Designing off-sample performance metrics

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Abstract

Modern machine learning systems are traditionally designed and tested with the overall goal of achieving the best possible performance on average. In this work, we consider an approach to building learning systems which treats the question of “how should we quantify good off-sample performance?” as a key design decision. We describe this proposal using a simple and general formulation, place the current dominant paradigm within the proper historical context, and then survey the literature for more recent developments that depart from tradition and can be viewed as special cases of our proposed methodology.

Contents

1 Background 2
2 Formalizing the performance of learning systems 2
3 Origins of expected loss minimization 4
4 Expected loss and learning problems 7
5 Survey of non-traditional methods 9
  5.1 Designing new empirical objectives 10
    5.1.1 M-estimators 10
    5.1.2 L-statistics 10
    5.1.3 Largest losses 11
    5.1.4 Exponential smoothing 11
    5.1.5 Location and deviation 11
  5.2 Designing new off-sample performance metrics 12
    5.2.1 Conditional value-at-risk 12
    5.2.2 L-risks 13
    5.2.3 OCE risk 13
    5.2.4 Location and deviation 14
    5.2.5 Psychologically motivated risks 15
    5.2.6 Distributional robustness 16
    5.2.7 Fairness 16

A Appendix 22
  A.1 Background on the OCE risk 22

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1 Background

This paper is concerned with the question of how to quantify performance in learning systems.\footnote{We have computer systems running machine learning software in mind as our primary application, but any system which can be reasonably modeled using the formulation to follow is of interest.} The widespread use of modern machine learning tools provides important socioeconomic context for this question. Machine learning techniques are developing rapidly, and together have become an important technology that supports the day-to-day activity of scientists, engineers, artists, physicians, and many others, not to mention the fact that machine learning underlies much of the online shopping experience, advertisements, financial transactions, and a lot of fun toys and games used by countless people worldwide.

Since there have already been so many successful learning systems applied in the real world, one might be inclined to assume that our question of quantifying performance must already have a satisfactory answer, since performance evaluation is indeed critical to providing feedback, and any learning system without a reliable mechanism for providing meaningful feedback is bound to fail. We argue, however, that there remains a lot of work to be done. Put in rather abstract terms, all learning systems involve some form of decision-making in an uncertain environment, and often face some requirement to generalize beyond limited experience. The dominant paradigm (particularly in machine learning) for evaluating performance has been to emphasize the degree of success in a task on average. While this is a perfectly natural way to define “good” performance, it is not the only way, and depending on the problem, it certainly need not be the best way.\footnote{We mean “best” in a multi-faceted sense: transparency, reliability, stability, and even in some cases final performance on average. Our literature review in §5 gives numerous concrete examples of this.}

Our goal in this work is to bring this limitation into clearer focus, in a concise but sufficiently descriptive form that is accessible to a diverse community of researchers who use or study learning systems. To achieve this, we first formulate a learning system in such a way which elevates the problem of “defining good performance” from an implicit assumption to an explicit design decision, highlighting methodological limitations of the existing standard approach (cf. §2). We then try to understand the current dominant paradigm within the proper historical context, looking at the key lines of thought that led to it (cf. §3), and the influential role it has played in the development of modern machine learning (cf. §4). We then shift our focus to more recent developments in learning algorithm design which can be seen as departures from tradition (cf. §5). In particular, many well-known works have considered the use of biased estimators in order to construct feedback that leads to more robust or stable algorithm performance (cf. §5.1), but it is only quite recently that focus has shifted away from the expected loss, to other performance metrics (cf. §5.2). This shift in approach is captured and generalized by the general design framework we introduce in §2.

2 Formalizing the performance of learning systems

When we say that a learning system “performs well,” what precisely do we mean? In this section, we give this notion a formal definition, by formulating a learning system in such a way that we capture the essential working parts of many important real-world systems, while maintaining a sufficient level of generality. A logical starting point is a non-empty set $\mathcal{H}$, called the hypothesis set.\footnote{Intuitively, this represents a set of candidate actions, choices, decision rules, and so forth. Mathematically, depending on the candidates we want to represent, the elements of the set $\mathcal{H}$ may be numbers, vectors, functions, or themselves sets of elements. In any case, each element $h \in \mathcal{H}$ only has meaning within the context of a task, which is characterized by a loss function.} Intuitively, this represents a set of candidate actions, choices, decision rules, and so forth. Mathematically, depending on the candidates we want to represent, the elements of the set $\mathcal{H}$ may be numbers, vectors, functions, or themselves sets of elements. In any case, each element $h \in \mathcal{H}$ only has meaning within the context of a task, which is characterized by a loss function.
\( \ell : \mathcal{H} \times \mathcal{Z} \rightarrow \mathbb{R} \) that assigns the value \( \ell(h; z) \) to \( h \), based on a data point \( z \in \mathcal{Z} \). A smaller loss is understood to imply better performance in the underlying task. Let \( \mathcal{Z} := (Z_1, Z_2, \ldots) \) denote a sequence of random data; we use the term learning process to refer to any sequence \((H_1, H_2, \ldots)\) which is allowed to depend on \( \mathcal{Z} \), and which satisfies \( H_n \in \mathcal{H} \) for all \( n \) almost surely.\(^3\) We use the term learning algorithm to refer to all the rules and transformations, potentially stochastic, which determine the learning process based on \( \mathcal{Z} \); using \( \mathcal{A} \) to express this explicitly, we have \( \mathcal{A}(\mathcal{Z}) = (H_1, H_2, \ldots). \)\(^4\) We say that a learning system is characterized by the task and the learning process, and thus in terms of elements we can control, the learning system is determined by \( \mathcal{H}, \ell, \) and \( \mathcal{A} \).

As mentioned in §1, our chief interest is with quantifying the performance of learning systems, within the context of a particular task. The fundamental idea underlying our approach is that the loss distribution characterizes performance. As a broad characterization, we say the distribution of losses \( \{\ell(H_i; Z_j) : i, j \in \mathbb{N}\} \) determines on-sample performance, but this alone does not entirely explain performance. A very important facet of learning is that of “generalizing” to new data. To capture this more formally, let \( Z' \) denote a random data point distinct from the elements of \( \mathcal{Z} \); for convenience, we will refer to \( Z' \) as a test point. We then say that the off-sample performance is determined by the distribution of \( (\ell(H_1; Z'), \ell(H_2; Z'), \ldots) \), noting that randomness comes from three sources: the data \( \mathcal{Z} \), the algorithm \( \mathcal{A} \), and the test point \( Z' \). We will often suppress the data dependence and write \( L_i(\cdot) := \ell(\cdot; Z_i) \) and \( L(\cdot) := \ell(\cdot; Z') \). With these notions in place, roughly speaking, the ultimate goal of learning is to achieve “good” off-sample performance.

We have thus formalized the notion of performance (both on- and off-sample), but we have yet to quantify it. In general, the distribution of a random process is unwieldy as a performance metric on its own; for reasons of theoretical tractability, ease of interpretation, and links to practical learning algorithms, a more concise numerical summary is desirable. Thus, our initial question of how to quantify the performance of learning systems is reduced to the problem of computing a concise numerical summary of the test loss distribution, i.e., the problem of designing a metric for off-sample performance.

