Probable Domain Generalization
via Quantile Risk Minimization

Abstract

Domain generalization (DG) seeks predictors which perform well on unseen test distributions by leveraging labeled training data from multiple related distributions or *domains*. To achieve this, ==DG is commonly formulated== as a worst-case optimization problem over the set of all possible domains. However, with worst-case shifts unlikely in practice, this generally leads to overly-conservative solutions. In fact, a recent study found that no DG algorithm outperformed empirical risk minimization in terms of average performance. In this work, we argue that DG is neither a worst-case problem nor an average-case problem, but rather a probabilistic one. To this end, we propose a probabilistic framework for DG, which we call *Probable Domain Generalization*, wherein our key idea is that distribution shifts seen during training should inform us of *probable* shifts at test time. To realize this, we explicitly relate training and test domains as draws from the same underlying meta-distribution, and propose a new optimization problem—*Quantile Risk Minimization* (QRM)—which requires that predictors *generalize with high probability*. We then prove that QRM: (i) produces predictors that generalize to new domains with a desired probability, given sufficiently many domains and samples; and (ii) recovers the causal predictor as the desired probability of generalization approaches one. In our experiments, we introduce a more holistic quantile-focused evaluation protocol for DG, and show that our algorithms outperform state-of-the-art baselines on real and synthetic data.

1 Introduction

Despite remarkable successes in recent years [1–3], machine learning systems often fail calamitously when presented with *out-of-distribution* (OOD) data [4–7]. In fact, evidence of state-of-the-art systems failing in the face of distribution shift is mounting rapidly—be it due to spurious correlations [8–10], changing sub-populations [11–13], changes in location or time [14–16], or other naturally-occurring variations [17–23]. These OOD failures are particularly concerning in safety-critical applications such as medical imaging [24–28] and autonomous driving [29–31], where they represent one of the most significant barriers to real-world deployment [32–35].

Domain generalization (DG) seeks to improve a system's OOD performance by leveraging datasets from multiple environments or *domains* at training time, each collected under different experimental conditions [36–38]. The goal is to build a predictor which exploits invariances across the training domains in the hope that these invariances also hold in related but distinct test domains [38–41]. To realize this goal, ==DG is commonly formulated== as a *worst-case* optimization problem over the set of all possible domains. However, this problem is generally intractable [42–44] and, with worst-case shifts unlikely in practice, leads to overly-conservative solutions—making large accuracy sacrifices in pursuit of adversarial robustness. In fact, a recent study [38] found that, across several popular datasets, no DG algorithm outperformed *empirical risk minimization* (ERM) in terms of *average performance*.

In this work, we argue that DG is neither a worst-case problem *nor* an average-case problem, but rather a probabilistic one. In particular, we advocate for predictors which perform well *with high probability* rather than in the worst case or on average. To this end, we propose a probabilistic

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Figure 1: **Overview of Probable Domain Generalization and quantile risk.** (a) Domains differ due to changes in (or interventions on) an underlying system of variables, e.g. hospitals with different equipment, procedures, etc. Hammers depict interventions. (b) Training and test domains are randomly sampled from the same underlying meta-distribution over domains $\mathbb{Q}(e)$. (c) Estimated risk distribution over training domains for a fixed predictor. The α-quantile is an upper bound on the test risk which holds with probability $\approx \alpha$.

framework for DG which we call *Probable Domain Generalization*. The key idea is that distribution shifts seen during training should inform us of *probable* shifts at test time since they represent the ways in which the underlying system tends to change (Fig. 1a). To realize this, we explicitly relate training and test domains as draws from the same underlying meta-distribution (Fig. 1b), and then propose *Quantile Risk Minimization* (QRM)—a new optimization problem for learning predictors that *generalize with high probability* (§ 3). The goal of QRM is to minimize the α-quantile of a predictor's risk distribution over training domains, leveraging the key insight that this α-quantile is an upper bound on the test risk which holds with probability α (Fig. 1c).

We then prove that QRM: (i) produces predictors that generalize to new domains with probability α, given sufficiently many domains and samples (§ 4); and (ii) recovers the causal predictor as $\alpha \to 1$, under weaker assumptions than Peters et al. [45]. Thus, α is an interpretable conservativeness-hyperparameter, with $\alpha = 1$ corresponding to the worst-case setting. In our experiments (§ 6), we introduce a more holistic quantile-focused evaluation protocol for DG, and demonstrate that: (i) the performance of DG algorithms was likely never "lost" [38], but rather invisible through the lens of average performance; and (ii) our algorithms outperform strong baselines on real and synthetic datasets.

Contributions. To summarize our main contributions, we:

- Propose *Quantile Risk Minimization* for learning predictors that generalize with probability α (§ 3).
- Prove that, given sufficiently many domains and samples, QRM does indeed produce predictors that generalize to new domains with probability α (Thm. 4.1).
- Prove that QRM recovers the causal predictor as $\alpha \to 1$ (Prop. 4.3 and Thm. 4.4).
- Demonstrate empirically that: (i) effective comparison of DG algorithms requires evaluating quantile performance; and (ii) our algorithms outperform strong baselines on real and synthetic data (§ 6).

