawa2020, Liu2021}. In these applications, numerical results suggest that RO and DRO can come at a degradation to the average-case performance \cite{Kurakin2017, Madry2018, Duchi2018}, though not universally, as Tsipras et al. (2019) observes that robust training can help reduce generalization error with very few training data. To connect, our result in this paper serves to justify a generalization performance of DRO even in the average case, without distributional shift, that can potentially outperform ERM.

To close this section, we discuss maximum mean discrepancy (MMD) \cite{Gretton2012}, which is the distance we will adopt in our DRO. MMD is a distance derived from the RKHS norm, by using test functions constrained by this norm as an Integral Probability Metric (IPM) \cite{Muller1997}. MMD is known to be less prone to the curse of dimensionality \cite{Shawe-Taylor2004, Smola2007, Grunewalder2012}, a property that we leverage in this paper, and such a property has allowed successful applications in statistical inference \cite{Gretton2012}, generative models \cite{Li2015, Sutherland2017} and reinforcement learning \cite{Nguyen2020}. Lastly, in using MMD in DRO, Staib and Jegelka (2019) obtains bounds in the form (3) and (6), where the latter relies on the complexity of the hypothesis class that is different from our complexity-free results. Zhu et al. (2020) studies the duality and optimization procedure for MMD DRO. Kirschner et al. (2020) applies MMD DRO in Bayesian optimization. For a recent comprehensive review of MMD, we refer readers to Muandet et al. (2017).

3. Main Results

We first present a general DRO bound:

\textbf{Theorem 1 (A General DRO Bound).} Let $\mathcal{X} \subset \mathbb{R}^d$ be a sample space, $P_0$ be a distribution on $\mathcal{X}$, $\{\xi_i\}_{i=1}^n$ be iid samples from $P_0$, and $\Theta$ be the solution space. For loss function $l: \Theta \times \mathcal{X} \to \mathbb{R}$, consider the DRO solution in (2) with ambiguity set $K$. For any $\epsilon > 0$, we have

$$\mathbb{P}[Z_0(\bar{\theta}^*) - Z_0(\theta_0^*) > \epsilon] \leq \mathbb{P}[P_0 \notin K] + \mathbb{P}[\bar{Z}(\theta_0^*) - Z_0(\theta_0^*) > \epsilon | P_0 \in K].$$

(7)
Theorem 1 states that the large deviations probability of the excess risk of a DRO solution is bounded by two terms. The first is the probability that $K$ does not include the true distribution $P_0$, and the second is the difference between the robust objective function $\tilde{Z}(\cdot)$ and the true objective function $Z_0(\cdot)$, at the true optimal solution $\theta^*_0$. This bound reveals a generalization tradeoff between the size of the ball (to control the first term) and the robust objective performance within the ball (to control the second term).

**Proof of Theorem 1.** We first write

$$Z_0(\theta^*) - Z_0(\theta^*_0) = (Z_0(\theta^*) - \tilde{Z}^*(\cdot)) + (\tilde{Z}^*(\cdot) - \tilde{Z}(\theta^*_0)) + (\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0)).$$

Note that the second term $\tilde{Z}(\theta^*) - \tilde{Z}(\theta^*_0) \leq 0$ almost surely by the DRO optimality of $\theta^*$. Therefore,

$$P[Z_0(\theta^*) - Z_0(\theta^*_0) > \varepsilon] \leq P[(Z_0(\theta^*) - \tilde{Z}(\theta^*)) + (\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0)) > \varepsilon]$$

$$\leq P[P_0 \notin K] + P[(Z_0(\theta^*) - \tilde{Z}(\theta^*)) + (\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0)) > \varepsilon, P_0 \in K].$$

Now, by definition of $\tilde{Z}(\cdot)$ as the worst-case objective function, we have $\tilde{Z}(\theta) \geq Z_0(\theta)$ for all $\theta \in \Theta$ as long as $P_0 \in K$. Thus,

$$P[Z_0(\theta^*) - Z_0(\theta^*_0) > \varepsilon] \leq P[P_0 \notin K] + P[\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0) > \varepsilon, P_0 \in K]$$

$$\leq P[P_0 \notin K] + P[\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0) > \varepsilon | P_0 \in K].$$

This completes our proof. □

A key feature of the bound in Theorem 1 is that it requires only the true loss function $l(\theta^*_0, \cdot)$. This contrasts sharply with ERM that relies on uniform bounds across the hypothesis class. To see where this distinction arises, note that in (8) we have divided $Z_0(\theta^*) - Z_0(\theta^*_0)$ into three parts where the second term is trivially $\leq 0$ and the third term depends only on the true loss. The key is that the first term satisfies

$$Z_0(\theta^*) - \tilde{Z}(\theta^*) = E_{\xi \sim P_0}[l(\theta^*, \xi)] - \max_{P \in K} E_{\xi \sim P}[l(\theta^*, \xi)] \leq 0$$

as long as $P_0 \in K$, thanks to the worst-case definition of the robust objective function $\tilde{Z}$. In contrast, in the ERM case, the same line of analysis gives

$$[Z_0(\theta^*) - \tilde{Z}(\theta^*)] + [\tilde{Z}(\theta^*) - \tilde{Z}(\theta^*_0)] + [\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0)]$$

and while the second and third terms are handled analogously, the first term needs to be handled by the uniform bound

$$\sup_{\theta \in \Theta} |E_{\xi \sim P_0}[l(\theta, \xi)] - E_{\xi \sim P}[l(\theta, \xi)]|$$

that requires empirical process analysis [Van Der Vaart and Wellner 1996] and the complexity of the hypothesis class $\{l(\theta, \cdot) : \theta \in \Theta\}$. Thus, in a sense, the worst-case nature of DRO “transfers” the uniformity requirement in the first term into alternate geometric requirements only on the true loss function.
3.1. Specialization to MMD DRO

