Deep Probabilistic Accelerated Evaluation: A Certifiable Rare-Event Simulation Methodology for Black-Box Autonomy

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Abstract

Evaluating the reliability of intelligent physical systems against rare catastrophic events poses a huge testing burden for real-world applications. Simulation provides a useful, if not unique, platform to evaluate the extremal risks of these AI-enabled systems before their deployments. Importance Sampling (IS), while proven to be powerful for rare-event simulation, faces challenges in handling these systems due to their black-box nature that fundamentally undermines its efficiency guarantee. To overcome this challenge, we propose a framework called Deep Probabilistic Accelerated Evaluation (D-PrAE) to design IS, which leverages rare-event-set learning and a new notion of efficiency certificate. D-PrAE combines the dominating point method with deep neural network classifiers to achieve superior estimation efficiency. We present theoretical guarantees and demonstrate the empirical effectiveness of D-PrAE via examples on the safety-testing of self-driving algorithms that are beyond the reach of classical variance reduction techniques.

1 Introduction

The unprecedented deployment of intelligent physical systems on many real-world applications comes with the need for safety validation and certification \cite{1,2}. For systems that interact with humans and are potentially safety-critical - which can range from medical systems to self-driving cars and personal assistive robots - it is imperative to rigorously assess their risks before their full-scale deployments. The challenge, however, is that these risks are often associated precisely to how AI reacts in rare and catastrophic scenarios which, by their own nature, are not sufficiently observed.

The challenge of validating the safety of intelligent systems described above is, unfortunately, insusceptible to traditional test methods. In the self-driving context, for instance, the goal of validation is to ensure the AI-enabled system reduces human-level accident rate (in the order of 1.5 per $10^8$ miles of driving), thus delivering enhanced safety promise to the public \cite{3,4,5}. Formal verification, which mathematically analyzes and verifies autonomous design, faces challenges when applied to black-box or complex models due to the lack of analytic tractability to formulate failure cases or consider all execution trajectories \cite{6}. Automated scenario selection approaches generate test cases based on domain knowledge \cite{7} or adaptive stress testing \cite{8}, which is more implementable

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but falls short of rigor. Test matrix approaches, such as Euro NCAP [9] use prepopulated test cases extracted from crash databases, but they only contain historical human-driver information. The closest analog to the latter for self-driving vehicles is “naturalistic tests”, which means placing them in real-world environments and gathering observations. This method, however, is economically prohibitive because of the rarity of the target conflict events [10] [11] [12] [13]. Because of all these limitations, simulation-based tests surface as a powerful, if not unique, approach to validate black-box autonomy designs [14]. This approach operates by integrating the target intelligent algorithm into an interacting virtual simulation platform that models the surrounding environment. By running enough Monte Carlo sampling of this (stochastic) environment, one hopes to observe catastrophic conflict events and subsequently conduct statistical analyses. This approach is flexible and scalable, as it hinges on building a virtual environment instead of physical systems, and provides a probabilistic assessment on the occurrences and behaviors of safety-critical events [15].

Nonetheless, similar to the challenge encountered by naturalistic tests, because of their rarity, safety-critical events are seldom observed in the simulation experiments. In other words, it could take an enormous amount of Monte Carlo simulation runs to observe one “hit”, and this in turn manifests statistically as a large estimation variance per simulation run relative to the target probability of interest (i.e., the so-called relative error; [16]). This problem, which is called rare-event simulation [17], is addressed conventionally under the umbrella of variance reduction, which includes a range of techniques from importance sampling (IS) [18] [19] to multi-level splitting [20] [21]. The main idea across all these techniques is to ensure the relative error is dramatically reduced (hence the name variance reduction), by analyzing the underlying model structures to gain understanding of the rare-event behaviors, and leveraging this knowledge to design good Monte Carlo schemes [22] [23]. For convenience, we call such relative error reduction guarantee an efficiency certificate.

Our main focus of this paper is on rare-event problems where the underlying model is unknown or too complicated to support analytical tractability. In this case, traditional variance reduction approaches fail to provide an efficiency certificate. Yet, this scenario is precisely the prominent case in intelligent system testing. In fact, we argue that the existing “black-box” variance reduction techniques (including for instance the cross-entropy method [24] [25] and particle approaches [26] [27]), not only do not provide correctness guarantees, but also could lead to dangerous under-estimation of the rare-event probability without noticed diagnostically. Our goal in this paper is to introduce an alternate framework, both theoretically justified and implementable, that allows the design of certifiable IS in the black-box setting. More precisely, it consists of three ingredients:

Relaxed efficiency certificate: We shift the estimation of target rare-event probability to a tight upper (and lower) bound, in a way that supports the integration of model errors into variance reduction without giving up estimation correctness.

Set-learning with one-sided error: We design learning algorithms to create outer (or inner) approximations of rare-event sets as special classification tasks that exhibit zero false negative rates, under a general geometric property called orthogonal monotonicity.

Deep-learning-based IS: We use a two-stage procedure, first to run deep neural network classifiers for set approximation, and second to assimilate the search of so-called dominant points in rare-event analysis, to create IS to that attains superior sampling efficiency with the relaxed certificate.

We call our framework consisting of the three ingredients above Deep Probabilistic Accelerated Evaluation (D-PrAE), where “Accelerated Evaluation” follows terminologies in recent approaches for the safety-testing of autonomous vehicles [28] [29]. To our best knowledge, this is the first approach for guaranteed rare-event simulation efficiency in settings beyond the analytical tractability heavily relied on in the traditional variance reduction literature. We envision our approach to open the door to further generalizations in the emerging applications of probabilistic AI-system risk evaluation.

2 Statistical Challenges in Black-Box Rare-Event Simulation

Our evaluation goal is the probabilistic assessment of a complex physical system invoking rare but catastrophic events in a stochastic environment. For concreteness, we write this rare-event probability \( \mu = P(X \in S_\gamma) \). Here \( X \) is a random vector in \( \mathbb{R}^d \) that denotes the environment, and is distributed according to \( \mu \). \( S_\gamma \) denotes a safety-critical set on the interaction between the physical system and the environment. The “rarity” parameter \( \gamma \in \mathbb{R} \) is considered a large number, with the property that
as \( \gamma \to \infty, \mu \to 0 \) (Think of, e.g., \( S_\gamma = \{ x : f(x) \geq \gamma \} \) for some risk function \( f \) and exceedance threshold \( \gamma \)). We will work with Gaussian \( p \) for the ease of analysis, but our framework is more general (i.e., apply to Gaussian mixtures and other light-tailed distributions). In the following, we explain intuitively the main concepts and challenges in black-box rare-event simulation, leaving the details to Appendix [A] where we also explain how we have generalized existing results.

**Monte Carlo Efficiency.** Suppose we use a Monte Carlo estimator \( \hat{\mu}_n \) to estimate \( \mu \), by running \( n \) simulation runs in total. Since \( \mu \) is tiny, the error of a meaningful estimation must be measured in relative term, i.e., we would like

\[
P(|\hat{\mu}_n - \mu| > \epsilon \mu) \leq \delta
\]

where \( \delta \) is some confidence level (e.g., \( \delta = 5\% \)) and \( 0 < \epsilon < 1 \). Suppose that \( \hat{\mu}_n \) is unbiased and is an average of \( n \) i.i.d. simulation runs, i.e., \( \hat{\mu}_n = (1/n) \sum_{i=1}^n Z_i \) for some random unbiased output \( Z_i \). We define the relative error \( RE = \text{Var}(Z_i)/\mu^2 \) as the ratio of variance (per-run) and squared mean. Importantly, to attain \( (1) \), a sufficient condition is \( n \geq RE/(\delta \epsilon^2) \). So, when \( RE \) is large, the required Monte Carlo size is also large.

**Challenges in Naive Monte Carlo.** Let \( Z_i = I(X_i \in S_\gamma) \) where \( I(\cdot) \) denotes the indicator function, and \( X_i \) is an i.i.d. copy of \( X \). Since \( Z_i \) follows a Bernoulli distribution, \( RE = (1 - \mu)/\mu \). Thus, the required \( n \) scales linearly in \( 1/\mu \) (when \( \mu \) is tiny). This demanding condition is a manifestation of the difficulty in hitting \( S_\gamma \). In the standard large deviations regime \([30, 31]\) where \( \mu \) is exponentially small in \( \gamma \), the required Monte Carlo size \( n \) would grow exponentially in \( \gamma \).

**Variance Reduction.** The severe burden when using naive Monte Carlo motivates techniques to drive down \( RE \). We use the term efficiency certificate to denote an estimator that achieves \( (1) \) with \( n = \tilde{O}(\log(1/\mu)) \), which can be attained with \( RE = \tilde{O}(\log(1/\mu)) \) (here \( \tilde{O}(\cdot) \) means polynomial growth). In the large deviations regime, this means \( n \) is reduced from exponential in the naive Monte Carlo to polynomial in \( \gamma \).