2 Background

Domain generalization (DG). In DG, predictors are trained on data drawn from multiple related training distributions or *domains* and then evaluated on related but unseen test domains. For example, in the `Camelyon17` dataset [46], the task is to predict if a given image of cells contains tumor tissue, and domains correspond to different hospitals in which these images were captured. More formally, we consider datasets $D^e = \{(x_i^e, y_i^e)\}_{i=1}^{n_e}$ collected from m different training domains or *environments* $\mathcal{E}_{\text{tr}} := \{e_1, \dots, e_m\}$, with each dataset D^e containing data pairs (x_i^e, y_i^e) sampled i.i.d. from $\mathbb{P}(X^e, Y^e)$. Then, given a suitable function class $\mathcal{F}$ and loss function ℓ, the goal of DG is to learn a predictor $f \in \mathcal{F}$ that generalizes to data drawn from a larger set of all possible domains $\mathcal{E}_{\text{all}} \supset \mathcal{E}_{\text{tr}}$. By letting $\mathcal{R}^e(f)$ denote the statistical risk of f in domain e, this is commonly [9, 22, 41, 47–49] formalized as the following minimax optimization problem:

$$\min_{f \in \mathcal{F}} \max_{e \in \mathcal{E}_{\text{all}}} \mathcal{R}^e(f) \qquad \text{where} \qquad \mathcal{R}^e(f) := \mathbb{E}_{\mathbb{P}(X^e, Y^e)}[\ell(f(X^e), Y^e)]. \qquad \text{(DG)}$$

As we only have access to data from a finite subset of $\mathcal{E}_{\text{all}}$ during training, solving (DG) is not just challenging but in fact impossible [41, 50, 51] without restrictions on how the domains may differ.

Causality and invariance in DG. Causal works on DG [9, 41, 45, 51, 52] describe domain differences using the language of causality and the notion of *interventions* [53, 54]. In particular, they

assume all domains share the same underlying *structural causal model* (SCM) [53], with different domains corresponding to different interventions (see Appendix A.1 for formal definitions and a simple example). Early work studied the problem of learning from multiple cause-effect datasets that share a functional mechanism but differ in noise distributions [39]. More generally, given (data from) multiple distributions, one can try to identify components which are stable, robust, or *invariant*, and find means to transfer them across problems [55–59]. Assuming that the mechanism of Y remains fixed or invariant[1] but all Xs may be intervened upon, recent works have shown that only the causal predictor: (i) has invariant predictive distributions [45], coefficients [9], or risks [41] across domains; and (ii) generalizes to arbitrary interventions on the Xs [9, 45, 52]. These works then exploit such insights by leveraging some form of invariance across domains to discover causal relationships which, through the invariant mechanism assumption, generalize to new domains.

3   Quantile Risk Minimization

In this section we introduce *Quantile Risk Minimization* (QRM) for achieving *probable* domain generalization. The core idea is to replace the worst-case perspective of (DG) with a probabilistic one. This approach is founded on a great deal of work in classical fields such as control theory [60, 61] and smoothed analysis [62], wherein approaches that yield high-probability guarantees are used in place of worst-case approaches in an effort to mitigate conservatism and computational limitations. This mitigation is of particular interest in domain generalization since generalizing to arbitrary domains is impossible [41, 50, 51]. Thus, motivated by this classical literature, our goal is to obtain predictors that are robust *with high probability* over domains drawn from $\mathcal{E}_{\text{all}}$, rather than in the worst-case.

A distribution over environments. We start by assuming the existence of a probability distribution $\mathbb{Q}(e)$ over the set of all environments $\mathcal{E}_{\text{all}}$. For instance, in the context of medical imaging, $\mathbb{Q}$ could represent a distribution over potential changes to a hospital's setup (see Fig. 1a) or simply a distribution over candidate hospitals. Given that such a distribution $\mathbb{Q}$ exists[2], we can think of the risk $\mathcal{R}^e(f)$ as a *random variable* for each $f \in \mathcal{F}$, where the randomness is engendered by the draw of $e \sim \mathbb{Q}$. This perspective gives rise to the following analogue of the optimization problem in (DG):

$$\min_{f \in \mathcal{F}} \operatorname*{ess\,sup}_{e \sim \mathbb{Q}} \mathcal{R}^e(f) \quad \text{where} \quad \operatorname*{ess\,sup}_{e \sim \mathbb{Q}} \mathcal{R}^e(f) = \inf \left\{ t \geq 0 : \Pr_{e \sim \mathbb{Q}} \left\{ \mathcal{R}^e(f) \leq t \right\} = 1 \right\} \quad (3.1)$$

Here, ess sup denotes the *essential-supremum* operator from measure theory, meaning that for each $f \in \mathcal{F}$, $\operatorname{ess\,sup}_{\mathbb{Q}} \mathcal{R}^e(f)$ is the least upper bound on $\mathcal{R}^e(f)$ that holds for almost every $e \sim \mathbb{Q}$. In this way, the ess sup in (3.1) is the measure-theoretic analogue of the max operator in (DG), with the subtle but critical difference being that the ess sup in (3.1) can neglect domains of measure zero under $\mathbb{Q}$. For example, for discrete $\mathbb{Q}$, (3.1) ignores domains which are impossible (zero probability) while (DG) does not, laying the foundation for ignoring domains which are *improbable*.

High-probability generalization. Although the minimax problem in (3.1) explicitly incorporates the distribution $\mathbb{Q}$ over environments, this formulation is no less conservative than (DG). Indeed, in many cases, (3.1) is equivalent to (DG); see Appendix B for details. Therefore, rather than considering the worst-case problem in (3.1), we propose the following generalization of (3.1) which requires that predictors generalize with probability α rather than in the worst-case:

$$\min_{f \in \mathcal{F}, t \in \mathbb{R}} t \qquad \text{subject to} \qquad \Pr_{e \sim \mathbb{Q}} \left\{ \mathcal{R}^e(f) \leq t \right\} \geq \alpha \qquad (3.2)$$

The optimization problem of (3.2) formally defines what we mean by *probable* domain generalization. In particular, we say that *a predictor f generalizes with risk t at level α* if f has risk at most t with probability at least α over domains sampled from $\mathbb{Q}$. In this way, the conservativeness parameter α controls the strictness of generalizing to unseen domains.