Let us briefly review how off-sample performance is traditionally evaluated in the context of both statistical learning theory and applied machine learning, among other fields. Without question, the de facto standard is \( \mathbf{E} \left[ \ell(H_n; Z') \mid H_n \right] \), namely the expected test loss conditioned on \( H_n \).\(^5\) From the perspective of algorithm design, this approach is congenial in that it suggests an obvious objective function by which to quantify off-sample performance:

\[
R(h) = \mathbf{E} \left[ \ell(h; Z') \mid \mathcal{Z} \right], \quad h \in \mathcal{H}.
\] (1)

When the learning problem can be expressed as simply minimizing this \( R(\cdot) \) over \( \mathcal{H} \), it is much easier to design effective learning algorithms. Roughly speaking, if the empirical distribution of the losses \( (\ell(\cdot; Z_1), \ell(\cdot; Z_2), \ldots) \) is similar to that of \( \ell(\cdot; Z') \), then minimizing the empirical mean of the former is a natural strategy that is often easy to implement. This is the basic idea underlying empirical risk minimization (ERM) and modern statistical learning theory [84, 85].

While the above approach is entirely natural, from the standpoint of evaluating off-sample performance, using (1) as a guide for algorithm design emphasizes performance on average. In many real-world situations, however, good performance on average may not be enough. As a

\(^3\)We use \( h \in \mathcal{H} \) or \( h_i \in \mathcal{H} \) to denote non-random quantities, in contrast to \( H_i \), where we use upper-case letters to emphasize randomness due to both the random data and randomness inherent to the learning process.

\(^4\)When we say “potentially stochastic,” we mean that even for a fixed, non-random sequence \((z_1, z_2, \ldots)\), it is possible that \( \mathcal{A}(z_1, z_2, \ldots) \) is random. Mathematically speaking, it is often convenient to let \( \mathcal{A} \) be a function with domain \( \mathcal{Z}^\infty \), which returns a sequence of measurable functions.

\(^5\)See our historical notes in §4, where we justify this claim.
simple example, the expected loss is quite sensitive to the distribution tails, whereas the median loss is not affected by the right-hand tails at all. The question of how to treat exceptionally large but rare losses is a value judgement; for some applications we can and should ignore such points, whereas for others, these points should be given equal weight. The latter scenario can be addressed fully using (1), but the former scenario cannot.

With these issues in mind, we are interested in a methodology which views the problem of how to quantify off-sample performance as a critical step in the overall process of designing a learning system. When we think about the design of learning systems, it is natural to focus on the specific choices of $\mathcal{H}$, $\ell$, and in particular the implementation details of $\mathcal{A}$. It is important to realize that underlying all these details is typically the expected test loss objective (1). However, as the simple “mean vs. median” example illustrates, the choice of what defines good off-sample performance is non-trivial, and often requires human intervention. Put simply, if we seek to methodically build a learning system that reliably meets our performance expectations, then a metric for quantifying off-sample performance should be explicitly designed.

To formalize these notions, let us first denote the class of random test losses indexed by the hypothesis set $\mathcal{H}$ as $L_{\mathcal{H}} = \{\ell(h; Z') : h \in \mathcal{H}\}$. Then, we call any function $R : L_{\mathcal{H}} \rightarrow \mathbb{R}$ an off-sample performance metric, using the more compact notation of $R(h) : R(\ell(h; Z'))$ for readability. Clearly (1) is just one special case of this. With this notation in place, the following is a general-purpose workflow for learning systems where off-sample performance is important.

1. **Task design and modeling.** Determine which $\mathcal{H}$ and $\ell$ to use; this effectively encodes $a \text{ priori}$ knowledge about the problem domain and the nature of the data.\(^6\)

2. **Off-sample performance metric design.** Determine $R : L_{\mathcal{H}} \rightarrow \mathbb{R}$ based on properties of the test loss distribution that we wish to prioritize.

3. **Algorithm design.** Determine $\mathcal{A}$ controlling the learning process $\mathcal{A}(Z) = (H_1, H_2, \ldots)$ in such a way that we expect $R(H_n)$ to approach an optimal value, given enough data.

4. **Performance analysis.** In theory, pursue bounds on $\mathbb{E}[R(H_n)]$ or $\mathbb{P}\{R(H_n) \in C\}$.\(^7\) In practice, empirically estimate $R(H_n)$ based on the empirical test loss distribution.

This four-step workflow highlights the central role played by the off-sample performance metric, in particular with respect to the design of learning algorithms. We have intentionally left our formulation as general as possible; “good performance” can be defined in terms of $R$ in a variety of ways (e.g., minimization, maximization, finding roots, etc.). This represents our alternative to the status quo, which we have claimed is centered around “average performance,” formalized in the objective (1). In §3 and §4 to follow, we justify this claim more thoroughly. Later, in §5, we survey some recent developments in the machine learning community, including some interesting special cases of the general framework just described.

### 3 Origins of expected loss minimization

The problem of decision-making under uncertainty has interested scholars for centuries. For an uncertain outcome which can be expressed numerically, the traditional “mathematical expecta-\(^6\)This knowledge can come in many forms and in varying degrees. It could be knowledge of a functional relationship linking inputs to outputs (up to a finite number of parameters), sparsity constraints, etc.

\(^7\)Here expectation and probability are with respect to both $Z$ and any randomness inherent to $\mathcal{A}$, and $C$ is an arbitrary set $C \subset \mathbb{R}$. A typical example when $R$ is negatively oriented (smaller is better) is to upper-bound the probability of the $\varepsilon$-bad event where $\varepsilon = (\varepsilon, \infty]$.}
tion" is the sum of all possible outcomes, weighted by the probability of each outcome. This notion was clearly described in letters from the Bernoullis and Gabriel Cramer dating back to the early 18th century [5]. With the expected value defined as a probability-weighted sum, then a problem of fundamental importance is how to evaluate outcomes, namely the process of assigning numerical values to real-world outcomes, which are appropriate within the context of the decisions that need to be made. The importance of this is highlighted by the “St. Petersburg paradox,” dating back to Nikolaus and Daniel Bernoulli [48]. Consider the following game: a fair coin is tossed until it turns up heads, and one receives a payment of $2^K$ dollars (or ducats), where $K$ is a random variable representing the number of tosses it took for heads to turn up. Note that $K$ is bounded below by 1, and unbounded above. The expected payout is $E[2^K] = 2(1/2) + 2^2(1/2^2) + \cdots = \infty$. While the expected payout is infinite, it seems irrational to pay a large amount to play this game, and thus arises the need to refine how we evaluate outcomes when making decisions. Essentially, this amounts to transforming the raw payouts in such a way that better reflects human preferences, say by introducing a function $f$ such that $E[f(2^K)] < \infty$. More generally, given any uncertain outcome $X$, the transformed value $f(X)$ is often called the utility of that outcome. The basic decision-making principle derived from this line of thought is simple: act in a way that maximizes the expected utility.