To this end, importance sampling (IS) is the most prominent technique to achieve efficiency certificate \([32]\). IS generates \( X \) from another distribution \( \tilde{p} \) (called IS distribution), and output \( \hat{\mu}_n = (1/n) \sum_{i=1}^n L(X_i)I(X_i \in S_\gamma) \) where \( L = dp/d\tilde{p} \) is the likelihood ratio, or the Radon-Nikodym derivative, between \( p \) and \( \tilde{p} \). Via a change of measure, it is easy to see that \( \hat{\mu}_n \) is unbiased for \( \mu \). The key is to control its \( RE \) by selecting a good \( \tilde{p} \). This requires analyzing the behavior of the likelihood ratio \( L \) under the rare event, and in turn understanding the rare-event sample path dynamics \([18]\).

**Perils of Black-Box Variance Reduction Algorithms.** Unfortunately, in black-box settings where complete model knowledge and analytical tractability are unavailable, the classical IS methodology faces severe challenges. To explain this, we first need to understand how efficiency certificate can be obtained based on the concept of dominant points. From now on, we consider input \( X \in \mathbb{R}^d \) from a Gaussian distribution \( N(\lambda, \Sigma) \) where \( \Sigma \) is positive definite.

**Definition 1.** A set \( A_\gamma \subset \mathbb{R}^d \) is a dominant set for the set \( S_\gamma \subset \mathbb{R}^d \) associated with the distribution \( N(\lambda, \Sigma) \) if for any \( x \in S_\gamma \), there exists at least one \( a \in A_\gamma \) such that \( (a - \lambda)^T \Sigma^{-1} (x - a) \geq 0 \). Moreover, this set is minimal in the sense that if any point in \( A_\gamma \) is removed, then the remaining set no longer satisfies the above condition. We call any point in \( A_\gamma \) a dominant point.

The dominant set comprises the “corner” cases where the rare event occurs \([33]\). In other words, each dominant point \( a \) encodes, in a local region, the most likely scenario should the rare event happen, and this typically corresponds to the highest-density point in this region. Locality here refers to the portion of the rare-event set that is on one side of the hyperplane cutting through \( a \) (see Figure [1](a)).

Intuitively, to increase the frequency of hitting the rare-event set (and subsequently to reduce variance), an IS would translate the distributional mean from \( \lambda \) to the global highest-density point in the rare-event set. The delicacy, however, is that this is insufficient to control the variance, due to the “overshoots” arising from sampling randomness. In order to properly control the overall variance, one needs to divide the rare-event set into local regions governed by dominant points, and using a mixture IS distribution that accounts for all of them:

**Theorem 1 (Certifiable IS).** Suppose \( S_\gamma = \bigcup_j S_\gamma^j \), where each \( S_\gamma^j \) is a “local” region corresponding to a dominant point \( a^j \in A_\gamma \) associated with the distribution \( N(\lambda, \Sigma) \), with conditions stated precisely in Theorem [5] in the Appendix. Then the IS distribution \( \sum_j \alpha_j N(a^j, \Sigma) \) achieves an efficiency certificate in estimating \( \mu = P(X \in S_\gamma) \).
On the contrary, if the Gaussian (mixture) IS distribution misses any of the dominant points, then the resulting estimate may be utterly unreliable for two reasons. First, not only that efficiency certificate may fail to hold, but its RE can be arbitrarily large. Second, even more dangerously, this poor performance can be empirically hidden and leads to a systematic under-estimation of the rare-event probability without detection. In other words, in a given experiment, we may observe a reasonable empirical relative error (i.e., sample variance over squared sample mean), yet the estimate is much lower than the correct value. These are revealed in the following example:

**Theorem 2** (Perils of under-estimation). Suppose we estimate \( \mu = P(X \geq \gamma \text{ or } X \leq -k\gamma) \) where \( X \sim p = N(0, 1) \) and \( 0 < k < 3 \). We choose \( \tilde{p} = N(\gamma, 1) \) as the IS distribution to obtain \( \hat{\mu}_n \). Then 1) The relative error of \( \hat{\mu}_n \) grows exponentially in \( \gamma \). 2) If \( n \) is polynomial in \( \gamma \), we have \( P\left(\left|\hat{\mu}_n - \Phi(\gamma)\right| > \varepsilon \Phi(\gamma)\right) = O\left(\frac{\gamma^2}{\varepsilon^2}\right) \) for any \( \varepsilon > 0 \) where \( \Phi(\gamma) = P(X \geq \gamma) < \mu \), and the empirical relative error \( = O(n^2) \) with probability higher than \( 1 - 1/2^n \).

We now explain why using black-box variance reduction algorithms can be dangerous - both in the sense of not having an efficiency certificate and, relatedly, the risk of an unnoticed systematic under-estimation. In the literature, there are two lines of techniques that apply to black-box problems. The first line is to use optimization to search for a good parametrization over a parametric class of IS. The objective criteria include the cross-entropy (with an oracle-best zero-variance IS distribution; [25, 24]) and estimation variance [34]. Without closed-form expressions, and also to combat the rare-event issue, one typically solves a sequence of empirical optimization problems, starting from a “less rare” problem (i.e., smaller \( \gamma \)) and gradually increasing the rarity with updated empirical objectives using better IS samples. Obtaining an efficiency certificate requires both a sufficiently expressive parametric IS class (enough mixtures) and parameter convergence (to account for all dominant points). In light of Theorem 2, one can construct examples where the converging IS distribution suffers from systematic under-estimation (see Appendix E). The second line of methods is the multi-level splitting or subsimulation [26, 27], a particle method in lieu of IS, which relies on enough mixing of descendant particles that can encounter similar issues as the cross-entropy method (see Appendix E). Thus, while both cross-entropy and multi-level splitting are powerful techniques, their use in rare-event problems with undefined structures should be properly cautioned.

### 3 The Deep Probabilistic Accelerated Evaluation Framework

We propose the D-PrAE framework to overcome the challenges faced by existing black-box variance reduction algorithms. This framework comprises two stages: First is to learn the rare-event set from a first-stage sample batch, by viewing set learning as a classification task. Second is to apply an efficiency-certified IS on the rare-event probability over the learned set. Algorithm 1 shows our main procedure. The key to achieving an ultimate efficiency certificate lies in how we learn the rare-event set in Stage 1, which requires two properties:

**Small one-sided generalization error:** “One-sided” generalization error here means the learned set is either an outer or an inner approximation of the unknown true rare-event set, with probability 1. Converting this into a classification, this means the false negative (or positive) rate is exactly 0. “Small” here then refers to the other type of error being controlled.

**Decomposability:** The learned set is decomposable according to dominant points in the form of Theorem 1, so that an efficient mixture IS can apply.
Algorithm 1: D-PrAE to estimate \( \mu = P(X \in S_\gamma) \).

**Input:** Black-box evaluator \( I(\cdot \in S_\gamma) \), sampling density \( q \), sample budgets \( n_1, n_2 \), input distribution \( N(\lambda, \Sigma) \).

**Output:** IS estimate \( \hat{\mu}_n \).

Stage 1 (Set Learning):
1. Sample \( \hat{X}_1, \ldots, \hat{X}_{n_1} \) from \( q \) and evaluate \( Y_i = I(\hat{X}_i \in S_\gamma) \) for \( i = 1, \ldots, n_1 \).
2. Train classifier with positive decision region \( \hat{S}_\gamma = \{ x : \hat{g}(x) \geq \hat{\kappa} \} \) using \( \{(\hat{X}_i, Y_i)\}_{i=1,\ldots,n_1} \).
3. Replace \( \kappa \) by \( \hat{\kappa} = \max \{ \kappa \in \mathbb{R} : (\hat{S}_\gamma)^c \subset \mathcal{H}(T_0) \} \).

Stage 2 (Mixture IS based on Searchdominant Points):
1. Start with \( \hat{A}_\gamma = \emptyset \).
2. While \( \{ x : \hat{g}(x) \geq \hat{\kappa}, (x_0^* - \lambda)^T \Sigma^{-1} (x_0^* - x^*) < 0, \forall x^* \in \hat{A}_\gamma \} \neq \emptyset \) do
3. Find a dominant point \( x^* \) by solving the optimization problem
   \[
   x^* = \arg \min_x (x - \lambda)^T \Sigma^{-1} (x - \lambda) \text{ s.t. } \hat{g}(x) \geq \hat{\kappa}, \ (x_0^* - \lambda)^T \Sigma^{-1} (x_0^* - x^*) < 0 \forall x^* \in \hat{A}_\gamma
   \]
   and update \( \hat{A}_\gamma \leftarrow \hat{A}_\gamma \cup \{ x^* \} \).
4. Sample \( X_1, \ldots, X_{n_2} \) from the mixture distribution \( \sum_{a \in \hat{A}_\gamma} (1/|\hat{A}_\gamma|) N(a, \Sigma) \).
5. Compute the IS estimator \( \hat{\mu}_n = (1/n_2) \sum_{i=1}^{n_2} L(X_i) I(X_i \in \hat{S}_\gamma^c) \), where the likelihood ratio
   \[
   L(X_i) = \phi(X_i; \lambda, \Sigma)/(\sum_{a \in \hat{A}_\gamma} (1/|\hat{A}_\gamma|) \phi(X_i; a, \Sigma)) \text{ and } \phi(\cdot; \alpha, \Sigma) \text{ denotes the density of } N(\alpha, \Sigma).
   \]

The first property ensures that, even though the learned set can contain errors, the learned rare-event probability is either an upper or lower bound of the truth. This requirement is important as it is extremely difficult to translate the impact of generalization errors into rare-event estimation errors. By Theorem 2, we know that any non-zero error implies the risk of missing out important regions of the rare-event set, undetectably. The one-sided generalization error allows a shift of our target to validate upper and lower bounds that can be correctly estimated, which is the core novelty of D-PrAE. To this end, we introduce a new efficiency notion:

**Definition 2.** We say an estimator \( \hat{\mu}_n \) satisfies an upper-bound relaxed efficiency certificate to estimate \( \mu \) if \( P(\hat{\mu}_n - \mu < -\epsilon \mu) \leq \delta \) with \( n \geq \tilde{O}(\log(1/\delta)) \), for \( 0 < \epsilon, \delta < 1 \).