A distribution over risks. The optimization problem presented in (3.2) offers a principled formulation for generalizing to unseen distributional shifts governed by $\mathbb{Q}$. However, $\mathbb{Q}$ is often unknown in practice and its support $\mathcal{E}_{\text{all}}$ may be high-dimensional or challenging to define [22]. While many previous works have made progress by limiting the scope of possible shift types over domains [19, 22, 48], in practice, such structural assumptions are often difficult to justify and impossible to test. For this reason, we start our exposition of QRM by offering an alternative view of (3.2) which elucidates how a predictor's *risk distribution* plays a central role in achieving probable domain generalization.

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[1]Arjovsky et al. [9] allow the noise variance of Y to vary.

[2]As $\mathbb{Q}$ is often unknown, our analysis does not rely on leveraging an explicit expression for $\mathbb{Q}$.

To begin, note that for each $f \in \mathcal{F}$, the distribution over domains $\mathbb{Q}$ naturally induces[3] a distribution $\mathbb{T}_f$ over the risks in each domain $\mathcal{R}^e(f)$. In this way, rather than considering the randomness of $\mathbb{Q}$ in the often-unknown and (potentially) high-dimensional space of possible shifts or interventions (Figs. 1a and 1b), one can consider it in the real-valued space of risks (Fig. 1c). This is analogous to statistical learning theory, where the analysis of convergence of empirical risk minimizers (i.e., of functions) is substituted by that of a weaker form of convergence, namely that of scalar risk functionals—a crucial step for VC theory [63]. From this perspective, the statistics of $\mathbb{T}_f$ can be thought of as capturing the sensitivity of f to different environmental shifts, summarizing the effect of different intervention types, strengths, and frequencies. To this end, (3.2) can be equivalently rewritten in terms of the risk distribution $\mathbb{T}_f$ as follows:

$$\min_{f \in \mathcal{F}} F_{\mathbb{T}_f}^{-1}(\alpha) \quad \text{where} \quad F_{\mathbb{T}_f}^{-1}(\alpha) := \inf \left\{ t \in \mathbb{R} : \Pr_{R \sim \mathbb{T}_f} \{R \leq t\} \geq \alpha \right\}. \tag{QRM}$$

Here, $F_{\mathbb{T}_f}^{-1}(\alpha)$ denotes the inverse CDF (or quantile) function of the risk distribution $\mathbb{T}_f$. By means of this reformulation, we elucidate how solving (QRM) amounts to finding a predictor with minimal α-quantile risk. That is, (QRM) requires that a predictor f satisfy the probabilistic constraint for at least an α-fraction of the risks $R \sim \mathbb{T}_f$, or, equivalently, for an α-fraction of the environments $e \sim \mathbb{Q}$. In this way, by varying α, (QRM) recovers several notable objectives for DG as special cases, namely a worst-case problem with $\alpha = 1$ and an average-case problem with $\alpha = 0.5$ (median).

Proposition 3.1. *For $\alpha = 1$, (QRM) is equivalent to the minimax problem of (3.1). Furthermore, if the mean and median of $\mathbb{T}_f$ coincide for all $f \in \mathcal{F}$, then for $\alpha = 1/2$, (QRM) is equivalent to (expected) risk minimization (RM, [63]) in which $\mathbb{T}_f$ is the uniform distribution*

$$\min_{f \in \mathcal{F}} \mathbb{E}_{R \sim \mathbb{T}_f} R = \min_{f \in \mathcal{F}} \mathbb{E}_{e \sim \mathbb{Q}} \mathcal{R}^e(f) \tag{3.3}$$

4 Algorithms for Quantile Risk Minimization

In this section we introduce two algorithms for empirically solving (QRM): empirical QRM (EQRM) and empirical superquantile RM (ESQRM).

4.1 Empirical QRM

Estimated risk distribution. In practice, given a predictor f and its empirical risks $\hat{\mathcal{R}}^{e_1}(f), \ldots, \hat{\mathcal{R}}^{e_m}(f)$ on the m training domains, we must form an *estimated* risk distribution $\widehat{\mathbb{T}}_f$. If we have prior knowledge about the form of $\mathbb{T}_f$ (e.g. Gaussian), we can simply estimate the parameters of this distribution (e.g. via the sample mean and variance). In the absence of such knowledge, we can use nonparametric methods like *kernel density estimation* (KDE, [64, 65]). Fig. 1c depicts the PDF and CDF for 10 training risks when using KDE with Gaussian kernels, while Fig. 2 compares the smoothed KDE CDF (black) to the unsmoothed empirical CDF (gray).

Importance of smoothing. As shown in Fig. 2, the KDE smoothing permits risk "extrapolation" [41] beyond our largest training risk, with the estimated α-quantile risk going to infinity as $\alpha \to 1$ (when kernels have full support). Critically, as detailed in Prop. 4.3 below, this unlocks *invariant prediction* for QRM. In Appendix C, we discuss the suitability of different data-dependent bandwidth-selection methods for our purposes, with different methods encoding different assumptions about right-tail heaviness and thus about projected OOD risk. In practice, we use Gaussian kernels with the Gaussian-optimal rule [66] or Silverman's rule-of-thumb [66].

Figure 2: Risk CDFs.

Empirical problem. Armed with a predictor's estimated risk distribution $\widehat{\mathbb{T}}_f$, we can approximately solve (QRM) using the following empirical analogue:

$$\widehat{\text{QRM}}_\alpha(f) := \min_{f \in \mathcal{F}} F_{\widehat{\mathbb{T}}_f}^{-1}(\alpha) \tag{4.1}$$

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[3]More formally, $\mathbb{T}_f$ can be defined as the push-forward measure of $\mathbb{Q}$ through the risk functional $\mathcal{R}^e(f)$; see Appendix B for a formal definition.