Our next step is to use Theorem 1 to derive complexity-free generalization bounds for a concrete DRO formulation. In the following, we use ambiguity set $K$ as a neighborhood ball of the empirical distribution measured by statistical distance, namely

$$K = \{ P \in \mathcal{P} : D_{\text{MMD}}(P, \hat{P}) \leq \eta \}$$  \hspace{1cm} (10)$$

for a threshold $\eta > 0$. Moreover, we specialize in MMD as the choice of distance $D_{\text{MMD}}(\cdot, \cdot)$. To this end, let $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a positive definite kernel function on $\mathcal{X}$ and $(\mathcal{H}, \langle \cdot, \cdot \rangle_\mathcal{H})$ be the corresponding RKHS. For any distributions $P$ and $Q$, the MMD distance is defined by the maximum difference of the integrals over the unit ball $\{ f \in \mathcal{H} : \| f \|_\mathcal{H} \leq 1 \}$. That is,

$$D_{\text{MMD}}(P, Q) := \sup_{f \in \mathcal{H} : \| f \|_\mathcal{H} \leq 1} \int f dP - \int f dQ.$$  

In the sequel, we adopt bounded kernels, i.e., $\sup_{x, x' \in \mathcal{X}} \sqrt{k(x, x')} < +\infty$, to conduct our analysis. This assumption applies to many popular choices of kernel functions and guarantees the so-called kernel mean embedding (KME) (Muandet et al. 2017) is well-defined in RKHS, namely $\mu_P := \int k(x, \cdot) dP \in \mathcal{H}$ for any distribution $P$. This well-definedness of KME gives two important implications. One is that MMD is equivalent to the norm distance in KME: $D_{\text{MMD}}(P, Q) = \| \mu_P - \mu_Q \|_\mathcal{H}$ (Borgwardt et al. 2006, Gretton et al. 2012). Second, it bridges the expectation and the inner product in the RKHS space (Smola et al. 2007):

$$\mathbb{E}_{x \sim P}[f(x)] = \int_x \langle f, k(x, \cdot) \rangle dP(x) = \langle f, \mu_P \rangle, \forall f \in \mathcal{H}.$$  \hspace{1cm} (11)

Both properties above will facilitate our analysis. We refer the reader to Appendix A for further details on KME.

**Theorem 2 (Complexity-Free Generalization for MMD DRO).** Adopt the notation and assumptions in Theorem [1]. Let $\mathcal{X}$ be a compact subspace of $\mathbb{R}^d$, $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a bounded continuous positive definite kernel, and $(\mathcal{H}, \langle \cdot, \cdot \rangle_\mathcal{H})$ be the corresponding RKHS. Suppose also that (i) $\sup_{x \in \mathcal{X}} \sqrt{k(x, x')} \leq K$; (ii) $l(\theta_0^*, \cdot) \in \mathcal{H}$ with $\| l(\theta_0^*, \cdot) \|_\mathcal{H} \leq M$. Then, for all $\delta \geq 0$, an MMD DRO solution, i.e., (2) using $K$ in (10), and ball size $\eta = \frac{K}{\sqrt{\mathcal{N}}} (1 + \sqrt{2 \log(1/\delta)})$, satisfies

$$Z_0(\tilde{\theta}^r) - Z_0(\theta^*_0) \leq \frac{2KM}{\sqrt{n}} (1 + \sqrt{2 \log(1/\delta)})$$

with probability at least $1 - \delta$.

Theorem 2 has a matching convergence rate with ERM $O(n^{-1/2})$. More importantly, this generalization bound depends only on the true loss function $l(\theta_0^*, \cdot)$. This is substantially distinct from
generalization bounds of ERM [Vapnik and Chervonenkis 1991, Vershynin 2018, Wainwright 2019] typically in the form:

\[ Z_0(\hat{\theta}^*) - Z_0(\theta_0^*) \leq \mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{n}} + \sqrt{\frac{d_{\text{comp}}}{n}}\right), \]

which crucially relies on a hypothesis class complexity measure \(d_{\text{comp}}\) such as the VC-dimension.

Proof of Theorem 2. Starting from the bound (7) in Theorem 1 we separate our proof into two parts. For \(\mathbb{P}[P_0 \notin \mathcal{K}]\), we set \(\eta = \frac{K}{\sqrt{n}}(1 + 2\sqrt{\log(1/\delta)})\), noting that:

**Proposition 1.** (Tolstikhin et al. 2017, Proposition A.1) Let \(k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}\) be a continuous positive definite kernel on nonempty compact set \(\mathcal{X} \subset \mathbb{R}^d\) with \(\sup_{x \in \mathcal{X}} \sqrt{k(x, x)} \leq K < \infty\). Then for any \(\delta \in (0, 1)\) with probability at least \(1 - \delta\),

\[ \|\mu_P - \mu_{P_0}\|_\mathcal{H} \leq \frac{K}{\sqrt{n}}(1 + 2\sqrt{\log(1/\delta)}). \]