Over the course of the 20th century, the theoretical foundations of this principle were substantially strengthened. Of particular historical significance is the seminal theory of games developed by von Neumann and Morgenstern [88], where expected utility $E[f(X)]$ appears in the context of axioms related to preferences over uncertain outcomes (or “lotteries”) that we expect any “rational” agent to satisfy. These axioms are typically stated with respect to a class of uncertain outcomes, here a set $\mathcal{X}$ of random variables. The famous “expected utility theorem” states that any agent satisfying these axioms (under $\mathcal{X}$) must assign its preferences based on expected utility, that is, there exists a utility function $f$ such that for any $X_1, X_2 \in \mathcal{X}$, we have $X_1 \preceq X_2$ (i.e., “$X_2$ is no worse than $X_1$”) if and only if $E[f(X_1)] \leq E[f(X_2)]$. As such, when the agent can choose between uncertain outcomes, it will choose the one with the largest expected utility. Due to the significant influence of this work, the decision-making principle of maximizing the expected utility is essentially synonymous with the “rational agent” model pervasive in the social sciences [77, 45].

Since the usual form of expected utility is a probability-weighted sum, one naturally runs into the question of where these probabilities come from, and what they mean. When betting...
on the outcome of a coin toss, under most conditions it is reasonable to say that the equal probability of heads and tails is a fact of nature, and the probabilities $P\{X = \text{“heads”}\} = P\{X = \text{“tails”}\} = 1/2$ are in this sense objectively determined. On the other hand, consider the question of “will the stock price of Company ABCD rise next quarter?” This is a typical example of uncertainty in the real world, and while the possible outcomes are crystal-clear (the price will either rise, or it will not), it is very difficult to conceive of any kind of objective probability that can be assigned to such an uncertain outcome. Depending on knowledge and past experience (among countless other factors), the probability that different parties assign to this event will assuredly differ, making probability an inherently subjective notion. Indeed, if we polled a handful of stock traders, employees of Company ABCD, and individuals with no interest or knowledge of the company, we would not be surprised if all these parties had very different expectations.

Historically, this dichotomy of objective and subjective probability has received a great deal of attention, and underlies much scholarly activity in many disciplines. For example, objective probability can be seen as underlying the principle of repeated sampling, which is central to the statistical methodology of Fisher [93]. Indeed, it is hard to justify a procedure of taking controlled random samples to estimate probability unless that probability is “well-defined” in an objective sense. In contrast, Bayesian statistical methods give the statistician the freedom to reflect opinion and knowledge (or a lack thereof) in the inferential procedure, through a prior distribution over the parameter set, which allows for a subjective interpretation of the probabilistic model. Given identical data sets, different statisticians can arrive at different conclusions. Arguably the most influential proponent of subjective probability is that of Leonard J. Savage; in his seminal work [69], he builds a theory of probability and statistics which is centered on “personal” probability. In the context of Bayesian inference, this approach can be implemented by emphasizing a subjective prior [93, Sec. 3.6]. Recalling the expected utility theorem described earlier, Savage proves an analogous theorem, but manages to do it without assuming given probabilities (used in computing an “objective” expected utility), and instead shows that the rational agent axioms imply a form of subjective expected utility maximization. This view of probability and decision-making is prevalent in modern game theory [55, Sec. 1.4], and the subjective expected utility theorem is a foundational result in the broader context of decision theory [74].

The final important historical development we should highlight is that of viewing statistical inference as a decision-making problem, in contrast with the classical notion of inference being a rather mechanical summary of data [93, Ch. 1–2]. Of particular importance is the work of Abraham Wald, whose work laid the foundations for statistical decision theory [89, 90, 91]. One key theme is that from the statistician’s perspective, different types of errors may naturally have a different importance, or weight. Starting with his seminal 1939 work [89], Wald introduces a general-purpose loss function (what he calls a “weight function”) that quantifies this decision-dependent importance, and captures a wide class of statistical problems by formulating them in terms of minimizing the expected loss, or what he calls the “risk.” Underlying this “risk,” of

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[13] Clearly, many decisions under uncertainty will inevitably involve subjective probabilities. Recent books by Taleb [76] and Kahneman [32] aimed at broad audiences give a lucid discussion of the potential ramifications that this subjectivity has on our interaction with complex systems, in particular those of a socioeconomic nature.

[14] For a textbook introduction to statistical inference that effectively describes the development of the field within the context of all the major schools of thought, Young and Smith [93] is a useful reference.

[15] See Mas-Colell et al. [45, Sec. 6.F] for a high-level description and useful references.

[16] Let us compare Wald’s terminology with ours (cf. §2). The “loss” of Wald [89] depends on an unknown true model parameter (denoted by $\theta$ in his notation), so his “loss” actually corresponds more closely to our off-sample performance metric $R(H_n)$, and his “risk” then amounts to our $E[R(H_n)]$, with expectation taken over $Z$ and
course, is a random loss. With Wald’s framework as context, a straightforward generalization beyond typical statistical models and tasks leads us directly to the random test loss $\ell(h; Z')$ that we introduced earlier in §2, depending on the candidate $h \in \mathcal{H}$. In particular, note that the class of test losses $\mathcal{L}_\mathcal{H} = \{\ell(h; Z') : h \in \mathcal{H}\}$ is in direct analogy with the class of “lotteries” $\mathcal{X} = \{X_1, X_2, \ldots\}$ discussed earlier in the context of expected utility. Furthermore, an important characteristic of the decision-theoretic approach to statistics is an emphasis upon the optimality of general inferential procedures, stated in terms that do not depend on any particular dataset [93, Ch. 1]. In short, the qualities of data-driven algorithms become an important object of analysis, which makes for a smooth methodological transition to machine learning problems.

4 Expected loss and learning problems

In this section, we provide some justification for our earlier statement that performance on average, i.e., minimization of the expected loss (1), is the dominant paradigm for performance evaluation in machine learning. A natural starting point is the Perceptron of Frank Rosenblatt in the late 1950s [65], and the 1962 proof of the convergence of the Perceptron learning algorithm (here, PLA) for linearly separable data.\footnote{See Novikoff [53] and Minsky and Papert [49, Ch. 11] for background on this result.} This important result is recognized as having effectively “started learning theory” [85, p. 5]. Making this a bit more concrete, given a dataset of $n$ points $Z = (Z_1, \ldots, Z_n)$, assumed to be input-output pairs $Z_i = (X_i, Y_i)$ with binary labels $Y_i \in \{-1, +1\}$, and denoting the random zero-one losses as $L_i(h) := I\{h(X_i) \neq Y_i\}$ for $i \in [n]$, the convergence theorem tells us that whenever perfect accuracy is possible, then the PLA output $A_{\text{PLA}}(Z) = (H_1, \ldots, H_n)$ will achieve it, namely that

$$\frac{1}{n} \sum_{i=1}^{n} L_i(H_n) = 0. \quad (2)$$

In the context of learning, the question is then how the PLA generalizes to new data. Given an independent test point $Z' = (X', Y')$ and writing $L(h) = I\{h(X') \neq Y'\}$, off-sample misclassification is characterized by $L(H_n)$. Since this is just a Bernoulli random variable, its distribution is characterized by its mean $\mathbb{E}[L(H_n)|Z] = \mathbb{P}\{H_n(X') \neq Y'|Z\}$. With the key fact of (2) in mind, the question of generalization can then be reduced to (uniform) control of the deviations between “relative frequencies of events and their probability,” which is precisely the topic of the seminal 1971 paper of Vapnik and Chervonenkis [86].