Note that (4.1) depends only on known quantities, so we can compute and minimize it in practice. Also note that in finance, when concerned with a distribution over potential losses, the α-quantile value is known as the *value at risk* (VaR) at level α [67]. Alg. 1 of Appendix E.1 details the EQRM algorithm.

Generalization bound. We now give a simplified version of our main generalization bound— Thm. D.1. The full version, stated and proved in Appendix D, provides specific finite-sample bounds on ϵ_1 and ϵ_2 below, depending on the hypothesis class $\mathcal{F}$, the empirical estimator $\widehat{\mathrm{QRM}}_\alpha$, and the assumptions made on the possible risk profiles of hypotheses $f \in \mathcal{F}$.

Theorem 4.1 (Simplified form of Thm. D.1, uniform convergence). *Given m domains and n samples in each, then with high probability over the training data,*

$$\sup_{f \in \mathcal{F}} \left| F_{\mathbb{T}_f}^{-1}(\alpha - \epsilon_2) - F_{\widehat{\mathbb{T}}_f}^{-1}(\alpha) \right| \le \epsilon_1, \tag{4.2}$$

where $\epsilon_1 \to 0$ as $n \to \infty$ and $\epsilon_2 \to 0$ as $m \to \infty$.

This states that, for m, n sufficiently large, the empirical α-quantile risk is a good estimate of the population α-quantile risk. Thus, a predictor f which minimizes the empirical problem in (4.1) should approximately minimize the population problem in (QRM). While many domains are required for this generalization bound to be tight, our empirical results in § 6 demonstrate that (E)QRM performs well in practice given only a few domains. In other words, while many domains are required for α to *precisely* estimate the true quantile, α can still be used as an interpretable conservativeness-hyperparameter given only a few domains, albeit with a less precise interpretation.

Recovering the causal predictor. We now state our causal recovery results, namely that: (i) QRM learns a minimal invariant-risk predictor as $\alpha \to 1$; and (ii) learning a minimal invariant-risk predictor is sufficient to recover the causal predictor under assumptions which are both weaker and more general than those of Peters et al. [45, Thm 2] and Krueger et al. [41, Thm 1] (Appendix A.2.3). For intuition on (i), we refer the reader to Appendices A.2.1 and A.2.2 where we illustrate how setting $\alpha \to 1$ eventually forces the risk variance over domains to 0. Together, these results provide the conditions under which QRM recovers the causal mechanism of Y as $\alpha \to 1$, as well as new insights into the fundamental connection between invariance (in particular, invariant *risks*, see Appendix G.1.2) and causality.

Definition 4.2. A predictor is said to be an *invariant-risk predictor* if its risk is equal almost surely across domains (i.e., $\mathrm{Var}_{e \sim \mathbb{Q}}[\mathcal{R}^e(f)] = 0$). A predictor is said to be a *minimal invariant-risk predictor* if it achieves the minimal possible risk over all possible invariant-risk predictors.

Proposition 4.3 (QRM learns a minimal invariant-risk predictor as $\alpha \to 1$, informal version of Props. A.4 and A.5). *Assume: (i) $\mathcal{F}$ contains an invariant-risk predictor with finite training risks; and (ii) no arbitrarily-negative training risks. Then, as $\alpha \to 1$, Gaussian and kernel QRM predictors (the latter with certain bandwidth-selection methods) converge to minimal invariant-risk predictors.*

Theorem 4.4 (The causal predictor is (often) the only minimal invariant-risk predictor). *Assume that: (i) Y is generated from a linear SEM, $Y = \beta^\mathsf{T} X + N$, with coefficients $\beta \in \mathbb{R}^d$ and noise N having constant variance and $\mathbb{E}[N] = 0$ across domains; (ii) $\mathcal{F}$ is the class of linear predictors, indexed by $\hat{\beta} \in \mathbb{R}^d$; (iii) all components of X are observed; (iv) the loss ℓ is squared-error; and (v) the system of equations*

$$\begin{aligned}
0 &\ge x^\mathsf{T} \mathbb{E}_{X \sim e_1}[XX^\mathsf{T}]x + 2x^\mathsf{T} \mathbb{E}_{N, X \sim e_1}[XN] \\
&= \cdots \\
&= x^\mathsf{T} \mathbb{E}_{X \sim e_m}[XX^\mathsf{T}]x + 2x^\mathsf{T} \mathbb{E}_{N, X \sim e_m}[XN].
\end{aligned} \tag{4.3}$$

has the unique solution $x = 0$. If $\hat{\beta}$ is a minimal invariant-risk predictor, then $\hat{\beta} = \beta$.

In Appendix A.2, we prove the formal versions of Prop. 4.3 (Props. A.4 and A.5) along with Thm. 4.4, provide some intuition and concrete examples regarding Assumption (v) of Thm. 4.4, and relate our α parameter to the β parameter of VREx [41, Eq. 8] for the special case of Gaussian estimators of $\mathbb{T}_f$.