For the second term \(\mathbb{P}[\tilde{Z}(\theta_0^*) - Z_0(\theta_0^*) > \varepsilon | P_0 \in \mathcal{K}]\) in (7), conditional on \(P_0 \in \mathcal{K}\) we have that

\[ \tilde{Z}(\theta_0^*) - Z_0(\theta_0^*) = \max_{P \in \mathcal{K}} \mathbb{E}_{\xi \sim P}[l(\theta_0^*, \cdot)] - \mathbb{E}_{\xi \sim P_0}[l(\theta_0^*, \cdot)] = \max_{P \in \mathcal{K}} \max_{P \in \mathcal{K}} \|l(\theta_0^*, \cdot)\|_\mathcal{H} \|\mu_P - \mu_{P_0}\|_\mathcal{H} \leq 2M\eta, \]

where the second line follows from (11). Then, we have

\[ \tilde{Z}(\theta_0^*) - Z_0(\theta_0^*) = \max_{P \in \mathcal{K}} \|l(\theta_0^*, \cdot)\|_\mathcal{H} \|\mu_P - \mu_{P_0}\|_\mathcal{H} \leq 2M\eta, \]

where the first inequality follows from the Cauchy-Schwarz inequality, and the last inequality holds since for all \(P \in \mathcal{K}\),

\[ \|\mu_P - \mu_{P_0}\|_\mathcal{H} \leq \|\mu_P - \mu_{\hat{P}}\|_\mathcal{H} + \|\mu_{\hat{P}} - \mu_{P_0}\|_\mathcal{H} \leq 2\eta, \]

by the triangle inequality. Hence,

\[ \mathbb{P}[\tilde{Z}(\theta_0^*) - Z_0(\theta_0^*) > \varepsilon | P_0 \in \mathcal{K}] \leq \mathbb{P}[\max_{P \in \mathcal{K}} \|l(\theta_0^*, \cdot)\|_\mathcal{H} \|\mu_P - \mu_{P_0}\|_\mathcal{H} > \varepsilon | P_0 \in \mathcal{K}] = 0, \]

provided that \(\varepsilon \geq 2M\eta\). Therefore, with probability at least \(1 - \delta\),

\[ Z_0(\hat{\theta}^*) - Z_0(\theta_0^*) \leq 2M\eta = \frac{2KM}{\sqrt{n}}(1 + \sqrt{2\log(1/\delta)}). \]

This completes our proof. \(\square\)

The key in the proof of Theorem 2 lies in the bounds

\[ \tilde{Z}(\theta_0^*) - Z_0(\theta_0^*) \leq \max_{P \in \mathcal{K}} \|l(\theta_0^*, \cdot)\|_\mathcal{H} D_{\text{MMD}}(P, P_0) \leq 2M\eta, \]

which use the compatibility between \(\mathcal{K}\) and the true loss function \(l(\theta^*, \cdot)\), more specifically the RKHS norm on \(l(\theta_0^*, \cdot)\), and the established dimension-free property of KME (Proposition 1).
Our general bound in Theorem 1 allows us to stitch these two ingredients together to obtain the complexity-free generalization bound for MMD DRO.

To close this section, we contrast our result with Staib and Jegelka (2019), who establishes generalization bounds for MMD DRO in the form of (3) and (6). In particular, the latter bound in Staib and Jegelka (2019) relies on \( \sup_{\theta \in \Theta} \| l(\theta, \cdot) \|_H \), which depends on the entire hypothesis class. The main implication there is to obtain ERM generalization bounds of the canonical order \( 1/\sqrt{n} \), but with a constant that depends on \( \sup_{\theta \in \Theta} \| l(\theta, \cdot) \|_H \) instead of more common complexity measures.

### 3.2. Extending to More General Loss Functions

In Theorem 2, we obtain complexity-free generalization bounds for MMD DRO as long as (i) \( \sup_{x \in X} \sqrt{k(x, x)} \leq K \); (ii) \( l(\theta_0^*, \cdot) \in \mathcal{H} \) with \( \| l(\theta_0^*, \cdot) \|_H \leq M \). Although (i) is natural for many kernels, e.g., Gaussian kernel \( k(x, x') = \exp(-\|x - x'\|_2^2/\sigma^2) \), (ii) is rather restrictive since many popular loss functions do not lie in the corresponding RKHS. For instance, a Gaussian kernel defined on any \( X \subseteq \mathbb{R}^d \) with nonempty interior induces an RKHS \( \mathcal{H} \) that does not contain any nonzero polynomial on \( X \) (Minh 2010). This motivates us to extend our framework to more general loss functions outside the kernel space \( \mathcal{H} \).

To tackle this, Staib and Jegelka (2019) suggests the use of universal kernels (Steinwart 2001) since under such kernels, by definition, any bounded continuous function can be approximated arbitrarily well (in \( L^\infty \) norm) by functions in \( \mathcal{H} \). However, the RKHS norm of the approximating function, which appears in the final generalization bound, may grow arbitrarily large as the approximation becomes finer (Cucker and Zhou 2007, Yu and Szepesvári 2012). This therefore requires analyzing a trade-off between the function approximation error and RKHS norm magnitude. More specifically, we define the approximation rate

\[
I(l(\theta_0^*, \cdot), R) := \inf_{g: \|g\|_H \leq R} \|l(\theta_0^*, \cdot) - g\|_\infty
\]

and, as a concrete example, we adopt the Gaussian kernel and the Sobolev space in order to quantify such a rate and establish Theorem 3 below.