The approach of the original “VC theory” goes well beyond hyperplanes and PLA. For any model $\mathcal{H}$ of binary classifiers, write $\hat{R}_n(h) := (1/n) \sum_{i=1}^{n} L_i(h)$ and $R(h) := \mathbb{P}\{h(X') \neq Y'\}$ for the empirical and true zero-one risk, respectively, and note that for the output $H_n$ of any learning algorithm (not restricted to PLA), we trivially have

$$\left|\hat{R}_n(H_n) - R(H_n)\right| \leq \sup_{h \in \mathcal{H}} \left|\hat{R}_n(h) - R(h)\right|. \quad (3)$$

The results of [86] enable us to characterize the convergence properties of the right-hand side of (3) based on properties of the model $\mathcal{H}$ that are of a combinatorial nature. Having this control is particularly useful for evaluating the performance of empirical risk minimizers, namely any algorithm which minimizes the empirical risk (such as PLA). Making this explicit, if we
constrain the learning algorithm such that $H_n$ minimizes $\hat{R}_n$, since for any fixed reference point $h^* \in \mathcal{H}$ we have $\hat{R}_n(H_n) \leq \hat{R}_n(h^*)$, it follows that
\[
R(H_n) - R(h^*) = R(H_n) - \hat{R}_n(H_n) + \hat{R}_n(H_n) - \hat{R}_n(h^*) + \hat{R}_n(h^*) - R(h^*) \leq 2 \sup_{h \in \mathcal{H}} |\hat{R}_n(h) - R(h)|.
\]
(4)

Assuming $R$ takes its minimum on $\mathcal{H}$, it is natural to take the reference point $h^* \in \mathcal{H}$ such that $R(h^*) = R^* := \inf \{R(h) : h \in \mathcal{H}\}$. This $R^*$ represents the best off-sample performance we can hope to achieve, and thus it is natural to ask that the learning algorithm be able to get arbitrarily close to this benchmark with sufficiently high probability, given enough data. More precisely, we can make the following requirement:
\[
\forall \varepsilon > 0, \quad \lim_{n \to \infty} \mathbb{P} \{R(H_n) - R^* > \varepsilon\} = 0.
\]
(5)

This is just convergence of $R(H_n) \to R^*$ in probability, also known as consistency of the learning algorithm. There is no conceptual reason to limit this analytical framework to the zero-one loss; any random loss $L(h) := \ell(h; Z')$ with a finite expectation $R(h) = \mathbb{E}[L(h)] < \infty$ can in principle be considered. Minimizing the expected value of a general-purpose loss over a hypothesis class $\mathcal{H}$ is precisely what Vapnik calls the general setting of learning [85, Ch. 1].

The requirement (5) can be stated in a different but equivalent fashion as follows: for any desired accuracy $\varepsilon > 0$ and confidence $0 < \delta < 1$, there must exist $N(\varepsilon, \delta) \in \mathbb{N}$ such that for any $n \geq N(\varepsilon, \delta)$, we have
\[
\mathbb{P} \{R(H_n) - R^* > \varepsilon\} \leq \delta.
\]
(6)

The condition (6) emphasizes precision and confidence requirements explicitly through the parameters $\varepsilon$ and $\delta$ respectively. The highly influential work of Valiant [80] considers a learning model which emphasizes precisely these points, with a particular interest in the computational complexity of achieving the $(\varepsilon, \delta)$-condition in (6). This became known as the PAC-learning model.\(^{18}\) In effect, the work of Valiant brought the consistency requirement to the community of computer scientists working on machine learning.\(^{19}\) In this community, as is mentioned by Kearns et al. [34], it should be noted that the emphasis on the expected value of a generic loss (i.e., the general setting of Vapnik) was largely due to the learning model studied by Haussler [26], in which the classical risk $\mathbb{E}[L(h)]$ plays a central role.\(^{20}\)

To conclude this section, given the historical context established in the preceding paragraphs, we give a brief overview highlighting how “learning as expected loss minimization” is emphasized in many influential and widely-read textbooks. Kearns and Vazirani [35] give an elementary

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\(^{18}\)The original idea of [80] was fleshed out further in subsequent works by Valiant [79, 81]. The naming of this model given in the main text (PAC: probably approximately correct) appears to date back to Angluin [2] and Angluin and Laird [3]. The textbook of Kearns and Vazirani [35] provides good additional background.

\(^{19}\)While the PAC-learning model was the first to receive widespread attention, clearly the general setting of Vapnik supersedes the PAC-learning model; the $(\varepsilon, \delta)$-condition (6) appears from the start of a book by Vapnik [82, Sec. 1.6], a 1982 English translation of a Russian book published in 1979. However, the work of Vapnik was not well-known by computer scientists in the West until the late 1980s, in particular due to the influential work of Blumer et al. [10], who introduced and built upon Vapnik and Chervonenkis [86]. As an aside, according to Vapnik [83, Ch. 2], L. Valiant did not know of his work when authoring the seminal 1984 article [80]. On the other hand, many probability theorists in the West were familiar with the work of Vapnik and Chervonenkis; see for example Dudley [19] or Pollard [57].

\(^{20}\)While the Haussler model is completely centered around $R(h) = \mathbb{E}[L(h)]$ as a performance metric, it should be mentioned that it includes a generalization of how to process this quantity. His learning model says to design an algorithm such that $H_n$ minimizes the expected “regret” $\mathbb{E}[f(H_n; R)]$, where $f$ can be a function like $f(h; R) = I\{D(R(h), R^*) > \varepsilon\}$ for an arbitrary metric $D$, or simply $f(h; R) = R(h) - R^*$.\(^{20}\)
introduction to the PAC-learning framework and basics of VC theory, with emphasis placed on computational tractability and tasks of interest in computer science. It goes without saying that all the books of Vapnik [82, 84, 85] are chiefly concerned with the problem of expected loss minimization. While restricted to the pattern recognition problem (binary classification), the highly influential text of Devroye et al. [15] characterizes the learning problem in terms of $E[L(H_n) | Z]$, formulated using the consistency condition (5). Expected loss is also central to the learning setup in the textbook of Ripley [60]. This setup is carried on by Anthony and Bartlett [4], in their text on neural network learning. A more modern textbook dealing with statistical and computational learning theory is Mohri et al. [50], and the expected loss plays a foundational role. Expected loss is used as a central criterion in the introductory text of Shalev-Shwartz and Ben-David [70], which also emphasizes links between stochastic optimization and machine learning. It is clear that these theory-oriented textbooks are centered around the expected loss, but this notion also appears frequently in more applied machine learning textbooks aimed at introducing key methods and tools to a general audience, albeit in more of a supplementary role. To give a few examples, we have MacKay [43, Ch. 36], Bishop [9, Ch. 1], Murphy [51, Ch. 5–6], Goodfellow et al. [24, Ch. 5], among others. Given this bibliographic evidence, along with the historical context provided in section 3 earlier, it is evident that the notion of expected loss as a metric for off-sample generalization has been pervasive in both the theory and practice of modern machine learning.