4.2 Empirical SQRM

Although the formulation presented in (4.1) is intuitive and interpretable, the quantile function is notoriously difficult to optimize [68]. Indeed, in many cases of interest, F^{-1} can be nonconvex and discontinuous, which induces an unfavorable optimization landscape [69, 70]. To circumvent this, we propose an alternative scheme in which we optimize the *superquantile* (SQ)—also known as the *conditional value at risk* (CVaR) or *expected tail loss*—at level α, which is defined[4] as follows:

$$\mathrm{SQ}_\alpha(R; \mathbb{T}_f) := \mathbb{E}_{R \sim \mathbb{T}_f}\left[R \mid R \geq F_{\mathbb{T}_f}^{-1}(\alpha) \right] \qquad (4.4)$$

SQ_α can be seen as the conditional expectation of a random variable R subject to R being larger than the α-quantile $F^{-1}(\alpha)$. In our case, where R represents the statistical risk on a randomly-sampled environment, SQ_α can be seen as the expected risk in the worst $100 \cdot (1 - \alpha)\%$ of cases/domains. Importantly, unlike the quantile, the superquantile has many desirable mathematical properties: (i) it is continuous in α; (ii) it is jointly convex in R and α; and (iii) it is the tightest convex surrogate for the inverse CDF [71, § 2]. Therefore, we also consider the following optimization problem:

$$\min_{f \in \mathcal{F}} \mathrm{SQ}_\alpha(R; \mathbb{T}_f) \qquad \text{(SQRM)}$$

We call the empirical analogue, which uses the empirical density rather than $\mathbb{T}_f$, empirical SQRM. Alg. 2 of Appendix E.1 details the ESQRM algorithm.

Connections to existing problems. It is straightforward to show that (SQRM) recovers the RM problem in (3.3) and the minimax problem in (3.2) as special cases with $\alpha = 0$ and $\alpha = 1$ respectively. Moreover, in Appendix F, we exploit the well-known duality properties of CVaR to show an alternative, view of (SQRM) as a distributionally-robust optimization problem, admitting close connections to previous work, including GroupDRO [48]; see Prop. F.1 and F.2 for details.

5 Related work

Robust optimization in DG. Throughout this paper, we follow an established line of work (see e.g., [9, 41, 49]) which formulates the DG problem through the lens of robust optimization [47]. To this end, various algorithms have been proposed for solving constrained [22] and distributionally robust [48] variants of the worst-case problem in (DG). Indeed, this robust formulation has a firm foundation in the broader machine learning literature, with notable works in adversarial robustness [72–76] and fair learning [77, 78] employing similar formulations. Unlike these past works, we consider a robust but non-adversarial formulation for DG, where predictors are trained to generalize with high probability rather than in the worst case. Moreover, the majority of this literature—both within and outside of DG—relies on specific structural assumptions (e.g. covariate shift) on the types of possible interventions or perturbations. In contrast, we make the weaker and more flexible assumption of iid-sampled domains, which ultimately makes use of the data/domains to determine the types of shifts that are possible or *probable*. We further discuss this important difference in § 7.

Other approaches to DG. Outside of robust optimization, many algorithms have been proposed for the DG setting which draw on insights from a diverse array of fields, including approaches based on tools from meta-learning [40, 79–82], kernel methods [83, 84], and information theory [49]. Also prominent are works that design regularizers to generalize OOD [85–87] and works that seek domain-invariant representations [88–90]. However, the majority of these works do not explicitly relate the domains seen during training and test time, which is a key feature of our approach. Moreover, many of these works employ hyperparameters which are difficult to interpret, which has no doubt contributed to the well-established model-selection problem in DG [38]. In contrast, in our framework, α can be easily interpreted in terms of the quantiles of the risk distribution. Finally, while many of the best-performing DG methods provide no theoretical results in the nonlinear setting (e.g.[9, 41, 82, 91]), QRM has both strong theoretical *and* empirical results in the nonlinear setting (see § 6).

High-probability generalization. As noted in § 3, relaxing worst-case problems in favor of probabilistic ones has a long history in control theory [42, 60, 61, 92, 93], operations research [94], and smoothed analysis [62]. Recently, this paradigm has been applied to several areas of machine learning, including perturbation-based robustness [95, 96], fairness [97], active learning [98], and reinforcement learning [99, 100]. However, it has not yet been applied to domain generalization.

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[4]This definition assumes that $\mathbb{T}_f$ is continuous; we present a more general definition in Appendix F.

Figure 3: **QRM on a toy linear regression dataset (A–D) and on ColoredMNIST (E–F). A:** Test risk at different quantiles or degrees of "OODness". Each α is optimal at the corresponding quantile. **B:** Estimated risk distributions. See Fig. 7 of Appendix G.1.1 for corresponding CDFs. **C:** Regression coefficients approach those of the causal predictor ($\beta_{\text{cause}} = 1$, $\beta_{\text{effect}} = 0$) as $\alpha \rightarrow 1$. **D:** Q-Q plot comparing the "true" risk quantiles (estimated with $m = 1000$) against "estimated" ones ($m < 1000$). Shown for $\alpha = 0.9$. **E:** Performance of different αs over increasingly OOD test domains. Dots show training-domain accuracies. **F:** KDE-estimated accuracy-CDFs depicting accuracy-robustness curves. Larger αs make lower accuracies (i.e. larger risks) less likely.

Quantile minimization. In financial optimization, VaR and CVaR [67, 69, 101] are central to the literature surrounding portfolio risk management, with numerous applications spanning banking regulations and insurance policies [68, 102]. In statistical learning theory, several recent papers have derived uniform convergence guarantees in terms of alternative risk functionals besides expected risk [98, 103–105]. These results focus on CVaR and closely related functionals that can be written in terms of expectations over the loss distribution. In contrast, our uniform convergence guarantee (Theorem D.1) shows uniform convergence of VaR, which *cannot* be written as such an expectation; this necessitates stronger conditions to obtain uniform convergence, which ultimately suggest regularizing the estimated risk distribution (e.g. by kernel smoothing).