**Theorem 3 (Complexity-Free Generalization for Sobolev Loss Functions).** Let \( (\mathcal{H}, \| \cdot \|_H) \) be the RKHS induced by \( k(x, x') = \exp(-\|x - x'\|_2^2/\sigma^2) \) on \( X = [0,1]^d \). Suppose that \( l(\theta_0^*, \cdot) \) is in the Sobolev space \( H^d(\mathbb{R}^d) \). Then, there exists a constant \( C \) independent on \( R \) but dependent on \( l(\theta_0^*, \cdot) \), \( d \), and \( \sigma \) such that for all \( \delta \geq 0 \), an MMD DRO solution (2) using \( K \) in (10) with \( \eta = \frac{1}{\sqrt{n}}(1 + \sqrt{2\log(1/\delta)}) \) satisfies

\[
Z_0(\bar{\theta}) - Z_0(\theta_0^*) \leq 2 \inf_{R \geq 1} \left\{ C(\log R)^{-d/4} + \frac{R}{\sqrt{n}}(1 + \sqrt{2\log(1/\delta)}) \right\}
\]

with probability at least \( 1 - \delta \).
For Gaussian kernels on $[0,1]^d$, $I(l(\theta^*_0, \cdot), R) \leq C(\log R)^{-d/16}$ [Cucker and Zhou 2007] which appears in the first term of (12) as the function approximation error. With such an approximation in place, we then use properties of the approximation function, say $g_R \in \mathcal{H}$, to establish the generalization bound of $g_R$ in the second term. This latter term depends on $g_R$’s RKHS norm magnitude $R$ and we take infimum over $R \geq 1$ to establish the aforementioned trade-off.

**Proof of Theorem 3.** For notational simplicity, we denote

$$g_R := \arg \inf_{\|g\|_R \leq R} \|l(\theta^*_0, \cdot) - g\|_{C^\infty}$$

for all $R \geq 1$, where $g_R$ is well-defined since for fixed $R$, $h(g) = \|l(\theta^*_0, \cdot) - g\|_{C^\infty}$ is a continuous function over a compact set $\{g : \|g\|_R \leq R\}$. Then, by Theorem 1 and Proposition 1, for any $\delta > 0$, once we set $\eta = \frac{1}{\sqrt{n}}(1 + \sqrt{2\log(1/\delta)})$, we have that

$$\mathbb{P}\left[Z_0(\tilde{\theta}^*) - Z_0(\theta^*_0) > \varepsilon\right] \leq \mathbb{P}[\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0) > \varepsilon | P_0 \in \mathcal{K}] + \eta.$$ 

By definition, we obtain

$$\tilde{Z}(\theta^*_0) - Z_0(\theta^*_0) = \max_{P \in \mathcal{K}} \left\{ \int l(\theta^*_0, \xi) P(d\xi) - \int l(\theta^*_0, \xi) P_0(d\xi) \right\} \leq \max_{P \in \mathcal{K}} \left\{ \int g_R P(d\xi) - \int g_R P_0(d\xi) + 2\|l(\theta^*_0, \cdot) - g_R\|_{C^\infty} \right\} \leq \max_{P \in \mathcal{K}} \{\|g_R\|_R \|\mu_P - \mu_{P_0}\|_{\mathcal{H}}\} + 2\|l(\theta^*_0, \cdot) - g_R\|_{C^\infty} \leq 2(\eta R + \|l(\theta^*_0, \cdot) - g_R\|_{C^\infty}),$$

where the second equality follows from the Cauchy-Schwarz inequality. We have $\|l(\theta^*_0, \cdot) - g_R\|_{C^\infty} = I(l(\theta^*_0, \cdot), R) \leq C(\log R)^{-d/16}$ according to Cucker and Zhou (2007) Theorem 6.1 (and see Zhou 2013 Proposition 18 for details on the constants). Then, taking infimum over $R \geq 1$ and combining the equations above yield the desired result.  

In Theorem 3 we have to pay an extra price on the solution quality as the loss function is less compatible with the chosen RKHS, i.e., $l(\theta^*_0, \cdot) \notin \mathcal{H}$, when compared to Theorem 2. This results in a worse convergence rate in $n$. For example, inserting $R = \sqrt{n}(\log n)^{-d/16}$ into (12) yields

$$O(\max\{C, \sqrt{\log(1/\delta)}\}(\log n)^{-16/d}).$$

That being said, our result can potentially be improved if the true loss function has more regularity that allows faster, e.g., polynomially decaying $I(l(\theta^*_0, \cdot), R) = O(R^{-\beta})$. Nonetheless, Theorem 3 shows that, even relaxing the RKHS assumption on the true loss function, i.e., $l(\theta^*_0, \cdot) \notin \mathcal{H}$, a generalization bound that is free of complexity measures of the hypothesis class, still holds.