5 Survey of non-traditional methods

Recall from §1 and §2 that our primary interest is with quantifying off-sample performance, without the restriction to the expected test loss (1). In particular, we contend that an important novelty of this work is that of bringing attention to off-sample performance metrics as an element of the learning system to be designed, rather than taken as a given. This is important since the underlying risk has a direct impact on feedback generation, interpretation of results, and transparency of the system design process. In this section, we provide a brief introduction to the existing machine learning literature which is relevant to this topic.

To get started, we first take a bird’s-eye view of the key trends in the existing literature. We identify two major trends that are relevant in the context of this work:

- **Designing new empirical objectives.** This category captures work on the design and analysis of learning algorithms that emphasize new training objective functions $\hat{R} \approx R$, while typically keeping $R(h) = E[L(h) | Z]$ as the ultimate objective function.

- **Designing new risk functions.** Here the focus is on using a novel risk function $R$ as the ultimate objective, where $R(\cdot) \neq E[L(\cdot)]$. In many cases, the risk design is such that novel learning algorithms can be readily derived based on the definition of $R$.

We discuss these two trends respectively in §5.1 and §5.2. While these two categories are fairly clear-cut, it should be noted that there is still some conceptual overlap between the two. For example, when designing a new objective function that can be computed based on training data, there may be a novel risk function which is implied by the new objective function (e.g., its expected value taken over the training data). The former category of literature tends to keep $E[L(h)]$ as the ultimate goal of learning, and thus often needs to deal with bias that arises due to introducing a non-traditional objective function. In the following sub-sections, we provide simple formulations using our notation, in order to highlight the salient features of key works from each category.
5.1 Designing new empirical objectives

In the literature to be introduced below, the main innovations are in the design of an objective function used for training. That is, the learning algorithms being studied almost invariably involve some explicit objective function \( \hat{\mathcal{R}}_n \) depending on at most \( n \) points from the training data \( \mathbf{Z} = (Z_1, Z_2, \ldots) \), and produce an output \( \mathcal{A}(\mathbf{Z}) = (H_1, H_2, \ldots) \) of the following form:

\[
H_n \in \arg \min_{h \in \mathcal{H}} \left[ \hat{\mathcal{R}}_n(h) \right].
\]  

(7)

Thus, learning algorithms are characterized by how \( \hat{\mathcal{R}}_n \) is designed, and how the minimization in (7) is implemented. For concreteness and simplicity, we shall assume for the rest of this sub-section that the training data is a sequence of \( n \) iid samples, \( \mathbf{Z} = (Z_1, \ldots, Z_n) \), and the corresponding losses are \( L_i(h) = \ell(h; Z_i) \), for \( i \in [n] \).

5.1.1 M-estimators

One of the most natural reasons to design novel objective functions is because the traditional empirical mean tends to be a sub-optimal estimator of the expected value when the loss distribution tends to be heavy-tailed.\(^{21}\) Seminal work from Brownlees et al.\(^{11}\) considers an alternative procedure using M-estimators of the true mean. Letting \( \rho : \mathbb{R} \to [0, \infty) \) be convex and differentiable, the idea is to set

\[
\hat{\mathcal{R}}_n(h) = \arg \min_{\theta \in \mathbb{R}} \left[ \frac{1}{n} \sum_{i=1}^{n} \rho \left( \frac{L_i(h) - \theta}{\sigma} \right) \right]
\]  

(8)

and minimize this \( \hat{\mathcal{R}} \) over \( \mathcal{H} \). Statistically, for regression problems with heavy-tailed data, it is possible to show that any minimizer of (8) enjoys desirable robustness properties that traditional ERM solutions do not\(^{11}\). This work is important because it is rigorously demonstrates the statistical merits of using biased, robust estimators as objective functions. The chief limitation is computational; all algorithmic elements are left abstract in\(^{11}\), since the minimization of (8) is a challenging optimization problem.\(^{22}\)

5.1.2 L-statistics

Another intuitive strategy for constructing an objective function based on a random sample of losses is to sort the losses and assign weights depending on rank, before summation. With \( n \) samples, let \( L_i(h) \) denote the \( i \)th-smallest loss under \( h \), i.e., depending on the choice of \( h \in \mathcal{H} \), the losses are sorted such that

\[
L_{(1)}(h) \leq L_{(2)}(h) \leq \ldots \leq L_{(n)}(h).
\]

Letting \( w_1, \ldots, w_n \) denote real-valued weights, summing to 1, we can construct an objective function as follows:

\[
\hat{\mathcal{R}}_n(h) = \sum_{i=1}^{n} w_i L_{(i)}(h).
\]  

(9)

---

\(^{21}\)Efficient construction of robust estimators of the mean is itself a hard problem being studied by many researchers. While M-estimators of location date back to Huber\(^{29}\), an important study from Catoni\(^{13}\) stimulated a flurry of activity over the past decade; see Lugosi and Mendelson\(^{41}\) for a review.

\(^{22}\)Since the M-estimator is itself defined as the solution of a minimization problem, minimizing that quantity as a function of \( h \in \mathcal{H} \) is what is termed a bi-level program.
This is an example of what is called an \textit{L-statistic}, namely a linear combination of order statistics [30]. This formulation captures a wide variety of possible objective functions. One can “trim” the extreme values by setting high-ranked weights to zero; indeed, robustness of the trimmed mean estimator is well-known [42, 41]. Conditions for uniform convergence of L-estimators are obtained by Khim et al. [36]. Applications to robust unsupervised learning, replacing average distortion with an L-statistic, have been studied by Maurer et al. [46].

5.1.3 Largest losses

Within the context of novel empirical objective functions, a particularly important special case of L-statistics is that of using a fixed fraction of the largest losses, ignoring all the smaller losses. To make this explicit, let \( L_{[i]}(h) \) denote the \( i \)-th largest loss under \( h \), i.e., we sort such that
\[
L_{[1]}(h) \geq L_{[2]}(h) \geq \ldots \geq L_{[n]}(h).
\]
With this notation in place, learning algorithms based on the \textit{k-largest loss}
\[
\hat{R}_n(h) = L_{[k]}(h)
\]

have been studied by Shalev-Shwartz and Wexler [71], who pay particular attention to \( k = n \), namely the “max loss.” A useful alternative studied by Fan et al. [21, 20] is the \textit{average top-k loss}, defined as
\[
\hat{R}_n(h) = \frac{1}{k} \sum_{i=1}^{k} L_{[i]}(h).
\]
A handy fact underlying this approach is that the map \((x_1, \ldots, x_n) \mapsto \sum_{i=1}^{k} x_{[i]}\) is convex.23

5.1.4 Exponential smoothing

A well-known smooth alternative to minimizing the largest loss is achieved by passing the losses through an exponential smoother before averaging:
\[
\hat{R}_n(h) = \frac{1}{\gamma} \log \left( \frac{1}{n} \sum_{i=1}^{n} e^{-\gamma L_i(h)} \right),
\]
where for \( \gamma > 0 \), this function gives a smooth approximation of \( L_{[n]}(\cdot) \) with known precision bounds [56]. Learning algorithms minimizing this objective have been called “tilted ERM” by Li et al. [39, 40], who provide lucid and informative analysis under any setting of \( \gamma \neq 0 \).