Invariant prediction and causality. As discussed in § 2, recent works have leveraged different forms of invariance across domains to discover causal relationships which, under the invariant mechanism assumption [54], generalize to new domains [9, 41, 45, 52, 106–108]. In particular, like QRM (as $\alpha \rightarrow 1$), Krueger et al. [41] leverage *invariant risks*, while Arjovsky et al. [9] leverage *invariant functions* or regression coefficients. We further discuss this important distinction in Appendix G.1.2. More recently, noting that causal parameters are often too conservative and thus that performing well out-of-distribution can require non-causal relationships, Rothenhäusler et al. [109] proposed *Anchor regression* for interpolating between causal and predictive parameters. However, the assumed shift types are even more restrictive than in the works above, despite nonlinear extensions [51].

6   Experiments

We now evaluate our algorithms on synthetic and real-world datasets. These evaluations illustrate the importance of multiple test domains in DG benchmarks, as well as the benefits of our algorithms in practice. Appendices E and G report further results and experimental details.

6.1   Synthetic datasets

Linear regression. We first consider a linear regression dataset based on the following linear SCM:

$$X_1 \leftarrow N_1, \qquad\qquad Y \leftarrow X_1 + N_Y, \qquad\qquad X_2 \leftarrow Y + N_2,$$

with $N_j \sim \mathcal{N}(0, \sigma_j^2)$. Here we have two features: one cause $X_1 = X_{\text{cause}}$ and one effect $X_2 = X_{\text{effect}}$ of Y. By fixing $\sigma_1^2 = 1$ and $\sigma_Y^2 = 2$ across domains but sampling $\sigma_2 \sim \text{LogNormal}(0, 0.5)$, we create

Table 1: `CMNIST` test acc.

Alg.	Initialization	
	Rand.	ERM
ERM	27.9 ± 1.5	27.9 ± 1.5
IRM	$\mathbf{52.5 \pm 2.4}$	69.7 ± 0.9
GrpDRO	27.3 ± 0.9	29.0 ± 1.1
SD	49.4 ± 1.5	70.3 ± 0.6
IGA	50.7 ± 1.4	57.7 ± 3.3
V-REx	$\mathbf{55.2 \pm 4.0}$	$\mathbf{71.6 \pm 0.5}$
SQRM	50.0 ± 11.0	28.2 ± 1.2
QRM	$\mathbf{53.4 \pm 1.7}$	$\mathbf{71.4 \pm 0.4}$
Oracle	72.1 ± 0.7	

Table 2: Avg. test accuracy on `PACS` and `VLCS`.

Algorithm	Training set		Cross-validation		Test set (oracle)	
	PACS	VLCS	PACS	VLCS	PACS	VLCS
ERM	85.5	77.5	83.0	77.2	86.7	77.6
IRM	83.5	78.5	83.0	76.3	84.5	76.9
GroupDRO	84.4	76.7	83.5	77.9	87.1	77.4
CORAL	86.2	**78.8**	82.6	**78.7**	87.1	77.7
V-REx	84.9	78.3	81.3	76.7	87.2	78.1
ARM	85.1	77.6	81.7	76.6	85.8	77.8
QRM	**86.6**	77.1	**85.1**	77.9	**87.4**	**78.8**

a dataset in which X_2 is more predictive of Y than X_1 but less stable. Importantly, as we know the true distribution over domains $\mathbb{Q}(e) = \text{LogNormal}(\sigma_2^e; 0, 0.5)$, we know the true risk quantiles. Fig. 3 depicts results for different α's with $m = 1000$ domains and $n = 100000$ samples in each, using the mean-squared-error (MSE) loss. Here we see that: **A:** for each true quantile (x-axis), the corresponding α has the lowest risk (y-axis), confirming that the empirical α-quantile risk is a good estimate of the population α-quantile risk; **B:** As $\alpha \to 1$, the estimated risk distribution of f_α approaches an invariant (or Dirac delta) distribution centered on the risk of the causal predictor; **C:** the regression coefficients approach those of the causal predictor as $\alpha \to 1$, trading predictive performance for robustness; and **D:** reducing the number of domains m reduces the accuracy of the estimated α-quantile risks. In Appendix G.1, we: (i) depict the risk CDFs corresponding to plot **B** above, and discuss how they depict the predictors' risk-robustness curves (G.1.1); and (ii) discuss the solutions of QRM on datasets in which σ_1^2, σ_2^2 and/or σ_Y^2 change over domains, compared to existing invariance-seeking algorithms like IRM [9] and VREx [41] (G.1.2).

ColoredMNIST. We next consider the `ColoredMNIST` or `CMNIST` dataset [9]. Here, the `MNIST` dataset is used to construct a binary classification task (0–4 or 5–9) in which digit color (red or green) is a highly-informative but spurious feature. In particular, the two training domains are constructed such that red digits have an 80% and 90% chance of belonging to class 0, while the single test domain is constructed such that they only have a 10% chance. The goal is to learn an invariant predictor which uses only digit shape—a stable feature having a 75% chance of correctly determining the class in all 3 domains. We compare with IRM [9], GroupDRO [48], SD [110], IGA [111] and VREx [41] using: (i) random initialization (Xavier method [112]); and (ii) random initialization followed by several iterations of ERM. The ERM initialization or pretraining directly corresponds to the delicate penalty "annealing" or warm-up periods used by most penalty-based methods [9, 41, 110, 111]. For all methods, we use a 2-hidden-layer MLP with 390 hidden units, the Adam optimizer, a learning rate of 0.0001, and dropout with $p = 0.2$. We sweep over five penalty weights for the baselines and five α's for QRM/SQRM. See Appendix E.2 for more details. Table 1 shows that: (i) all methods struggle without ERM pretraining, explaining the need for penalty-annealing strategies in previous works and corroborating the results of [113, Table 1]; (ii) with ERM pretraining, QRM matches or outperforms IRM and VREx, even approaching oracle performance (that of ERM trained on grayscale digits). These results suggest ERM pretraining as an effective strategy for DG methods—a strategy we employ in the next section.