### 4. Numerical Experiments

We conduct simple experiments to study the numerical behaviors of our MMD DRO and comparisons with ERM on simulated data, which serves to illustrate the potential of MMD DRO in...
improving generalization and validate our developed theory. We adapt the experiment setups from 
Duchi and Namkoong (2019, Section 5.2) and consider a quadratic loss with linear perturbation:
\[ l(\theta, \xi) = \frac{1}{2} \| \theta - v \|_2^2 + \xi^T (\theta - v), \]
where \( \xi \sim \text{Unif}[-B, B]^d \) with constant \( B \) varying from \( \{1, 10, 100\} \) in the experiment. Here, \( v \) is chosen uniformly from \( [1/2, 1]^d \) and is known to the learner in advance. In applying MMD DRO, we use Gaussian kernel \( k(x, x') = \exp(-\|\xi - \xi'\|_2^2/\sigma^2) \) with \( \sigma \) set to the median of \( \{\|\xi_i - \xi_j\|_2 \mid \forall i, j\} \) according to the well-known median heuristic (Gretton et al. 2012). To solve MMD DRO, we adopt the semi-infinite dual program and the constraint sampling approach from Zhu et al. (2020), where we uniformly sample a constraint set of size equal to the data size \( n \). The sampled program is then solved by CVX (Grant and Boyd 2014) and MOSEK (ApS 2021). Each experiment is the average performance of 500 independently trials. Our computational environment is a Mac mini with Apple M1 chip, 8 GB RAM and all algorithms are implemented in Python 3.8.3.

In Figure 1(a), we present the excess risks of ERM and DRO, i.e., \( Z_0(\theta_{\text{data}}) - Z_0(\theta^*) \), where \( \theta_{\text{data}} \) denotes the ERM or DRO solution. We set \( d = 5 \) and tune the ball size via the best among \( \eta \in \{0.01, 0.1, 0.2, \ldots, 1.0\} \) (more details to be discussed on Figure 1(b) momentarily). Figure 1(a) shows that, as \( n \) increases, both DRO and ERM incur a decreasing loss. More importantly, DRO appears to perform much better than ERM. For \( n = 200 \) and \( B = 100 \) for instance, the expected loss of DRO is less than \( 10^{-19} \), yet that of ERM remains at around \( 10^1 \).

We attribute the outperformance of DRO to our complexity-free generalization behavior. This can be supported by an illustration on the effect of ball size \( \eta \). In Figure 1(b), we present excess risk \( Z_0(\theta_{\text{data}}) - Z_0(\theta^*) \) for \( d = 5, n = 50 \), and varying \( B, \eta \). We see that the excess risk of the DRO solution drops sharply when \( \eta \) is small, and then for sufficiently big \( \eta \), i.e., \( \eta \in [0.2, 1] \), it remains at a fixed level of \( 10^{-19} \), which is close to the machine accuracy of zero (such an “L”-shape excess
loss also occurs under other choices of sample size $n$, and we leave out those results to avoid redundancy). Such a phenomenon coincides with our theorems. First, note that $\theta_0^* = v$ and the optimal loss function satisfies $\|l(\theta_0^*, \cdot)\|_H = \|0\|_H = 0$, so that our assumptions in Theorem 2 are satisfied. Recall that by Theorem 1,

$$
\Pr[Z_0(\bar{\theta}^*) - Z_0(\theta_0^*) > \varepsilon] \leq \Pr[P_0 \notin K] + \Pr[Z(\theta_0^*) - Z_0(\theta_0^*) > \varepsilon | P_0 \in K].
$$

(13)

Conditioning on $P_0 \in K$, $\bar{\theta}^* = \theta_0^* = v$ with $Z(\bar{\theta}^*) = Z_0(\theta_0^*) = 0$. Therefore, (13) yields $\Pr[Z_0(\bar{\theta}^*) - Z_0(\theta_0^*) > \varepsilon] \leq \Pr[P_0 \notin K]$. The proof of Theorem 2 reveals that for all $\delta > 0$, if the ball size is big enough, namely $\delta \geq K \sqrt{n (1 + \sqrt{2 \log(1/\delta)})}$, then the excess risk will vanish, i.e., $Z_0(\bar{\theta}^*) - Z_0(\theta_0^*) = 0$, with probability at least $1 - \delta$. This behavior shows up precisely in Figure 1(b).

Our discussion above is not to suggest the choice of $\eta$ in practice. Rather, it serves as a conceptual proof for the correctness of our theorem. In fact, to the best of our knowledge, none of the previous results, including the multiple approaches to explain the generalization of DRO reviewed in Section 2, can explain the strong outperformance of DRO with the “L”-shape phenomenon in this example. These previous results focus on either absolute bounds (Section 2.1) or using variability regularization (Section 2.2) whose bounds, when converted to excess risks, typically increase in $\eta$ when $\eta$ is sufficiently large and, moreover, involve complexity measures on the hypothesis class due to the use of uniform bounds (e.g., the $\phi$-divergence case in Duchi and Namkoong 2019 Theorems 3, 6 and the Wasserstein case in Gao 2020 Corollaries 2, 4). Our developments in Section 3 thus appear to provide a unique explanation for the significant outperformance of DRO in this example.

### Appendix A: Review on KME

We first review the definition of kernel mean embedding (KME).

**Definition 1** (Kernel Mean Embedding). Given a distribution $P$, and a positive definite kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, i.e., $\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j k(x_i, x_j) \geq 0$ holds for any $x_1, \ldots, x_n \in \mathcal{X}$, given $n \in \mathbb{N}, a_1, \ldots, a_n \in \mathbb{R}$, the KME of $P$ is defined by: $\mu_P := \int k(x, \cdot) P(dx)$.

We have the following property.