5.1.5 Location and deviation

The notion of minimizing a sum of location and deviation estimators has a long history, with a particularly well-known example being the mean-variance objective due to Markowitz [44], used in classical work on portfolio optimization. Denoting the empirical mean and variance of the training loss given an iid sample as
\[
\bar{L}_n(h) := \frac{1}{n} \sum_{i=1}^{n} L_i(h), \quad \bar{V}_n(h) := \frac{1}{n(n-1)} \sum_{i<j} (L_i(h) - L_j(h))^2,
\]

23For more on this optimization task, see Ogryczak and Tamir [54].
then using a weight parameter \( \eta \geq 0 \) the resulting objective is

\[
\hat{R}_n(h) = \Gamma_n(h) + \eta \sqrt{\frac{\nabla_n(h)}{n}}.
\]  

(14)

This formulation is used by Maurer and Pontil [47] to derive the “sample variance penalization” (SVP) class of learning programs based on empirical Bernstein inequalities. Bounds are clear, but computation is hard. To make computation easier, Duchi and Namkoong [18, 17] consider optimizing the traditional risk under a “distributional robustness” constraint, namely a worst-case bound over all “close” distributions, which preserves convexity; we revisit this line of work later in §5.2.6.

5.2 Designing new off-sample performance metrics

Here we pay close attention to examples from the literature which are characterized by introducing non-traditional off-sample performance metrics into the learning system. Recall from §2 that given a hypothesis set \( \mathcal{H} \) and test losses \( \mathcal{L}_H = \{L(h) : h \in \mathcal{H}\} \), we use \( R : \mathcal{L}_H \rightarrow \mathbb{R} \) as general-purpose notation for any off-sample performance metric. In contrast with §5.1, where we dealt with empirical objectives that can be computed based on the training data, the risk function here is an ideal quantity depending on the test distribution, and \( R(\cdot) \) can never be evaluated exactly in practice. Regarding terminology, in the special case where \( R \) is negatively oriented (smaller is better), in much of the literature \( R \) is called a risk function.

5.2.1 Conditional value-at-risk

The subject of quantifying “risk” is of particular importance in the financial sector, from which many risk functions have been proposed. Within the context of machine learning, by far the best-known example is that of conditional value-at-risk (CVaR), which in words is the expected loss, conditioned on a “bad event” characterized by exceeding a particular quantile level. Making this more concrete, let us denote the distribution function and \( \beta \)-level quantile of \( L(h) \) respectively by

\[
F_h(u) := \mathbb{P}\{L(h) \leq u\}, \quad Q_{\beta}(h) := \inf \{u \in \mathbb{R} : F_h(u) \geq \beta\}
\]  

(15)

The quantile \( Q_{\beta}(h) \) is also known as the value-at-risk. With these definitions in place, CVaR is defined for any \( 0 < \beta < 1 \) as

\[
R(h) = \frac{1}{1-\beta} \mathbb{E} \left[ L(h) I_{\{L(h) \geq Q_{\beta}(h)\}} \right].
\]  

(16)

While at first glance this quantity may not appear to imply any efficient approximate minimizers, tractability of both computation and mathematical analysis is likely the chief reason CVaR has been so popular. Seminal work that popularized this quantity in the financial community is due to Rockafellar and Uryasev [61, 62]. The key is characterizing CVaR using a convex program [61, Thm. 1], namely showing that CVaR as defined in (16) can be characterized as

\[
R(h) = \min_{\theta \in \mathbb{R}} r(h, \theta), \quad \text{where} \quad r(h, \theta) := \theta + \frac{1}{1-\beta} \mathbb{E} [L(h) - \theta]_+.
\]  

(17)

Early work in the machine learning literature that explicitly defined CVaR as the underlying risk function is due to Kashima [33]. Connections to specialized machine learning methods are
elucidated by Takeda and Sugiyama [75]. Using CVaR as the underlying risk, it is straightforward to derive novel ERM procedures, oriented to the new risk. For example, analysis of stochastic sub-gradient methods under CVaR was done by Cardoso and Xu [12] and Soma and Yoshida [73] under sub-Gaussian assumptions, with Holland and Haress [28] introducing a robust procedure with analogous guarantees under heavy-tailed data.

5.2.2 L-risks

A very flexible class of risk functions can be constructed using a weighted sum of the loss distribution quantiles. Let $f : [0, 1] \to \mathbb{R}_+$ be a weighting function which is non-negative, non-decreasing, and integrates to 1 over the unit interval. Then, we define the L-risk incurred by $h \in H$ as

$$R(h) = \int_0^1 Q_u(h) f(u) \, du.$$  \hfill (18)

This is the “population” version of the L-statistic (9) considered in §5.1, and is itself a well-known concept in statistics [30]. The name “L-risk” is used by Khim et al. [36] in the machine learning literature, though this quantity is also well-known as a spectral risk in the financial literature [1]. It should be mentioned that CVaR is a special case of an L-risk: having fixed some $0 < \beta < 1$, if we set the weight function to $f(u) = I_{\{\beta<u\leq1\}}/(1 - \beta)$, then the L-risk (18) is in fact equal to CVaR (16), a fact that follows since $\beta$-level CVaR can be equivalently written as an integral over the quantile.\textsuperscript{24}

5.2.3 OCE risk

Another broad class of risks can be defined using a straightforward generalization of the characterization of CVaR seen in (17). Let $\phi : \mathbb{R} \to \mathbb{R}$ be proper closed convex, non-decreasing, such that $\phi(0) = 0$ and $1 \in \partial \phi(0)$. Then, we define the optimized certainty equivalent (OCE) risk as

$$R(h) = \inf_{\theta \in \mathbb{R}} (\theta + \mathbb{E}[\phi(L(h) - \theta)]).$$  \hfill (19)

This quantity was originally proposed by Ben-Tal and Teboulle [6] in the context of uncertain payoffs, rather than uncertain losses.\textsuperscript{25} The appearance of the OCE risk in this general form in the machine learning literature is recent, with lucid work by Lee et al. [37], who obtain conditions for the uniform convergence of the empirical OCE risk. Veraguas et al. [87] have also recently considered OCE risk minimization from the perspective of stochastic optimization. The OCE risk family captures several important special cases; perhaps the most obvious is that of CVaR, achieved by setting $\phi(u) = [u]_+/(1 - \beta)$. Another important special case is obtained when we set $\phi(u) = (e^{\gamma u} - 1)/\gamma$, resulting in a risk of the form

$$R(h) = \frac{1}{\gamma} \log \left( \mathbb{E} \left[ e^{\gamma L(h)} \right] \right).$$  \hfill (20)

This is the “population” version of the exponentially smoothed objective (12) seen earlier, and it has a rather long history of use in reinforcement learning, as detailed by García and Fernández [23, Sec. 3.2.1]. As described by Föllmer and Knispel [22], this special case is often called the entropic risk in a financial context.