Compared with the efficiency certificate in [1], Definition 2 is relaxed to only requiring \( \hat{\mu}_n \) to be an upper bound of \( \mu \), up to an error of \( \epsilon \mu \). An analogous lower-bound relaxed efficiency certificate can be seen in Appendix D. From a risk quantification viewpoint, the upper bound for \( \mu \) is more crucial, and the lower bound serves to assess an estimation gap. The following provides a handy certification:

**Proposition 1 (Achieving relaxed efficiency certificate).** Suppose \( \hat{\mu}_n \) is upward biased, i.e., \( \bar{\mu} := E[\hat{\mu}_n] \geq \mu \). Moreover, suppose \( \hat{\mu}_n \) takes the form of an average of \( n \) i.i.d. simulation runs \( Z_i \), with \( \text{RE} = \text{Var}(Z_i)/\bar{\mu}^2 = \tilde{O}(\log(1/\bar{\mu})) \). Then \( \hat{\mu}_n \) possesses the upper-bound relaxed efficiency certificate.

Proposition 1 stipulates that a relaxed efficiency certificate can be attained by an upward biased estimator that has a logarithmic relative error with respect to the biased mean (and hence also the original target probability). Appendix C shows an extension of Proposition 1 to two-stage procedures, where the first stage determines the upward biased mean. This upward biased mean, in turn, can be obtained by learning an outer approximation for the rare-event set, giving:

**Corollary 1 (Set-learning + IS).** Consider estimating \( \mu = P(X \in S_\gamma) \). Suppose we can learn a set \( \hat{S}_\gamma \) with any number of i.i.d. samples \( D_{n_1} \) (drawn from some distribution) such that \( \hat{S}_\gamma \supset S_\gamma \) with probability 1. Also suppose that there is an efficiency certificate for an IS estimator for \( \bar{\mu}(D_{n_1}) := P(X \in \hat{S}_\gamma) \). Then a two-stage estimator where a constant \( n_2 \) number of samples \( D_{n_2} \) are first used to construct \( \hat{S}_{n_1} \), and \( n_2 = \tilde{O}(\log(1/\bar{\mu}(D_{n_1})) \) samples are used for the IS in the second stage, achieves the upper-bound relaxed efficiency certificate.
To execute the procedure in Corollary 1, we need to learn an outer approximation of the rare-event set. To this end, consider set learning as a classification problem: We draw \( \tilde{X}_1, \ldots, \tilde{X}_n \) from some sampling distribution that has sufficient presence throughout the space (e.g., uniform over a large box centered at the mean of \( p \)). For each \( \tilde{X}_i \), we evaluate \( Y_i := I(\tilde{X}_i \in S_\gamma) \), i.e., \( Y_i = 1 \) if \( \tilde{X}_i \) is in the rare-event set \( S_\gamma \), and 0 otherwise. We consider the pairs \( \{(\tilde{X}_i, Y_i)\} \) where \( \tilde{X}_i \) is regarded as the feature and \( Y_i \) as the binary label, and construct a classifier, say \( \hat{g}(x) : \mathbb{R}^d \to [0, 1] \), from some hypothesis class \( \mathcal{G} \) that (nominally) signifies \( P(Y = 1|X = x) \). The learned rare-event set \( S_\gamma \) is taken to be \( \{x : \hat{g}(x) \geq \kappa\} \) for some threshold \( \kappa \in \mathbb{R} \).

The outer approximation requirement \( S_\gamma \supseteq S_\gamma \) means that all true positive (i.e., 1) labels must be correctly classified, or in other words, the false negative (i.e., 0) rate is zero, i.e.,

\[
P(X \in S_\gamma^c, Y = 1) = 0
\]  

(2)

Typically, achieving such a zero “Type I” misclassification rate is impossible for any finite sample except in degenerate cases. However, this is achievable under a mild geometric premise on the rare-event set \( S_\gamma \) that we call orthogonal monotonicity. To facilitate discussion, suppose from now on that the rare-event set is known to lie entirely in the positive quadrant \( \mathbb{R}^d_+ \), so in learning the set, we only consider sampling points in \( \mathbb{R}^d_+ \) (analogous development can be extended to the entire space).

**Definition 3.** We call a set \( S \subseteq \mathbb{R}^d_+ \) orthogonally monotone if for any two points \( x, x' \in \mathbb{R}^d_+ \), we have \( x \leq x' \) (where the inequality is defined coordinate-wise) and \( x \in S \) implies \( x' \in S \) too.

Definition 3 means that any point that is more “extreme” than a point in the rare-event set must also lie inside the same set. This is an intuitive assumption that commonly holds in rare-event settings. Note that, even with such a monotonicity property, the boundary of the rare-event set can be very complex. The key is that, with orthogonal monotonicity, we can now produce a classification procedure that satisfies (2). In fact, the simplest approach is to use what we call an orthogonally monotone hull:

**Definition 4.** For a set of points \( D = \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^d_+ \), we define the orthogonally monotone hull of \( D \) (with respect to the origin) as \( \mathcal{H}(D) = \bigcup_i \mathcal{R}(x_i) \), where \( \mathcal{R}(x_i) \) is the rectangle that contains both \( x_i \) and the origin as two of its corners.

In other words, the orthogonally monotone hull consists of the union of all the rectangles each wrapping each point \( x_i \) and the origin 0. Now, denote \( T_0 = \{\tilde{X}_i : Y_i = 0\} \) as the non-rare-event sampled points. Evidently, if \( S_\gamma \) is orthogonally monotone, then \( \mathcal{H}(T_0) \subseteq S_\gamma^c \) (where complement is with respect to \( \mathbb{R}^d_+ \), or equivalently, \( \mathcal{H}(T_0)^c \supseteq S_\gamma \), i.e., \( \mathcal{H}(T_0)^c \) is an outer approximation of the rare-event set \( S_\gamma \). Figure (1b) shows this outer approximation (and also the inner counterpart). Moreover, \( \mathcal{H}(T_0)^c \) is the smallest region (in terms of set volume) such that (2) holds, because any smaller region could exclude a point that has label 1 with positive probability.

**Lazy-Learner IS.** We now consider an estimator for \( \mu \) where in Stage 1, we sample a constant \( n_1 \) i.i.d. random points from some density, say \( q \). Then, we use the mixture IS depicted in Theorem 1 to estimate \( P(X \in \mathcal{H}(T_0)^c) \) in Stage 2. Since \( \mathcal{H}(T_0)^c \) takes the form \( \bigcup_i \mathcal{R}(\tilde{X}_i)^c \), it has a finite number of dominant points, which can be found by a sequential algorithm (similar to the one that we will discuss momentarily). We call this the “lazy-learner” approach. Its problem, however, is that \( \mathcal{H}(T_0)^c \) tends to have a very rough boundary. This generates a large number of dominant points, many of which are unnecessary in that they do not correspond to any “true” dominant points in the original rare-event set \( S_\gamma \) (see the middle of Figure (1d)). This in turn leads to a large number of mixture components that degrades the IS efficiency, as the RE bound in Theorem 1 scales linearly with the number of mixture components.