**Proposition 2.** (Smola et al. 2007) For a positive definite kernel $k$ defined on compact space $\mathcal{X} \times \mathcal{X}$, let $H$ be the induced RKHS. If $\mathbb{E}_{x \sim P} [k(x, x)] < +\infty$, then $\mu_P \in H$ for all $P \in \mathcal{P}$.

It is easy to verify that for a bounded kernel, $\mathbb{E}_{x \sim P} [k(x, x)] < +\infty$ for all distribution $P$. Therefore, as a corollary of Proposition 2 for any bounded kernel, KME is well-defined in RKHS, i.e., $\mu_P \in H$.

The following proposition provides the properties of KME that we utilize in Section 3.1. Specifically, Proposition 3(i) establishes the equivalence between MMD and the norm distance in KME. Proposition 3(ii) bridges the expectation to inner product in RKHS in (11).

**Proposition 3.** Assume the condition in Proposition 2 for the existence of the kernel mean embeddings $\mu_p, \mu_q$ is satisfied. Then,
(i) (Borgwardt et al. 2006, Gretton et al. 2012) $D_{MMD}(P,Q) = \|\mu_P - \mu_Q\|_H$;

(ii) (Smola et al. 2007) $\mathbb{E}_{x \sim P}[f(x)] = \langle f, \mu_P \rangle_H$.

Finally, we review the result in Cucker and Zhou (2007) used in Section 3.2.

**Theorem 4.** (Cucker and Zhou 2007, Theorem 6.1) Let $(\mathcal{H}, \| \cdot \|_H)$ be the RKHS induced by $k(x,x') = \exp(-\|x - x'\|^2/\sigma^2)$ on $X = [0,1]^d$. Suppose that $l(\theta^*_0, \cdot)$ is in the Sobolev space $H^d(\mathbb{R}^d)$. Then, there exists a constant $C$ independent on $R$ but dependent on $f, d,$ and $\sigma$ such that

$$\inf_{\|g\|_H \leq R} \|l(\theta^*_0, \cdot) - g\|_{C^\infty} \leq C(\log R)^{\frac{d}{16}}, \forall R \geq 1.$$

**Acknowledgments**

We gratefully acknowledge support from the National Science Foundation under grants CAREER CMMI-1834710 and IIS-1849280.

**References**

ApS M (2021) *The MOSEK optimization toolbox for Python manual. Version 9.2.46*. URL [https://docs.mosek.com/9.2/pythonfusion/index.html](https://docs.mosek.com/9.2/pythonfusion/index.html).

Bartlett PL, Bousquet O, Mendelson S, et al. (2005) Local Rademacher complexities. *The Annals of Statistics* 33(4):1497–1537.

Bayraksan G, Love DK (2015) Data-driven stochastic programming using phi-divergences. *Tutorials in Operations Research*, 1–19 (INFORMS).

Ben-Tal A, Den Hertog D, De Waegenaere A, Melenberg B, Rennen G (2013) Robust solutions of optimization problems affected by uncertain probabilities. *Management Science* 59(2):341–357.

Ben-Tal A, El Ghaoui L, Nemirovski A (2009) *Robust Optimization* (Princeton University Press).

Bertsimas D, Brown DB, Caramanis C (2011) Theory and applications of robust optimization. *SIAM Review* 53(3):464–501.

Bertsimas D, Gupta V, Kallus N (2018) Robust sample average approximation. *Mathematical Programming* 171(1-2):217–282.

Blanchet J, Kang Y (2021) Sample out-of-sample inference based on Wasserstein distance. *Operations Research*.

Blanchet J, Kang Y, Murthy K (2019a) Robust Wasserstein profile inference and applications to machine learning. *Journal of Applied Probability* 56(3):830–857.

Blanchet J, Murthy K (2019) Quantifying distributional model risk via optimal transport. *Mathematics of Operations Research* 44(2):565–600.

Blanchet J, Murthy K, Si N (2019b) Confidence regions in Wasserstein distributionally robust estimation. *arXiv preprint arXiv:1906.01614*.
Borgwardt KM, Gretton A, Rasch MJ, Kriegel HP, Schölkopf B, Smola AJ (2006) Integrating structured biological data by kernel maximum mean discrepancy. *Bioinformatics* 22(14):e49–e57.

Chen L, Ma W, Natarajan K, Simchi-Levi D, Yan Z (2018) Distributionally robust linear and discrete optimization with marginals. *Available at SSRN 3159473*.

Chen R, Paschalidis IC (2018) A robust learning approach for regression models based on distributionally robust optimization. *Journal of Machine Learning Research* 19(13).

Chen X, He S, Jiang B, Ryan CT, Zhang T (2020) The discrete moment problem with nonconvex shape constraints. *Operations Research*.

Cucker F, Zhou DX (2007) *Learning Theory: An Approximation Theory Viewpoint*, volume 24 (Cambridge University Press).

Delage E, Ye Y (2010) Distributionally robust optimization under moment uncertainty with application to data-driven problems. *Operations Research* 58(3):595–612.

Dhara A, Das B, Natarajan K (2021) Worst-case expected shortfall with univariate and bivariate marginals. *INFORMS Journal on Computing* 33(1):370–389.

Doan XV, Li X, Natarajan K (2015) Robustness to dependency in portfolio optimization using overlapping marginals. *Operations Research* 63(6):1468–1488.

Duchi J, Hashimoto T, Namkoong H (2020) Distributionally robust losses for latent covariate mixtures. *arXiv preprint arXiv:2007.13982*.