\textsuperscript{24}For this basic fact as well as more general representations using CVaR, see Shapiro [72].

\textsuperscript{25}See §A.1 for additional background, and discussion of the link between the payoff and loss settings.
5.2.4 Location and deviation

Just as described in §5.1, it is natural to evaluate performance using both “location” and “deviation” properties of the loss distribution.\textsuperscript{26} Making this explicit, let $R_{\text{loc}}$ and $R_{\text{dev}}$ respectively denote risk functions capturing some concept of location and deviation. Assuming the scale of the two functions is comparable, then it is natural to define a risk using the sum of these two base risks:\textsuperscript{27}

$$R(h) = R_{\text{loc}}(h) + R_{\text{dev}}(h).$$  \hfill (21)

Special cases of the general form given by (21) are abundant, especially in the financial risk optimization literature (cf. [66, Sec. 4]). By far the most common choice of location is that of the expected loss $R_{\text{loc}}(L) = \mathbb{E}[L]$, where we suppress the dependence on $h$ for readability. The classical mean-variance risk of Markowitz [44] just sets the deviation as $R_{\text{dev}}(L) = \mathbb{E}[(L - \mathbb{E}[L])^2]$, though the scale of the location and deviation do not match in this case. Aligning the units and generalizing to

$$R_{\text{dev}}(L) = (\mathbb{E}|L - \mathbb{E}[L]|^p)^{1/p}$$  \hfill (22)

for some $1 \leq p < \infty$, we get a general class $R(L) = \mathbb{E}[L] + R_{\text{dev}}(L)$ of what are called mean-deviation risk functions.\textsuperscript{28} Since this class of risks under (22) does not in general satisfy monotonicity, the resulting risk $R(h)$ need not be convex in $h$, even if $L(h)$ is. A common technique to enforce monotonicity is to replace the absolute value $| \cdot |^{1/p}$ in (22) with the positive part $\lfloor \cdot \rfloor_+$, where $\lfloor u \rfloor_+ = \max\{u, 0\}$. The resulting risk

$$R(L) = \mathbb{E}[L] + (\mathbb{E}[L - \mathbb{E}[L]]_+^p)^{1/p}$$  \hfill (23)

is known as the mean-semi-deviation (or upper semi-variance). Further extensions of this same idea are readily obtained by considering upper deviations beyond a threshold $\theta \in \mathbb{R}$ which can be pre-fixed manually as in

$$R(L) = \mathbb{E}[L] + (\mathbb{E}[L - \theta]^p_+)^{1/p}$$  \hfill (24)

or even optimized over as

$$R(L) = \mathbb{E}[L] + \inf_{\theta \in \mathbb{R}} (\mathbb{E}[L - \theta]_+^p)^{1/p}.$$  \hfill (25)

Both of these examples appear in the survey of Ruszczyński and Shapiro [67]. A new class of risks studied by Holland [27] bridges the gap between traditional location-deviation risk and the OCE risk described previously, by considering

$$R(L) = \inf_{\theta \in \mathbb{R}} (\theta + \mathbb{E}[\rho(L - \theta)])$$

$$= \theta(L) + \mathbb{E}[\rho(L - \theta(L))]$$

where $\rho$ is convex and non-negative, but is allowed to be non-monotonic. The minimizer $\theta(L)$ is well-defined for a large class of functions $\rho$, and interpreted as a location, $\theta(L)$ is monotonic.

\textsuperscript{26}We use the term \textit{deviation} to emphasize that we are considering \textit{dispersion} properties of the loss distribution that are measured by the tendency to \textit{deviate} from some location.

\textsuperscript{27}Historically in statistics, it was common for the terms “scale” and “dispersion” to be used interchangeably (e.g., “estimates of scale” in Huber and Ronchetti [30]), but for our purposes these are distinct notions; dispersion is a property that does not change with arbitrary shifts, whereas the scale depends critically on the location.

\textsuperscript{28}We follow the nomenclature of Ruszczyński and Shapiro [66].
and translation-equivariant. With all these different risk examples as context, it is clear that given a location, we can use that location for “centering,” and to use the location of the centered distribution as an indicator of deviation:

\[ R_{\text{dev}}(L) := R_{\text{loc}}(L - R_{\text{loc}}(L)). \]  

(27)

Deviation functions of the form (27) are central to the axiomatic characterization of deviations due to Rockafellar et al. [64] (cf. their Thm. 2).

5.2.5 Psychologically motivated risks

A unique and interesting direction is designing risks which attempt to mirror human tendencies for risk aversion (or preference) when making decisions under uncertainty. In terms of the machine learning literature, essentially the only salient example is an application of the metrics used in the cumulative prospect theory (CPT) of Tversky and Kahneman [77]. To make our explanation as clear as possible, let us begin with an arbitrary random variable \( X \). Let \( V(\cdot) \) be a “value” function, and let \( F \) denote the true distribution function of \( X \), namely \( F(u) = P\{X \leq u\} \). The CPT score assigned to \( X \) is defined by taking the expectation using a modified distribution function \( \tilde{F} \), namely

\[ \text{CPT}(X) := \int_{\mathbb{R}} V(x) \tilde{F}(dx). \]  

(28)

Thus, the CPT score is characterized by the value function \( V \) and the transformation \( F \mapsto \tilde{F} \). Setting 0 as a threshold, using indicators \( I\{X \geq 0\} \) and \( I\{X < 0\} \) the CPT score typically treats these two mutually exclusive events differently. To do this, we construct value functions \( V_+ \) and \( V_- \) and differentiable weighting functions \( w_+ \) and \( w_- \) for each of these cases, setting

\[ V(x) = I\{x \geq 0\} V_+(x) + I\{x < 0\} V_-(x) \]

\[ \tilde{F}(x) = I\{x \geq 0\} w_+(F(x)) + I\{x < 0\} w_-(F(x)). \]

Putting these pieces together, the resulting CPT score takes the more explicit form

\[ \text{CPT}(X) = \int_{-\infty}^{0} V_-(x) w_-'(F(x)) F(dx) + \int_{0}^{\infty} V_+(x) w_+'(F(x)) F(dx) \]  

(29)

where \( w'_+ \) and \( w'_- \) are the derivatives of the weight functions. The threshold of 0 is of course arbitrary; this can be set to any value. The important concepts here are as follows: (a) “gains” and “losses” relative to some threshold are treated differently in human psychology; (b) small probabilities tend to be underweighted, large probabilities tend to be overweighted. See Rieger and Wang [59] for a useful background reference. Taking this from CPT scores to a natural notion of CPT risk just amounts to setting \( X = L(h) \), with our usual shorthand notation \( \text{CPT}(h) := \text{CPT}(L(h)) \) for each \( h \in \mathcal{H} \). While the general-purpose CPT score itself is well-known, literature on the CPT risk in machine learning remains quite sparse. Concentration bounds for estimators of the CPT risk (pointwise in \( h \)) are given by Bhat and Prashanth [8]. To the best of our knowledge, it appears that Leqi et al. [38] are the first to consider learning with CPT risks, under the catchy name “human-aligned risks,” although their studies are limited to an empirical analysis of learning using ERM implementations of certain special sub-classes of CPT risks.
5.2.6 Distributional robustness