**Deep-Learning-Based IS.** Our main approach is a deep-learning alternative that resolves the statistical degradation of the lazy learner. We train a neural network classifier, say \( \hat{g} \), using all the Stage 1 samples \( \{(\tilde{X}_i, Y_i)\} \), and obtain an approximate non-rare-event region \( (\hat{S}_\gamma)^c = \{x : \hat{g}(x) < \kappa\} \), where \( \kappa \) is say 1/2. Then we adjust \( \kappa \) minimally away from 1/2, say to \( \hat{\kappa} \), so that \( (\hat{S}_\gamma)^c \subseteq \mathcal{H}(T_0) \), i.e., \( \hat{\kappa} = \max\{\kappa \in \mathbb{R} : (\hat{S}_\gamma)^c \subseteq \mathcal{H}(T_0)\} \). Then \( \hat{S}_\gamma^c \supseteq \mathcal{H}(T_0)^c \supseteq S_\gamma \), so that \( \hat{S}_\gamma^c \) is an outer approximation for \( S_\gamma \) (see Figure (1c), where \( \hat{\kappa} = 0.68 \)). Stage 1 in Algorithm 1 shows this procedure. With this, we can run mixture IS to estimate \( P(X \in \hat{S}_\gamma^c) \) in Stage 2.
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(ERM) to train

\(\sup \) ERM. Suppose the density \(q \) has bounded support \(K \subset [0, M]^d \) and \(0 < q_1 \leq q(x) \leq q_0 \) for any \(x \in K \). Also suppose there exists a function \(h \) such that for any \(g \in G \), \(g(x) \geq \kappa \) implies \(\ell(g(x), 0) \geq h(\kappa) > 0 \). (e.g., if \(\ell \) is the squared loss, then \(h(\kappa) \) could be chosen as \(h(\kappa) = \kappa^2 \)). Then, with probability at least \(1 - \delta \),

\[
P_{X \sim q}(X \in \bar{\mathcal{S}}^c / \mathcal{S}) \leq \frac{R(g^*) + 2 \sup_{g \in G} |R_{n_1}(g) - R(g)|}{h(\kappa^* - t(\delta, n_1))v \text{dLip}(g^*) - \|\hat{g} - g^*\|_{\infty}}.
\]

Here, Lip(\(g^*\)) is the Lipschitz parameter of \(g^*\), and \(t(\delta, n_1) = 3 \left( \frac{\log(n_1 q_1) + d \log M + \log \frac{1}{\delta}}{n_1 q_1} \right)^{\frac{1}{2}} \).

Theorem 4 reveals a tradeoff between overfitting (measured by \(\sup_{g \in G} |R_{n_1}(g) - R(g)| \) and \(\|\hat{g} - g^*\|_{\infty} \)) and underfitting (measured by \(R(g^*) = \inf_{g \in G} R(g) \)). Appendix B discusses related results on the sharp estimates of these quantities for deep neural networks, a more sophisticated version of Theorem 4 that applies to the cross-entropy loss, a corresponding bound for the lazy learner, as well as results to interpret Theorem 4 under the original distribution \(p \).

4 Numerical Experiments

We implement and compare the estimated probabilities and the RE’s of deep-learning-based IS for the upper bound (D-PrAE UB) and lazy-learner IS (LL UB). We also show the corresponding lower-bound estimator (D-PrAE LB and LL LB), the cross entropy method (CE), and na"ive Monte Carlo (NMC), in a 2-dimensional example and the safety-testing of a self-driving algorithm in a car-following scenario. These two experiments are representative as the former is low-dimensional (visualizable) yet with extremely rare events while the latter is high-dimensional, challenging for most of the existing methods.
**2D Example.** We estimate \( \mu = P(X \in \mathcal{S}_\gamma) \) where \( X \sim N([5, 5]^T, 0.25I_{2 \times 2}) \), and \( \gamma \) ranging from 1.8 to 2.6. We use \( n = 30,000 \) (10,000 for Stage 1 and 20,000 for Stage 2). Figure 1 illustrates the shape of \( \mathcal{S}_\gamma \), which has two dominant points. This probability is microscopically small (e.g., \( \gamma = 1.8 \) gives \( \mu = 4.1 \times 10^{-24} \)) and serves to investigate our performance in ultra-extreme situations.

![Figure 2: 2-dimensional example. Naive Monte Carlo failed in all cases and hence not shown.](image)

Figure 2 compares all approaches to the benchmark, which we compute via a proper mixture IS with 50,000 samples assuming full knowledge of \( \mathcal{S}_\gamma \). It shows several observations. First, D-PrAE and LL (both UB and LB) always provide valid bounds that contain the truth. Second, the UB for LL is consistently 2 order of magnitude more conservative than D-PrAE, attributed to the overly many dominant points (e.g., 34 vs 2 when \( \gamma = 2.6 \)). Correspondingly, the RE of LL UB blows up to 300\%, compared to 3\% for D-PrAE UB. Third, CE, which ends up using only one dominant point, under-estimates the truth by 50\%, yet it gives an over-confident RE, e.g., < 1\% when \( \gamma < 2.2 \), showing a systematic undetected under-estimation. Lastly, NMC fails to give a single hit in all cases (thus not shown on the graphs). Among all approaches, D-PrAE stands out as giving reliable and tight bounds with low RE.

**Self-Driving Example.** We consider simulating the crash probability in a car-following scenario involving a human-driven lead vehicle (LV) followed by an autonomous vehicle (AV). The AV is controlled by the Intelligent Driver Model (IDM) to maintain safety distance while ensuring smooth ride and maximum efficiency, which is widely used for autonomy evaluation and microscopic transportation simulations [37, 38, 39]. The state at time \( t \) is given by 6 states consisting of the position, velocity, and acceleration of both LV and AV. The dynamic system has a stochastic input \( u_t \) related to the acceleration of the LV and subject to uncertain human behavior. We consider an evaluation horizon \( T = 60 \) seconds and draw a sequence of 15 Gaussian random actions at a 4-second epoch, leading to a 15-dimensional LV action space. A (rare-event) crash occurs at time \( t \leq T \) if the longitudinal distance \( r_t \) between the two vehicles is negative, with \( \gamma \) parameterizing the AV maximum throttle and brake pedals. This rare-event set is analytically challenging (see [10] for a similar setting). More details are in Appendix F.

![Figure 3: Self-driving example. Naive Monte Carlo failed in all cases and hence not shown.](image)

Figure 3 shows the performances of competing approaches, using \( n = 10,000 \). D-PrAE and LL (UB and LB) appear consistent in giving upper and lower bounds for the target probability. Once again, D-PrAE produces tighter bounds than LL (\( 10^{-2} \) vs \( 10^{-6} \) in general). LL UB has 5,644 dominant points when \( \gamma = 1 \) vs 42 in D-PrAE, and needs 4 times more computational time to search for them than D-PrAE. Moreover, the RE of D-PrAE is around 3 times lower than LL across the range (in both UB and LB). Thus, D-PrAE outperforms LL in both tightness, computation speed, and RE. CE seems to give a stable estimation. However, we have evidence to believe it is under-estimated. We run a modification of D-PrAE that replaces \( \mathcal{S}_\gamma \) by \( \mathcal{S}_\gamma \) in the last step of Algorithm 1 (D-PrAE IS) and find a consistent positive gap over CE. D-PrAE IS lacks an efficiency certificate and thus could be under-estimated, and the fact that its estimate is higher than CE suggests CE is under-estimated.
Summary of Practical Benefits. Our investigation shows strong evidence of the practical benefits of using D-PrAE for rare-event estimation. It generates tight bounds for the target, with low RE, and requires reasonable computation effort in training deep-learning classifiers and IS. For example, if one were to assess whether the AV crash rate is below $10^{-8}$ for $\gamma = 1.0$, only 1000 simulation runs would be needed to get around 1% RE, taking about 400 seconds in total. This is in contrast to 3.7 months for naive Monte Carlo, and 1.1 hours for other methods that have no efficiency certificate. Results suggest that D-PrAE could be a game-changer once embedded in simulation software for safety evaluation of black-box autonomy.

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References

[1] Philip Koopman and Michael Wagner. Autonomous vehicle safety: An interdisciplinary challenge. *IEEE Intelligent Transportation Systems Magazine*, 9(1):90–96, 2017.

[2] Jonathan Uesato, Ananya Kumar, Csaba Szepesvari, Tom Erez, Avraham Ruderman, Keith Anderson, Nicolas Heess, Pushmeet Kohli, et al. Rigorous agent evaluation: An adversarial approach to uncover catastrophic failures. *arXiv preprint arXiv:1812.01647*, 2018.

[3] A. Evan. Fatal Tesla Self-Driving Car Crash Reminds Us That Robots Aren’t Perfect. *IEEE Spectrum*, 2016.

[4] Nidhi Kalra and Susan M Paddock. Driving to safety: How many miles of driving would it take to demonstrate autonomous vehicle reliability? *Transportation Research Part A: Policy and Practice*, 94:182–193, 2016.

[5] NTSB. Preliminary Report, Highway HWY16FH018, 2016.

[6] Edmund M Clarke, Thomas A Henzinger, Helmut Veith, and Roderick Bloem. *Handbook of model checking*, volume 10. Springer, 2018.

[7] Joachim Wegener and Oliver Bühler. Evaluation of different fitness functions for the evolutionary testing of an autonomous parking system. In *Genetic and Evolutionary Computation Conference*, pages 1400–1412. Springer, 2004.

[8] Mark Koren, Saud Alsaif, Ritchie Lee, and Mykel J Kochenderfer. Adaptive stress testing for autonomous vehicles. In *2018 IEEE Intelligent Vehicles Symposium (IV)*, pages 1–7. IEEE, 2018.

[9] NHTSA. The new car assessment program suggested approaches for future program enhancements. *DOT HS*, 810:698, 2007.

[10] Ding Zhao, Xianan Huang, Huei Peng, Henry Lam, and David J LeBlanc. Accelerated evaluation of automated vehicles in car-following maneuvers. *IEEE Transactions on Intelligent Transportation Systems*, 19(3):733–744, 2017.