Duchi J, Namkoong H (2018) Learning models with uniform performance via distributionally robust optimization. *arXiv preprint arXiv:1810.08750*.

Duchi JC, Glynn PW, Namkoong H (2021) Statistics of robust optimization: A generalized empirical likelihood approach. *Mathematics of Operations Research*.

Duchi JC, Namkoong H (2019) Variance-based regularization with convex objectives. *Journal of Machine Learning Research* 20:68–1.

Esfahani PM, Kuhn D (2018) Data-driven distributionally robust optimization using the Wasserstein metric: Performance guarantees and tractable reformulations. *Mathematical Programming* 171(1-2):115–166.

Gao R (2020) Finite-sample guarantees for Wasserstein distributionally robust optimization: Breaking the curse of dimensionality. *arXiv preprint arXiv:2009.04382*.

Gao R, Chen X, Kleywegt AJ (2017) Wasserstein distributionally robust optimization and variation regularization. *arXiv preprint arXiv:1712.06050*.

Gao R, Kleywegt AJ (2016) Distributionally robust stochastic optimization with Wasserstein distance. *arXiv preprint arXiv:1604.02199*.

Ghaoui LE, Oks M, Oustry F (2003) Worst-case value-at-risk and robust portfolio optimization: A conic programming approach. *Operations Research* 51(4):543–556.
Glasserman P, Xu X (2014) Robust risk measurement and model risk. *Quantitative Finance* 14(1):29–58.

Goh J, Sim M (2010) Distributionally robust optimization and its tractable approximations. *Operations Research* 58(4-Part-1):902–917.

Goodfellow IJ, Shlens J, Szegedy C (2015) Explaining and harnessing adversarial examples. *International Conference on Learning Representations*.

Gotoh Jy, Kim MJ, Lim AE (2018) Robust empirical optimization is almost the same as mean–variance optimization. *Operations Research Letters* 46(4):448–452.

Gotoh Jy, Kim MJ, Lim AE (2021) Calibration of distributionally robust empirical optimization models. *Operations Research*.

Grant M, Boyd S (2014) CVX: Matlab software for disciplined convex programming, version 2.1.

Gretton A, Borgwardt KM, Rasch MJ, Schölkopf B, Smola A (2012) A kernel two-sample test. *Journal of Machine Learning Research* 13(1):723–773.

Grünewälder S, Lever G, Gretton A, Baldassarre L, Patterson S, Pontil M (2012) Conditional mean embeddings as regressors. *International Conference on Machine Learning*.

Gupta V (2019) Near-optimal Bayesian ambiguity sets for distributionally robust optimization. *Management Science* 65(9):4242–4260.

Hanasusanto GA, Roitch V, Kuhn D, Wiesemann W (2015) A distributionally robust perspective on uncertainty quantification and chance constrained programming. *Mathematical Programming* 151(1):35–62.

Hansen LP, Sargent TJ (2008) *Robustness* (Princeton University Press).

Hashimoto T, Srivastava M, Namkoong H, Liang P (2018) Fairness without demographics in repeated loss minimization. *International Conference on Machine Learning*, 1929–1938 (PMLR).

Jiang R, Guan Y (2016) Data-driven chance constrained stochastic program. *Mathematical Programming* 158(1):291–327.

Kirschner J, Bogunovic I, Jegelka S, Krause A (2020) Distributionally robust Bayesian optimization. *Artificial Intelligence and Statistics*, 2174–2184 (PMLR).

Kuhn D, Esfahani PM, Nguyen VA, Shafieezadeh-Abadeh S (2019) Wasserstein distributionally robust optimization: Theory and applications in machine learning. *Operations Research & Management Science in the Age of Analytics*, 130–166 (INFORMS).

Kurakin A, Goodfellow IJ, Bengio S (2017) Adversarial machine learning at scale. *International Conference on Learning Representations*.

Lam H (2016) Robust sensitivity analysis for stochastic systems. *Mathematics of Operations Research* 41(4):1248–1275.

Lam H (2018) Sensitivity to serial dependency of input processes: A robust approach. *Management Science* 64(3):1311–1327.
Lam H (2019) Recovering best statistical guarantees via the empirical divergence-based distributionally robust optimization. *Operations Research* 67(4):1090–1105.

Lam H, Mottet C (2017) Tail analysis without parametric models: A worst-case perspective. *Operations Research* 65(6):1696–1711.

Lam H, Zhou E (2017) The empirical likelihood approach to quantifying uncertainty in sample average approximation. *Operations Research Letters* 45(4):301 – 307, ISSN 0167-6377.

Li B, Jiang R, Mathieu JL (2017) Ambiguous risk constraints with moment and unimodality information. *Mathematical Programming* 1–42.

Li Y, Swersky K, Zemel R (2015) Generative moment matching networks. *International Conference on Machine Learning*, 1718–1727 (PMLR).

Liu J, Shen Z, Cui P, Zhou L, Kuang K, Li B, Lin Y (2021) Stable adversarial learning under distributional shifts. *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 35, 8662–8670.

Madry A, Makelov A, Schmidt L, Tsipras D, Vladu A (2018) Towards deep learning models resistant to adversarial attacks. *International Conference on Learning Representations*.

Minh HQ (2010) Some properties of Gaussian reproducing kernel Hilbert spaces and their implications for function approximation and learning theory. *Constructive Approximation* 32(2):307–338.