Fig. 3 depicts the behavior of QRM with different αs. Here we see that: **E:** increasing α leads to more consistent performance across domains, eventually forcing the model to ignore color and focus on invariant, shaped-based prediction; and **F:** a predictor's estimated accuracy-CDF depicts its accuracy-robustness curve, just as its estimated risk-CDF depicts its risk-robustness curve. Note that $\alpha = 0.5$ gives the best worst-case risk over the two training domains—the preferred solution of DRO [48]—while $\alpha \to 1$ sacrifices risk for increased invariance or robustness.

6.2 DomainBed datasets: between synthetic and real-world shifts

We next consider two large-scale datasets from the DomainBed [38] suite: `PACS` and `VLCS`. While both of these datasets encode real-world shifts, each contains only four domains – three for training and one for testing – and therefore it is not possible to analyze the tail performance of our algorithms. However, in line with a litany of recent work, we offer a comparison of QRM to a range of standard baselines in Table 2 in terms of the average performance across each choice of test domain; we

Table 3: QRM test risks on `iWildCam`.

Alg.	Mean risk	Quantile risk						
		0.0	0.25	0.50	0.75	0.90	0.99	1.0
ERM	1.31	0.015	0.42	0.76	2.25	2.73	4.99	5.25
IRM	1.53	0.098	0.52	1.24	1.86	2.36	6.95	7.46
GroupDRO	1.73	0.091	0.68	1.65	2.18	3.36	5.29	5.54
CORAL	1.27	0.024	0.45	0.73	2.12	2.66	4.50	4.98
$QRM_{0.25}$	2.03	0.024	0.46	2.70	3.01	3.48	5.03	5.26
$QRM_{0.50}$	1.11	**0.004**	0.24	0.68	1.71	2.15	4.04	4.11
$QRM_{0.75}$	1.05	0.009	**0.21**	0.68	1.50	2.35	4.88	5.45
$QRM_{0.90}$	**0.98**	0.047	0.28	**0.63**	**1.26**	**1.81**	4.11	4.48
$QRM_{0.99}$	0.99	0.12	0.35	0.64	1.30	2.00	**3.44**	**3.55**

Table 4: QRM test risks on `OGB-MolPCBA`.

Alg.	Mean risk	Quantile risk						
		0.0	0.25	0.50	0.75	0.90	0.99	1.0
ERM	**0.051**	0.0	0.004	0.017	0.060	0.13	0.49	16.04
IRM	0.073	0.098	0.52	1.24	1.86	2.36	6.95	7.46
GroupDRO	0.21	0.091	0.68	1.65	2.18	3.36	5.29	**5.54**
CORAL	0.055	0.0	0.12	0.32	1.23	2.01	5.76	7.44
$QRM_{0.25}$	0.054	0.0	0.003	0.016	0.059	0.13	0.48	15.46
$QRM_{0.50}$	0.052	0.0	0.003	0.015	0.059	0.13	0.48	11.33
$QRM_{0.75}$	0.052	0.0	0.003	0.015	0.059	0.13	0.47	12.15
$QRM_{0.90}$	0.052	0.0	0.003	0.015	0.059	0.12	0.47	10.81
$QRM_{0.99}$	0.053	0.0	0.003	**0.014**	**0.055**	**0.11**	**0.46**	7.16

Table 5: SQRM test risks on `iWildCam`.

Alg.	Superquantile risk						
	0.0	0.25	0.50	0.75	0.90	0.99	1.0
ERM	1.31	1.91	2.58	3.69	4.83	9.58	9.58
IRM	1.53	1.95	2.52	3.49	4.85	7.46	7.46
GroupDRO	1.73	2.20	2.80	3.68	4.46	5.54	5.54
CORAL	1.27	2.10	2.67	3.52	4.90	8.29	9.21
$SQRM_{0.25}$	1.18	1.53	2.10	2.99	4.09	6.03	6.03
$SQRM_{0.50}$	1.16	1.51	2.03	2.89	3.91	5.95	5.95
$SQRM_{0.75}$	**1.08**	**1.41**	**1.94**	**2.71**	**3.64**	**4.55**	**4.55**

Table 6: SQRM test risks on `OGB-MolPCBA`.

Alg.	Superquantile risk						
	0.0	0.25	0.50	0.75	0.90	0.99	1.0
ERM	**0.051**	0.081	0.12	0.20	0.36	1.30	16.04
IRM	0.073	0.095	0.14	0.23	0.42	2.00	38.91
GroupDRO	0.21	0.28	0.42	0.80	1.85	16.22	730.64
CORAL	0.055	0.101	0.24	0.35	0.62	3.84	63.88
$SQRM_{0.10}$	0.054	**0.071**	**0.10**	**0.17**	**0.29**	**0.90**	16.04
$SQRM_{0.20}$	0.061	0.081	0.12	0.20	0.36	1.28	8.78
$SQRM_{0.30}$	0.060	0.079	0.16	0.20	0.35	1.21	**7.03**
$SQRM_{0.40}$	0.060	0.079	0.11	0.20	0.35	1.20	7.70

include a full set of results with additional baselines in Appendix G.2. Observe that on `PACS`, we beat state-of-the-art algorithms across all three model-selection methods, with a notable 2-percentage-point improvement for the cross-validation selection method. On `VLCS`, we match the state-of-the-art, with a slight improvement of nearly 1-percentage-point for the oracle selection method.