[11] Mansur Arief, Peter Glynn, and Ding Zhao. An accelerated approach to safely and efficiently test pre-production autonomous vehicles on public streets. In *2018 21st International Conference on Intelligent Transportation Systems (ITSC)*, pages 2006–2011. IEEE, 2018.

[12] Joan Claybrook and Shaun Kildare. Autonomous vehicles: No driver... no regulation? *Science*, 361(6397):36–37, 2018.

[13] Matthew O’Kelly, Aman Sinha, Hongseok Namkoong, Russ Tedrake, and John C Duchi. Scalable end-to-end autonomous vehicle testing via rare-event simulation. In *Advances in Neural Information Processing Systems*, pages 9827–9838, 2018.

[14] Anthony Corso, Robert J Moss, Mark Koren, Ritchie Lee, and Mykel J Kochenderfer. A survey of algorithms for black-box safety validation. *arXiv preprint arXiv:2005.02979*, 2020.
[15] Philip Koopman and Michael Wagner. Toward a framework for highly automated vehicle safety validation. Technical report, SAE Technical Paper, 2018.

[16] Søren Asmussen and Peter W Glynn. Stochastic Simulation: Algorithms and Analysis, volume 57. Springer Science & Business Media, New York, 2007.

[17] James Bucklew. Introduction to rare event simulation. Springer Science & Business Media, 2013.

[18] Sandeep Juneja and Perwez Shahabuddin. Rare-event simulation techniques: an introduction and recent advances. Handbooks in Operations Research and Management Science, 13:291–350, 2006.

[19] Jose Blanchet and Henry Lam. State-dependent importance sampling for rare-event simulation: An overview and recent advances. Surveys in Operations Research and Management Science, 17(1):38–59, 2012.

[20] Paul Glasserman, Philip Heidelberger, Perwez Shahabuddin, and Tim Zajic. Multilevel splitting for estimating rare event probabilities. Operations Research, 47(4):585–600, 1999.

[21] Manuel Villén-Altamirano and José Villén-Altamirano. Restart: a straightforward method for fast simulation of rare events. In Proceedings of Winter Simulation Conference, pages 282–289. IEEE, 1994.

[22] Jose Blanchet and Henry Lam. Rare event simulation techniques. In Proceedings of the 2011 Winter Simulation Conference (WSC), pages 146–160. IEEE, 2011.

[23] Thomas Dean and Paul Dupuis. Splitting for rare event simulation: A large deviation approach to design and analysis. Stochastic processes and their applications, 119(2):562–587, 2009.

[24] Pieter-Tjerk De Boer, Dirk P Kroese, Shie Mannor, and Reuven Y Rubinstein. A tutorial on the cross-entropy method. Annals of operations research, 134(1):19–67, 2005.

[25] Reuven Y Rubinstein and Dirk P Kroese. The cross-entropy method: a unified approach to combinatorial optimization, Monte-Carlo simulation and machine learning. Springer Science & Business Media, 2013.

[26] Siu-Kui Au and James L Beck. Estimation of small failure probabilities in high dimensions by subset simulation. Probabilistic engineering mechanics, 16(4):263–277, 2001.

[27] Frédéric Cérou and Arnaud Guyader. Adaptive multilevel splitting for rare event analysis. Stochastic Analysis and Applications, 25(2):417–443, 2007.

[28] Ding Zhao, Henry Lam, Huei Peng, Shan Bao, David J LeBlanc, Kazutoshi Nobukawa, and Christopher S Pan. Accelerated evaluation of automated vehicles safety in lane-change scenarios based on importance sampling techniques. IEEE transactions on intelligent transportation systems, 18(3):595–607, 2016.

[29] Z. Huang, H. Lam, D. J. LeBlanc, and D. Zhao. Accelerated evaluation of automated vehicles using piecewise mixture models. IEEE Transactions on Intelligent Transportation Systems, 19(9):2845–2855, Sep. 2018.

[30] Ofer Zeitouni Amir Dembo. Large deviations techniques and applications. Springer-Verlag, 2010.

[31] PaulDupuis and Richard S Ellis. A weak convergence approach to the theory of large deviations, volume 902. John Wiley & Sons, 2011.

[32] Peter W Glynn and Donald L Iglehart. Importance sampling for stochastic simulations. Management science, 35(11):1367–1392, 1989.

[33] John S Sadowsky and James A Bucklew. On large deviations theory and asymptotically efficient monte carlo estimation. IEEE transactions on Information Theory, 36(3):579–588, 1990.
[34] Bouhari Arouna. Adaptive monte carlo method, a variance reduction technique. *Monte Carlo Methods and Applications*, 10(1):1–24, 2004.

[35] Vincent Tjeng, Kai Xiao, and Russ Tedrake. Evaluating robustness of neural networks with mixed integer programming. *arXiv preprint arXiv:1711.07356*, 2017.

[36] Zhiyuan Huang, Henry Lam, and Ding Zhao. Designing importance samplers to simulate machine learning predictors via optimization. In *2018 Winter Simulation Conference (WSC)*, pages 1730–1741. IEEE, 2018.

[37] Martin Treiber, Ansgar Hennecke, and Dirk Helbing. Congested traffic states in empirical observations and microscopic simulations. *Physical Review E*, 62(2):1805–1824, Aug 2000.

[38] X. Wang, R. Jiang, L. Li, Y. Lin, X. Zheng, and F. Wang. Capturing car-following behaviors by deep learning. *IEEE Transactions on Intelligent Transportation Systems*, 19(3):910–920, 2018.

[39] P. F. Orzechowski, K. Li, and M. Lauer. Towards responsibility-sensitive safety of automated vehicles with reachable set analysis. In *2019 IEEE International Conference on Connected Vehicles and Expo (ICCVE)*, pages 1–6, 2019.

[40] Antonius Bernardus Dieker and Michel Mandjes. Fast simulation of overflow probabilities in a queue with gaussian input. *ACM Transactions on Modeling and Computer Simulation (TOMACS)*, 16(2):119–151, 2006.

[41] Jurgen Gartner. On large deviations from the invariant measure. *Theory of Probability & Its Applications*, 22(1):24–39, 1977.

[42] Richard S Ellis et al. Large deviations for a general class of random vectors. *The Annals of Probability*, 12(1):1–12, 1984.

[43] Nick Harvey, Christopher Liaw, and Abbas Mehrabian. Nearly-tight VC-dimension bounds for piecewise linear neural networks. In Satyen Kale and Ohad Shamir, editors, *Proceedings of the 2017 Conference on Learning Theory*, volume 65 of *Proceedings of Machine Learning Research*, pages 1064–1068, Amsterdam, Netherlands, 07–10 Jul 2017. PMLR.

[44] Yuan Cao and Quanquan Gu. Tight sample complexity of learning one-hidden-layer convolutional neural networks. In *Advances in Neural Information Processing Systems 32*, pages 10612–10622. Curran Associates, Inc., 2019.

[45] Aad W. van der Vaart and Jon A. Wellner. Weak convergence and empirical processes. *Springer Series in Statistics*, 1996.

[46] Cem Anil, James Lucas, and Roger Grosse. Sorting out Lipschitz function approximation. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 291–301, Long Beach, California, USA, 09–15 Jun 2019. PMLR.

[47] Zhou Lu, Hongming Pu, Feicheng Wang, Zhiqiang Hu, and Liwei Wang. The expressive power of neural networks: A view from the width. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 6231–6239. Curran Associates, Inc., 2017.

[48] Frédéric Cérou, Arnaud Guyader, et al. Fluctuation analysis of adaptive multilevel splitting. *The Annals of Applied Probability*, 26(6):3319–3380, 2016.

[49] Gareth O Roberts, Jeffrey S Rosenthal, et al. General state space markov chains and mcmc algorithms. *Probability surveys*, 1:20–71, 2004.

[50] Paul Glasserman, Philip Heidelberger, Perwez Shahabuddin, and Tim Zajic. A large deviations perspective on the efficiency of multilevel splitting. *IEEE Transactions on Automatic Control*, 43(12):1666–1679, 1998.
Appendices

We present supplemental results and discussions. Appendix A expands Section 2 regarding Monte Carlo efficiency and variance reduction. Appendix B provides further details on Algorithm 1, in particular the mixed integer formulation used to solve the underlying optimization problems. Appendix C expands the efficiency and conservativeness results in Section 3. Appendix D presents the lower-bound relaxed efficiency certificate and estimators in parallel to the upper-bound results in Section 3. Appendix E provides an overview of the cross-entropy method and multi-level splitting (or subset simulation) and discusses their perils for black-box problems. Appendix F illustrates further experimental results. Finally, Appendix G shows all technical proofs.

A Further Details for Section 2

This section expands the discussions in Section 2, by explaining in more detail the notion of relative error, challenges in naive Monte Carlo, the concept of dominant points, and the perils of black-box variance reduction algorithms.