Muandet K, Fukumizu K, Sriperumbudur B, Schölkopf B (2017) Kernel mean embedding of distributions: A review and beyond. *Foundations and Trends® in Machine Learning* 10(1-2):1–141, ISSN 1935-8237.

Müller A (1997) Integral probability metrics and their generating classes of functions. *Advances in Applied Probability* 429–443.

Nguyen TT, Gupta S, Venkatesh S (2020) Distributional reinforcement learning with maximum mean discrepancy. *arXiv preprint arXiv:2007.12354*.

Petersen IR, James MR, Dupuis P (2000) Minimax optimal control of stochastic uncertain systems with relative entropy constraints. *IEEE Transactions on Automatic Control* 45(3):398–412.

Popescu I (2005) A semidefinite programming approach to optimal-moment bounds for convex classes of distributions. *Mathematics of Operations Research* 30(3):632–657.

Rockafellar RT (2007) Coherent approaches to risk in optimization under uncertainty. *OR Tools and Applications: Glimpses of Future Technologies*, 38–61 (Informs).

Ruszczynski A, Shapiro A (2006) Optimization of convex risk functions. *Mathematics of Operations Research* 31(3):433–452.

Sagawa S, Koh PW, Hashimoto TB, Liang P (2020) Distributionally robust neural networks. *International Conference on Learning Representations*.

Scarf H (1958) A min-max solution of an inventory problem. *Studies in the Mathematical Theory of Inventory and Production*. 
Shafieezadeh-Abadeh S, Kuhn D, Esfahani PM (2019) Regularization via mass transportation. *Journal of Machine Learning Research* 20(103):1–68.

Shawe-Taylor J, Cristianini N, et al. (2004) *Kernel Methods for Pattern Analysis* (Cambridge University Press).

Sinha A, Namkoong H, Duchi JC (2018) Certifying some distributional robustness with principled adversarial training. *International Conference on Learning Representations*.

Smola A, Gretton A, Song L, Schölkopf B (2007) A Hilbert space embedding for distributions. *International Conference on Algorithmic Learning Theory*, 13–31 (Springer).

Staib M, Jegelka S (2019) Distributionally robust optimization and generalization in kernel methods. *Advances in Neural Information Processing Systems*, 9131–9141.

Steinwart I (2001) On the influence of the kernel on the consistency of support vector machines. *Journal of Machine Learning Research* 2(Nov):67–93.

Sutherland DJ, Tung H, Strathmann H, De S, Ramdas A, Smola AJ, Gretton A (2017) Generative models and model criticism via optimized maximum mean discrepancy. *International Conference on Learning Representations*.

Sutter T, Van Parys BP, Kuhn D (2020) A general framework for optimal data-driven optimization. *arXiv preprint arXiv:2010.06606*.

Tolstikhin I, Sriperumbudur BK, Muandet K (2017) Minimax estimation of kernel mean embeddings. *Journal of Machine Learning Research* 18(1):3002–3048.

Tsipras D, Santurkar S, Engstrom L, Turner A, Madry A (2019) Robustness may be at odds with accuracy. *International Conference on Learning Representations*.

Van Der Vaart AW, Wellner JA (1996) *Weak Convergence and Empirical Processes* (Springer).

Van Parys BP, Esfahani PM, Kuhn D (2020) From data to decisions: Distributionally robust optimization is optimal. *Management Science*.

Van Parys BP, Goulart PJ, Kuhn D (2016) Generalized Gauss inequalities via semidefinite programming. *Mathematical Programming* 156(1-2):271–302.

Vapnik V, Chervonenkis A (1991) The necessary and sufficient conditions for consistency in the empirical risk minimization method. *Pattern Recognition and Image Analysis* 1(3):283–305.

Vershynin R (2018) *High-Dimensional Probability: An Introduction with Applications in Data Science*, volume 47 (Cambridge University Press).

Wainwright MJ (2019) *High-Dimensional Statistics: A Non-Asymptotic Viewpoint*, volume 48 (Cambridge University Press).

Wiesemann W, Kuhn D, Sim M (2014) Distributionally robust convex optimization. *Operations Research* 62(6):1358–1376.
Xu H, Caramanis C, Mannor S (2009) Robustness and regularization of support vector machines. *Journal of Machine Learning Research* 10(7).

Xu H, Caramanis C, Mannor S (2010) Robust regression and Lasso. *IEEE Transactions on Information Theory* 56(7):3561–3574.

Xu H, Mannor S (2012) Robustness and generalization. *Machine Learning* 86(3):391–423.

Yu Y, Szepesvári C (2012) Analysis of kernel mean matching under covariate shift. *International Conference on Machine Learning*.

Zhang Y, Shen S, Mathieu JL (2016) Distributionally robust chance-constrained optimal power flow with uncertain renewables and uncertain reserves provided by loads. *IEEE Transactions on Power Systems* 32(2):1378–1388.

Zhao C, Jiang R (2017) Distributionally robust contingency-constrained unit commitment. *IEEE Transactions on Power Systems* 33(1):94–102.

Zhou DX (2013) Density problem and approximation error in learning theory. *Abstract and Applied Analysis*, volume 2013 (Hindawi).

Zhu JJ, Jitkrittum W, Diehl M, Schölkopf B (2020) Kernel distributionally robust optimization. *arXiv preprint arXiv:2006.06981* .