6.3 Real-world datasets

We now evaluate our methods on the real-world or *in-the-wild* distribution shifts of WILDS [12]. We focus our evaluation on `iWildCam` [114] and `OGB-MolPCBA` [115, 116]—two large-scale classification datasets which have numerous test domains and thus facilitate a comparison of the risk distributions and their quantiles. Additional comparisons (e.g. using average accuracy) can be found in Appendix G.3. Our results demonstrate that, across two distinct data types (images and molecular graphs), QRM and SQRM offer superior quantile and superquantile performance respectively.

Figure 4: **Test risk distributions on iWildCam and OGB-MolPCBA.** Each distribution shows that for larger values of α, QRM_α and $SQRM_\alpha$ tend to display superior tail performance relative to ERM.

iWildCam. We first consider the `iWildCam` image-classification dataset which has 243 training domains and 48 test domains. Here, the label Y is 1 of 182 different animal species and the domain e is the camera trap which took the photo. In Table 3, we observe that QRM_α does indeed tend to optimize the α-risk quantile, with larger αs during training resulting in lower test-time risks at the corresponding quantiles. Similarly, Table 5 shows that $SQRM_\alpha$ effectively optimizes the superquantile function, with $\alpha = 0.75$ yielding particularly low values relative to ERM. In the two leftmost panes of Fig. 4, we plot the (smoothed) test-time risk distributions. Here we see a clear trend: as α increases, the tails of the risk distribution tend to drop below ERM, which corroborates the superior quantile and superquantile performance reported in Tables 3 and 5.

Note that, in both Tables 3 and 5, QRM and SQRM tend to record lower *average* risks than ERM. This has several plausible explanations. First, the number of testing domains (48) is relatively small,

which could result in a biased sample with respect to the training domains. Second, the test domains may not represent i.i.d. draws from $\mathbb{Q}$, with WILDS [12] test domains tending to be more challenging.

OGB-MolPCBA. We next consider the `OGB-MolPCBA` (or `OGB`) dataset, which is a molecular graph-classification benchmark containing 44,930 training domains and 43,793 test domains with an average of 3.6 samples per domain. Tables 4 and 6 show that ERM achieves the lowest *average* test risk on `OGB`, in contrast to the `iWildCam` results, while QRM_α and $SQRM_\alpha$ still achieve stronger quantile and superquantile performance. Of particular note is the fact that our methods significantly outperform ERM with respect to worst-case performance (columns/quantiles labeled 1.0); when QRM_α and $SQRM_\alpha$ are run with large values of α, we reduce the worst-case risk by more than a factor of two. In Fig. 4, we again see that the risk distributions of QRM_α and $SQRM_\alpha$ have lighter tails than that of ERM.

A new evaluation protocol for DG. The analysis provided in Tables 3-6 and Fig. 4 diverges from the standard evaluation protocol in DG [12, 38]. Rather than evaluating an algorithm's performance *on average* across test domains, we seek to understand *the distribution of its performance*—particularly in the tails by means of the quantile and superquantile functions. This new evaluation protocol lays bare the importance of multiple test domains in DG benchmarks, allowing predictors' risk distributions to be analyzed and compared. Indeed, as DG is neither a worst-case nor an average-case problem, solely reporting a predictor's worst or average risk over test domains can be misleading when assessing its ability to generalize OOD (as shown in Tables 3-6). This underscores the necessity of incorporating tail risk measures into a more holistic evaluation protocol for DG, ultimately providing a more nuanced and complete picture of a predictor's ability to generalize OOD. ==In practice, which measure is preferred will depend on the application-of-interest,== e.g. ==via a human-specified quantile-of-interest.==

7   Discussion

On the assumption of i.i.d. domains. For α to approximate the probability of generalizing, training and test domains must be i.i.d.-sampled. While this is rarely true in practice—e.g. hospitals have shared funders, service providers, foundation dates, etc.—we can better satisfy this assumption by subscribing to a new data collection process in which we collect training data from domains which are representative of how the underlying system tends to change. For example: (i) randomly select 100 US hospitals; (ii) gather and label data from these hospitals; (iii) train our system with the desired α; (iv) deploy our system to all US hospitals where it will be successful with probability $\approx \alpha$. While this process may seem expensive, time-consuming and vulnerable (e.g. new hospitals), it offers a promising path to machine learning systems which *generalize with high probability*. Moreover, it is worth noting the alternative: prior works achieve generalization by assuming that only particular types of shifts can occur, e.g. covariate shifts [22, 117, 118], label shifts [118, 119], concept shifts [120], measurement shifts [19], mean shifts [109], shifts which leave the mechanism of Y invariant [9, 39, 41, 45], etc. In real-world settings, where the shift mechanisms are often unknown, such assumptions are both difficult to justify and impossible to test. Future work could look to relax the i.i.d.-domains assumption by leveraging knowledge of domain dependencies (e.g. time).

Interpretable model selection. α approximates the probability with which our predictor will generalize with risk below the associated α-quantile value. Thus, α represents an interpretable parameterization of the risk-robustness trade-off. Such interpretability is critical for model selection in DG, and for practitioners with application-specific requirements on performance and/or robustness.

The wider value of risk distributions. As demonstrated in § 6, a predictor's risk distribution has value beyond quantile-minimization—it estimates the probability associated with each level of risk. Thus, regardless of the algorithm used, risk distributions can be used to analyze trained predictors.

8   Conclusion

We have presented QRM for achieving *probable* domain generalization, motivated by the argument that DG should seek predictors which generalize with high probability rather than in the worst-case or on-average. By explicitly relating training and test domains as draws from the same underlying meta-distribution, we proposed to learn predictors with minimal α-quantile risk under the training domains. Theoretically, we proved that α does indeed approximate the probability of generalizing and that QRM recovers the causal predictor as $\alpha \to 1$. Empirically, we demonstrated the importance of *multiple* test domains and tail performance in DG benchmarks, and that our algorithms perform well in practice.

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