A.1 Explanation of the Role of Relative Error

As described in Section 2, to estimate a tiny $\mu$ using $\hat{\mu}_n$, we want to ensure a high accuracy in relative term, namely, (1). Suppose that $\hat{\mu}_n$ is unbiased and is an average of $n$ i.i.d. simulation runs, i.e., $\hat{\mu}_n = (1/n) \sum_{i=1}^{n} Z_i$ for some random unbiased output $Z_i$. The Markov inequality gives that

$$P(|\hat{\mu}_n - \mu| > \epsilon \mu) \leq \frac{\text{Var}(\hat{\mu}_n)}{\epsilon^2 \mu^2} = \frac{\text{Var}(Z_i)}{n \epsilon^2 \mu^2}$$

so that

$$\frac{\text{Var}(Z_i)}{n \epsilon^2 \mu^2} \leq \delta$$

ensures (1). Equivalently,

$$n \geq \frac{\text{Var}(Z_i)}{\delta \epsilon^2 \mu^2} = \frac{\text{RE}}{\delta \epsilon^2}$$

is a sufficient condition to achieve (1), where $\text{RE} = \text{Var}(Z_i)/\mu^2$ is the relative error defined as the ratio of variance (per-run) and squared mean.

A.2 Further Explanation on the Challenges in Naive Monte Carlo

We have seen in Section 2 that for the naive Monte Carlo estimator, where $Z_i = I(X_i \in S_\gamma)$, the relative error is $\text{RE} = \mu(1-\mu)/\mu^2 = (1-\mu)/\mu$. Thus, when $\mu$ is tiny, the sufficient condition for $n$ to attain (1) scales at least linearly in $1/\mu$. In fact, this result can be seen to be tight by analyzing $n\hat{\mu}_n$ as a binomial variable. To be more specific, we know that $P(|\hat{\mu}_n - \mu| > \epsilon \mu) = P(|n\hat{\mu}_n - n\mu| > \epsilon n\mu)$ and that $n\hat{\mu}_n$ takes values in $\{0, 1, \ldots, n\}$. Therefore, if $n\mu \to 0$, then $P(|\hat{\mu}_n - \mu| > \epsilon \mu) \to 1$, and hence (1) does not hold.

Moreover, the following provides a concrete general statement that an $n$ that grows only polynomially in $\gamma$ would fail to estimate $\mu$ that decays exponentially in $\gamma$ with enough relative accuracy, of which (1) fails to hold is an implication.

**Proposition 2.** Suppose that $\mu = P(X \in S_\gamma)$ is exponentially decaying in $\gamma$ and $n$ is polynomially growing in $\gamma$. Define $\hat{\mu}_n = (1/n) \sum_{i=1}^{n} I(X_i \in S_\gamma)$. Then for any $0 < \varepsilon < 1$,

$$\lim_{\gamma \to \infty} P(|\hat{\mu}_n - \mu| > \varepsilon \mu) = 1.$$

We have used the term efficiency certificate to denote an estimator that achieves (1) with $n = \tilde{O}(\log(1/\mu))$. In the rare-event literature, such an estimator is known as “logarithmically efficient” or “weakly efficient” [18, 19].
A.3 Further Explanations of Dominant Points

We have mentioned that a certifiable IS should account for all dominant points, defined in Definition 1. We provide more detailed explanations here. Roughly speaking, for $X \sim N(\lambda, \Sigma)$ and a rare-event set $S_\gamma$, the Laplace approximation gives $P(X \in S_\gamma) \approx e^{-\inf_{a \in S_\gamma} \frac{1}{2} (a-\lambda)^T \Sigma^{-1} (a-\lambda)}$ (see the proof of Theorem 5).

Thus, to obtain an efficiency certificate, IS estimator given by $Z = L(X)I(X \in S_\gamma)$, where $X \sim \tilde{p}$ and $L = dp/d\tilde{p}$, needs to have $\hat{V}ar(Z) \leq E[Z^2] \approx e^{-\inf_{a \in S_\gamma} \frac{1}{2} (a-\lambda)^T \Sigma^{-1} (a-\lambda)}$ (where $\hat{V}ar(\cdot)$ and $E[\cdot]$ denote the variance and expectation under $\tilde{p}$, and $\approx$ is up to some factor polynomial in $\inf_{a \in S_\gamma} \frac{1}{2} (a-\lambda)^T \Sigma^{-1} (a-\lambda)$; note that the last equality relation cannot be improved, as otherwise it would imply that $\hat{V}ar(Z) = E[Z^2] - (E[Z])^2 < 0$).

Now consider an IS that translates the mean of the distribution from $\mu$ to $a^* = \arg \min_{a \in S_\gamma} (a-\lambda)^T \Sigma^{-1} (a-\lambda)$, an intuitive choice since $a^*$ contributes the highest density among all points in $S_\gamma$ (this mean translation also bears the natural interpretation as an exponential change of measure; [17]). The likelihood ratio is $L(x) = e^{(a^*-\mu)^T \Sigma^{-1} (a^*-\mu)} \cdot e^{-\frac{1}{2} (x-a^*)^T \Sigma^{-1} (x-a^*)}$.

If the “overshoot” $(a^*-\lambda)^T \Sigma^{-1} (x-a^*)$, i.e., the remaining term in the exponent of $L(x)$ after moving out $-(a^*-\lambda)^T \Sigma^{-1} (x-a^*)$, satisfies $(a^*-\lambda)^T \Sigma^{-1} (x-a^*) \geq 0$ for all $x \in S_\gamma$, then the expectation in the right hand side of (3) is bounded by 1, and an efficiency certificate is achieved. This, however, is not true for all set $S_\gamma$, which motivates the following definition of the dominant set and points in Definition 1.

For instance, if $S_\gamma$ is convex, then, noting that $(x-\lambda)^T \Sigma^{-1}$ is precisely the gradient of the function $(1/2)(x-\lambda)^T \Sigma^{-1} (x-\lambda)$, we get that $a^*$ gives a singleton dominant set since $(a^*-\lambda)^T \Sigma^{-1} (x-a^*) \geq 0$ for all $x \in S_\gamma$ is precisely the first order optimality condition of the involved quadratic optimization.

In general, if we can decompose $S_\gamma = \bigcup_j S_\gamma^j$ where $S_\gamma^j = \{ x : (a_j^*-\lambda)^T \Sigma^{-1} (x-a_j) \geq 0 \}$ for a dominant point $a_j \in A_\gamma$, then each $S_\gamma^j$ can be viewed as a “local” region where the dominant point $a_j$ is the highest-density, or the most likely point such that the rare event occurs.

**Theorem 5** (Certifiable IS). Suppose that $A_\gamma$ is the dominant set for $S_\gamma$ associated with the distribution $N(\lambda, \Sigma)$. Then we can decompose $S_\gamma = \bigcup_j S_\gamma^j$ where $S_\gamma^j$’s are disjoint, $a_j \in S_\gamma^j$ and $S_\gamma^j \subset \{ x : (a_j^*-\lambda)^T \Sigma^{-1} (x-a_j) \geq 0 \}$ for $a_j \in A_\gamma$. Denote $a^* = \arg \min \{(a_j^*-\lambda)^T \Sigma^{-1} (a_j^*-\lambda) : a_j \in A_\gamma\}$. Assume that each component of $a^*$ is of polynomial growth in $\gamma$. Moreover, assume that there exist invertible matrix $B$ and positive constant $\varepsilon$ such that $\{ x : B(x-a^*) \geq 0, (x-a^*)^T \Sigma^{-1} (x-a^*) \leq \varepsilon^2 \} \subset S_\gamma$. Then the IS distribution $\sum_j a_j N(\lambda, \Sigma)$ achieves an efficiency certificate in estimating $\mu = P(X \in S_\gamma)$, i.e., if we let $Z = I(X \in S_\gamma) L(X)$ where $L$ is the corresponding likelihood ratio, then $E[Z^2]/E[Z]^2$ is at most polynomially growing in $\gamma$. This applies in particular to $S_\gamma = \{ x : f(x) \geq \gamma \}$ where $f(x)$ is a piecewise linear function.

We contrast Theorem 5 with existing works on dominant points. The latter machinery has been studied in [33, 40]. These papers, however, consider regimes where the Gärtner-Ellis Theorem [41, 42] can be applied, which requires the considered rare-event set to scale proportionately with the rarity parameter. This is in contrast to this point in the dominant points used in Theorem 5.

A.4 Further Explanation of the Example in Theorem 2

In the theorem, there are two dominant points $\gamma$ and $-k\gamma$ but the IS design only considers the first one. As a result, there could exist “unlucky” scenario where the sample falls into the rare-event set, so that $I(X \in S_\gamma) = 1$, while the likelihood ratio $L(X)$ explodes, which leads to a tremendous estimation variance. Part 2 of the theorem further shows how this issue is undetected empirically, as the empirical RE appears small (polynomially in $n$ and hence $\gamma$ by our choice of $n$) while the estimation concentrates at a value that can be severely under the correct one (especially when $k < 1$).

This is because the samples all land on the neighborhood of the solely considered dominant point. If the missed dominant point is a significant contributor to the rare-event probability, then the empirical
performance would look as if the rare-event set is smaller, leading to a systematic under-estimation. Note that this phenomenon occurs even if the estimator is unbiased, which is guaranteed by IS by default.