An influential line of recent work looks at learning procedures which are robust to a certain degree of distributional shift between training and testing. To formulate this objective in a straightforward way, let $\mathcal{L}$ denote a set of integrable random losses, and define a new risk as

$$R(h) = \sup_{L \in \mathcal{L}} E[L(h)].$$  

(30)

This minimax objective asks the learner to perform well in the “worst-case” scenario, as characterized by $\mathcal{L}$. It is traditional for this worst-case scenario to be stated explicitly in terms of a shift in the data distribution. That is, starting with our training data sequence $Z = (Z_1, Z_2, \ldots)$, let us assume $Z_1, Z_2, \ldots$ are iid with a common distribution function $F_{TR}$. Then, using any divergence function $D$, define $\mathcal{L}$ such that the test data distribution is no more than $\delta$-far away from the training data:

$$\mathcal{L} = \{L(\cdot) = \ell(\cdot; Z') : Z' \sim F \text{ where } D(F; F_{TR}) \leq \delta\}.$$  

(31)

A particularly important special case is the class of risks implied by (30) and (31), where the divergence function $D$ is chosen to be an $f$-divergence [14]. Seminal work is due to Namkoong and Duchi [52] (see also Duchi and Namkoong [16]), who study efficient methods to actually solve learning problems of this form, and in the literature these solutions are naturally called distributionally robust. It is interesting to note that CVaR (16) is a special case [16]. As is typical of minimax objectives, in order to actually solve the problem, the learner must place a sufficient amount of weight on the worst-performing examples, which can lead to instability and inefficiency in learning. To alleviate such issues, recent work by Zhai et al. [94] considers using (30) with a choice of $\mathcal{L}$ that is more sophisticated than that of (31), designed to balance robustness to distribution shift as well as outliers.

5.2.7 Fairness

A topic of increasing importance that of ensuring the fairness of decisions made using machine learning systems. This is a big topic with literature that is growing rapidly, but here we highlight a representative example that shows how risk function design has links to algorithm fairness. Assume that our test data $Z'$ includes some sensitive features, and can be written $Z' = (Z'_0, S)$, where $S$ denotes the sensitive sub-group of features, and $Z'_0$ denotes the remaining features. For example, if “sex” is the only sensitive feature, then $S$ would be a random variable taking values in {“male”, “female”}. An intuitive and persuasive notion of fairness is that for better or for worse, algorithm performance should be uniform across sensitive sub-groups.

To make this concrete, consider the $S$-conditional expected loss:

$$R(h; S) := E[L(h) \mid S].$$  

(32)

Since $R(h; S)$ is a random quantity, notions of fairness can be described by properties of its distribution over the random draw of $S$. Recently, Williamson and Menon [92] took arguably the most natural approach, defining fairness in terms of sub-group deviations. For example, one might require that the learning algorithm output $A(Z) = (H_1, H_2, \ldots)$ satisfy a $\varepsilon$-fairness requirement of $\text{var}[R(H_n; S) \mid H_n] \leq \varepsilon$. To enforce this in practice, it is natural to consider objectives of the form

$$R(h) = E[R(h; S)] + \text{var}[R(h; S)]$$  

(33)

16
where expectation and variance in (33) are taken with respect to \( S \). Of course, this notion generalizes well beyond variance to more general deviations of random variables \([64, 63]\); see Williamson and Menon \([92]\) for an axiomatic treatment of fairness as sub-group deviations which admits convex objectives. Furthermore, while \( R(h; S) = \mathbb{E}[L(h) | S] \) was defined here using the conditional expected loss, this can in principle be generalized to a much larger class of \( S \)-conditional location parameters.

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A Appendix

A.1 Background on the OCE risk

Here we give a brief background on the optimized certainty equivalent (OCE) risk (19) discussed in §5.2. Let random variable $X$ represent some uncertain future payout (larger is better), and let $f : \mathbb{R} \to \mathbb{R}$ be a utility function (cf. §3). The certainty equivalent of $X$ under $f$, denoted $C_f(X)$, is defined as any (non-random) quantity which satisfies

$$f(C_f(X)) = E_f(X).$$

That is, receiving a payout $C_f(X)$ with certainty is just as good as receiving the uncertain payout $X$, from the standpoint of expected utility under $f$. The core idea of Ben-Tal and Teboulle [6] in defining their “new” certainty equivalent is that if receiving a certain payout at present causes a reduction in the uncertain payout to be received in the future, it is then natural to optimize the amount to receive now. More concretely, they consider

$$C^*_f(X) := \sup_{\theta \in \mathbb{R}} [\theta + E f(X - \theta)].$$

as the best possible allocation payouts across time. It should be noted that when we say this allocation is “best,” it is measured as a sum of quantities with different units. Instead of just measuring in terms of utility, the first term in $C^*_f(X)$ is the raw payout, whereas the second term is in terms of utility. Regarding the naming, (35) was originally called NCE (new certainty equivalent) in Ben-Tal and Teboulle [6]. Two decades later, the authors published an updated work on this quantity [7], in which they called it OCE.

In the recent work of Lee et al. [37], they consider using the OCE idea in the context of random losses, to define risk functions for machine learning tasks. More explicitly, as given in (19), they consider risks of the form

$$R(h) = \inf_{\theta \in \mathbb{R}} [\theta + E \phi(L(h) - \theta)].$$

Linking this quantity up with the original OCE for payoffs is straightforward. Losses can be considered negative payouts, and thus if we start with a utility function $f$, the function $\phi$ is naturally defined $\phi(u) = -f(-u)$. There are two minus signs here. Note that $u$ passed to $\phi$.

See Mas-Colell et al. [45, Defn. 6.C.2] for more background on this notion.
will be a loss, and thus since we need to pass \( f \) a payout, we pass it \( -u \). Furthermore, since \( \phi(\cdot) \) is to be minimized, while \( f(\cdot) \) is to be maximized, we use \(-f\) to obtain negative utility, or what Lee et al. [37] call “disutility.” Then establishing the link is straightforward, since

\[
\inf_{\theta \in \mathbb{R}} [\theta + \mathbb{E} \phi(L(h) - \theta)] = \inf_{\theta \in \mathbb{R}} [\theta - \mathbb{E} [f (-L(h) + \theta)]]
\]

we have that the preceding minimizing is equivalent to the following maximization:

\[
\sup_{\theta \in \mathbb{R}} (-1) [\theta - \mathbb{E} [f (-L(h) + \theta)] = \sup_{\theta \in \mathbb{R}} [-\theta + \mathbb{E} [f (-L(h) + \theta)]
\]

\[
= \sup_{\theta \in \mathbb{R}} [\theta + \mathbb{E} [f (-L(h) - \theta)]].
\]

Since negative losses are interpreted as payouts, setting \( X = -L(h) \) we obtain precisely the utility-based OCE given in (35). These facts lead us to clear connections between the OCE risk and the certainty equivalent under an exponential utility function [22, Sec. 2].