B Further Details on Implementing Algorithm\[1\]

We provide further details on implementing Algorithm\[1\]. In particular, we present how to solve the optimization problem

\[
x^* = \arg \min_x (x - \lambda)^T \Sigma^{-1}(x - \lambda) \quad \text{s.t.} \quad g(x) \geq \hat{\kappa}, \quad (x_j^* - \lambda)^T \Sigma^{-1}(x - x_j^*) < 0 \quad \forall x_j^* \in \hat{A}_j
\]

(4)

to obtain the next dominant point in the sequential cutting-plane approach in Stage 2. Moreover, we also present how to tune \(\hat{\kappa}\) to achieve (5). This requires checking, for a given \(\kappa\), whether \((S_{\kappa}^c)^c \subset \mathcal{H}(T_0)\). We use an MIP to check \((S_{\kappa}^c)^c \subset \mathcal{H}(T_0)\). Recall that \(\mathcal{H}(T_0) = \bigcup_{i=1}^{d} \mathcal{Y}_i = \{x \in \mathbb{R}^d_+ : x \leq X_i\}\). We want to check if \(\{x \in \mathbb{R}^d_+ : \hat{g}(x) \leq \kappa\}\) for a

MIP formulations for ReLU-activated neural net classifier. The problem (4) can be reformulated into a mixed integer program (MIP), in the case where \(\hat{g}(x)\) is trained via a ReLU-activated neural net classifier, which is used in our deep-learning-based IS. Since the objective is convex quadratic and second set of constraints is linear in (4), we focus on the first constraint \(g(x) \geq \gamma\). The neural net structure \(g(x)\) in our approach (say with \(n\) layers) can be represented as \(g(x) = (g_{n_0}, \ldots, g_{1})(x)\), where each \(g_i(\cdot)\) denotes a ReLU-activated layer with linear transformation, i.e. \(g_i(\cdot) = \max\{LT(\cdot), 0\}\), where \(LT(\cdot)\) denotes a certain linear transformation in the input. In order to convert \(g(\cdot)\) into an MIP constraint, we introduce \(M\) as a practical upper bound for \(x_1, \ldots, x_n\) such that \(|x_i| < M\). The key step is to reformulate the ReLU function \(y = \max\{x, 0\}\) into

\[
\begin{align*}
y &\leq x + M(1 - z) \\
y &\geq x \\
y &\leq M z \\
y &\geq 0 \\
z &\in \{0, 1\}.
\end{align*}
\]

For simple ReLU networks, the size of the resulting MIP formulation depends linearly on the number of neurons in the neural network. In particular, the number of binary decision variables is linearly dependent on the number of ReLU neurons, and the number of constraints is linearly dependent the total number of all neurons (here we consider the linear transformations as independent neurons).

The MIP reformulation we discussed can be generalized to many other popular piecewise linear structures in deep learning. For instance, linear operation layers, such as normalization and convolutional layers, can be directly used as constraints; some non-linear layers, such as ReLU and max-pooling layers, introduce non-linearity by the “max” functions. A general reformulation for the max functions can be used to convert these non-linear layers to mixed integer constraints.

Consider the following equality defined by a max operation \(y = \max\{x_1, x_2, \ldots, x_n\}\). Then the equality is equivalent to

\[
\begin{align*}
y &\leq x_i + 2M(1 - z_i), \quad i = 1, \ldots, n \\
y &\geq x_i, \quad i = 1, \ldots, n \\
\sum_{i=1}^{n} z_i &= 1 \\
z_i &\in \{0, 1\}.
\end{align*}
\]

Tuning \(\hat{\kappa}\). We illustrate how to tune \(\hat{\kappa}\) to achieve (5). This requires checking, for a given \(\kappa\), whether \((S_{\kappa}^c)^c \subset \mathcal{H}(T_0)\). Then, by discretizing the range of \(\kappa\) or using a bisection algorithm, we can leverage this check to obtain (5). We use an MIP to check \((S_{\kappa}^c)^c \subset \mathcal{H}(T_0)\). Recall that \(\mathcal{H}(T_0) = \bigcup_{i=1}^{d} \mathcal{Y}_i = \{x \in \mathbb{R}^d_+ : x \leq X_i\}\). We want to check if \(\{x \in \mathbb{R}^d_+ : \hat{g}(x) \leq \kappa\}\) for a
given $\kappa$ lies completely inside the hull, where $\hat{g}(x)$ is trained with a ReLU-activated neural net. This can be done by solving an optimization problem as follows. First, we rewrite $\mathcal{H}(T_0)$ as
$$\{ x \in \mathbb{R}^d : \min_{i=1,\ldots,n} \max_{j=1,\ldots,d} \{ x^j - \tilde{X}^j_i \} \leq 0 \},$$
where $x^j$ and $x^j_i$ refer to the $j$-th components of $x$ and $\tilde{X}_i$, respectively. Then we solve
$$\max_{x \in \mathbb{R}^d} \min_{i=1,\ldots,n} \max_{j=1,\ldots,d} \{ x^j - \tilde{X}^j_i \} \quad \text{subject to} \quad \hat{g}(x) \leq \kappa \quad x \geq 0$$
(6)

If the optimal value is greater than 0, this means $\{ x \in \mathbb{R}^d : \hat{g}(x) \leq \kappa \}$ is not completely inside $\mathcal{H}(T_0)$, and vice versa. Now, we rewrite (6) as
$$\max_{x \in \mathbb{R}^d, \beta \in \mathbb{R}} \beta \quad \text{subject to} \quad \max_{i=1,\ldots,n} \{ x^j - \tilde{X}^j_i \} \geq \beta \forall i = 1,\ldots,n \quad \hat{g}(x) \leq \kappa \quad x \geq 0$$
(7)

We then rewrite (7) as an MIP by introducing a large real number $M$ as a practical upper bound for all coordinates of $x$:
$$\max_{x \in \mathbb{R}^d, \beta \in \mathbb{R}} \beta \quad \text{subject to} \quad x^j - \tilde{X}^j_i + 4M(1 - z_{ij}) \geq \beta \forall i = 1,\ldots,n, j = 1,\ldots,d \quad \sum_{j=1}^{d} z_{ij} \geq 1 \forall i = 1,\ldots,n \quad z_{ij} \in \{0,1\} \forall i = 1,\ldots,n, j = 1,\ldots,d \quad \hat{g}(x) \leq \kappa \quad x \geq 0$$
(8)

Note that the set of points $T_0$ to be considered in constructing $\mathcal{H}(T_0)$ can be reduced to its “extreme points”. More concretely, we call a point $x \in T_0$ an extreme point if there does not exist any other point $x' \in T_0$ such that $x \leq x'$. We can eliminate all points $x \in T_0$ such that $x \leq x'$ for another $x' \in T_0$, and the resulting orthogonal monotone hull would remain the same. If we carry out this elimination, then in (7) we need only consider $X_i$ that are extreme points in $\mathcal{H}(T_0)$, which can reduce the number of integer variables needed to add. In practice, we can also randomly remove points in $T_0$ to further reduce the number of integer variables. This would not affect the correctness of our approach, but would increase the conservativeness of the final estimate.

C Further Results for Section 3

Here we present and discuss several additional results for Section 3 regarding estimation efficiency and conservativeness. The latter includes further theorems on the lazy-learner classifier and classifiers constructed using the difference of two functions, translation of the false positive rate under the Stage 1 sampling distribution to under the original distribution, and interpretations and refinements of the conservativeness results.

C.1 Extending Upper-Bound Relaxed Efficiency Certificate to Two-Stage Procedures

We present an extension of Proposition 1 to two-stage procedures, which is needed to set up Corollary 1

**Proposition 3** (Extended relaxed efficiency certificate). Suppose constructing $\hat{\mu}_n = \hat{\mu}_{n_2}(D_{n_1})$ consists of two stages, with $n = n_1 + n_2$: First we sample $D_{n_1} = \{ \tilde{X}_1,\ldots,\tilde{X}_{n_1} \}$, where $\tilde{X}_i$ are i.i.d. (following some sampling distribution), and given $D_{n_1}$, we construct $\hat{\mu}_{n_2}(D_{n_1}) = (1/n_2) \sum_{i=1}^{n_2} Z_i$ where $Z_i$ are i.i.d. conditional on $D_{n_1}$ (following some distribution). Suppose $\hat{\mu}_n$ is conditionally upward biased almost surely, i.e., $\overline{\pi}(D_{n_1}) := E[\hat{\mu}_n|D_{n_1}] \geq \mu$, and the conditional relative error given $D_{n_1}$ in the second stage satisfies $RE(D_{n_1}) := Var(Z_i|D_{n_1})/\overline{\pi}(D_{n_1})^2 = O(\log(1/\overline{\pi}(D_{n_1})))$. If $n_1 = O(\log(1/\mu))$ (such as a constant number), then $\hat{\mu}_n$ possesses the upper-bound relaxed efficiency certificate.
C.2 Conservativeness of Lazy Learner

We provide a result to quantify the conservativeness of the lazy-learner IS in terms of the false positive rate. Recall that the lazy learner constructs the outer approximation of the rare-event set using \( \mathcal{H}(T_0)^c \), which is the complement of the orthogonal monotone hull of the set of all non-rare-event samples. The conservativeness is measured concretely by the set difference between \( \mathcal{H}(T_0)^c \) and \( \mathcal{S}_\gamma \), for which we have the following result:

**Theorem 6** (Conservativeness of lazy learner). Suppose that the density \( q \) has bounded support \( K \subset [0, M]^d \), and \( 0 < q_i \leq q(x) \leq q_u \) for any \( x \in K \). Then, with probability at least \( 1 - \delta \),

\[
P_{X \sim q}(X \in \mathcal{H}(T_0)^c \setminus \mathcal{S}_\gamma) \leq M^{d-1} q_u \left( \frac{\sqrt{d}}{2} \right)^{d-1} w_d t(\delta, n_1)
\]

\[
= \sqrt{\frac{e}{\pi (d-1)}} \left( \frac{1}{2} \pi e \right)^{d-1} \frac{1}{q_u} q_u t(\delta, n_1)(1 + O(d^{-1})).
\]

Here \( t(\delta, n_1) = \left( \frac{\log(n_1 q_i) + d \log M + \log \frac{1}{\delta} \log 1}{n_1 q_i} \right)^{\frac{3}{2}} \), \( w_d \) is the volume of a \( d \)-dimensional Euclidean ball of radius 1, and the last \( O(\cdot) \) is as \( d \) increases.

C.3 Translating the False Positive Rate to under the Original distribution

Theorems 4 and 6 are stated with respect to \( q \), the sampling distribution used in the first stage. We explain how to translate the false positive rate results to under the original distribution \( p \). In the discussion below, we will consider Theorem 4 (and Theorem 6 can be handled similarly). In this case, our target is to give an upper bound to \( P_{X \sim p}(X \in \mathcal{S}_\gamma) \) based on the result of Theorem 4.

If the true input distribution \( p \) does not have a bounded support, we can first choose \( M \) to be large enough so that \( P_{X \sim p}(X \notin [0, M]^d) \) is small compared to the probability of \( \mathcal{S}_\gamma \). We argue that we do not need \( M \) to be too large here. Indeed, if \( p \) is light tail (e.g., a distribution with tail probability exponential in \( M \)), then the required \( M \) grows at most polynomially in \( \gamma \).

Having selected \( M \), and with the freedom in selecting \( q \) in Stage 1, we could make sure that \( P_{X \sim p}(X \notin [0, M]^d) \) is bounded away from 0 (e.g., we can choose \( q \) to be the uniform distribution over \([0, M]^d\)). Then, by Theorem 4 and a change of measure argument, we can give a bound for \( P_{X \sim p}(X \in [0, M]^d, X \in \mathcal{S}_\gamma) \). Finally, we bound the false positive rate with respect to \( p \) by \( P_{X \sim p}(X \in \mathcal{H}(T_0)^c \setminus \mathcal{S}_\gamma) \leq P_{X \sim p}(X \notin [0, M]^d) + P_{X \sim p}(X \in [0, M]^d, X \in \mathcal{H}(T_0)^c \setminus \mathcal{S}_\gamma) \).

C.4 Conservativeness Results for Classifiers Constructed Using Differences of Two Trained Functions

Theorem 4 presents a conservativeness result when \( \hat{g} \) is trained with an empirical risk minimization (ERM). In this subsection, we will show a more sophisticated version of Theorem 4, which corresponds more closely to the \( \hat{g} \) that we implemented in our experiments. Suppose that the Stage 1 samples are generated in the same way as in Algorithm 1. We let \( \mathcal{F} := \{ f_0 \} \) denote the function class induced by the model. Here a main difference with previously is that we allow functions in \( \mathcal{F} \) to be 2-dimensional, and both the loss function and the classification boundary will be constructed from these 2-dimensional functions.

Suppose that \( f_0 \) is the output a neural network with 2 neurons in the output layer, and denote them as \( f_{0,0}, f_{0,1} \). Let the loss function evaluated at the \( i \)-th sample be \( \ell(f_0(X_i), Y_i) \). For example, the cross-entropy loss is given by \(- \left[ I(Y_i = 0) \log \frac{e^{f_{0,0}(X_i)}}{e^{f_{0,0}(X_i)} + e^{f_{0,1}(X_i)}} + I(Y_i = 1) \log \frac{e^{f_{0,1}(X_i)}}{e^{f_{0,0}(X_i)} + e^{f_{0,1}(X_i)}} \right] \).

Like in the ERM approach in Theorem 4, we compute \( \hat{f} = f_0 \in \mathcal{F} \) which is the minimizer of the empirical risk, i.e., \( \hat{f} = \arg \min_{f_0 \in \mathcal{F}} R_{n_1}(f_0) \). For each function \( f_0 \in \mathcal{F} \), define function \( g_{0,1} \) as \( g_0 := f_{0,1} - f_{0,0} \). In this modified approach, the learned rare-event set would be given by \( \mathcal{S}_\gamma := \{ x : \hat{g}_0(x) \geq \kappa \} \), and to make sure that \( \mathcal{S}_\gamma \subset \hat{S}_\gamma \), we would replace \( \kappa \) by \( \hat{\kappa} := \min \{ \hat{g}_0(x) : x \notin \mathcal{H}(T_0) \} \) as in Step 1 of Algorithm 1.
We give a theorem similar to Theorem 4 for this more sophisticated procedure. To this end, we begin by giving some definitions similar to the set up of Theorem 4. Let \( R(f_0) := E_{X \sim q}(\ell(f_0(X), I(X \in S_\gamma^c))) \) denote the true risk function. Let \( f^* = \arg \min f_{\in \mathcal{F}} R(f) \) denote the true risk minimizer within function class \( \mathcal{F} \). Define \( g^* = f^*_1 - f^*_0 \) accordingly and let \( \kappa^* := \min_{\theta \in \mathcal{S}} g^*(x) \) denote the true threshold associated with \( f^* \) in obtaining the smallest outer rare-event approximation.

**Theorem 7.** Suppose that the density \( q \) has bounded support \( K \subset [0, M]^d \) and \( 0 < q_1 \leq q(x) \leq q_w \) for any \( x \in K \). Also suppose that there exists a function \( h \) such that for any \( f_\theta \in \mathcal{F} \), if \( g_\theta(x) \geq \kappa \), we have \( \ell(f_\theta(x), 0) \geq h(\kappa) > 0 \) (for the cross entropy loss, this happens if we know that \( f_\theta \) has a bounded range). Then, for the set \( S_\gamma^c \), with probability at least \( 1 - \delta \),

\[
P_{X \sim q}(X \in S_\gamma^c, X \in S_\gamma^c) \leq \left( h(\kappa^* - t(\delta, n_1)\sqrt{d}Lip(g^*) - \|\hat{g} - g^*\|_\infty) \right)^{-1} \left( R(f^*) + 2 \sup_{f_\theta \in \mathcal{F}} |R_{n_1}(f_\theta) - R(f_0)| \right)
\]

Here \( Lip(g^*) \) is the Lipschitz parameter of \( g^* \), and \( t(\delta, n_1) \) is defined as in Theorem 4.

**C.5 Implications of Theorem 4 and Related Results in the Literature**

First, we explain the trade-off between overfitting and underfitting. If the function class \( \mathcal{G} \) is not rich, then \( R(g^*) = \inf_{g \in \mathcal{G}} R(g) \) may be big because of the lack of expressive power. On the other hand, if the function class is too rich, then the generalization error will be huge. Here, the generalization error is represented by \( \sup_{g \in \mathcal{G}} |R_{n_1}(g_\theta) - R(g_\theta)| \) as well as \( t(\delta, n_1)\sqrt{d}Lip(g^*) + \|\hat{g} - g^*\|_\infty \), which characterize the difference between the right hand side of the bound in the theorem and its limit as \( n_1 \to \infty \).

Another question is how to give a more refined bound for the false positive rate based on Theorem 4 that depends on explicit constants of the classification model or training process. This would involve theoretical results for deep neural networks that are under active research. Let us examine the terms appearing in Theorem 4 and give some related results. In machine learning theory, the term \( \sup_{g_\theta \in \mathcal{G}} |R_{n_1}(g_\theta) - R(g_\theta)| \) is often bounded by the Rademacher complexity of the function class (some results about the Rademacher complexity for neural networks are in [33, 44]). The convergence of \( \|\hat{g} - g^*\|_\infty \) to 0 as \( n_1 \to \infty \) is implied by the convergence of the parameters, which is in turn justified by the empirical process theory [45]. A bound for \( Lip(g^*) \) could be potentially derived by adding norm constraints to the parameters in the neural network [46]. On the other hand, if we let the network size grow to infinity, the class of neural networks can approximate any continuous function [47], and hence \( R(g^*) \) can be arbitrarily small when the neural network is complex enough. However, if we restrict the choices of networks, for instance by the Lipschitz constant, then no results regarding the sufficiency of its expressive power for arbitrary functions are available in the literature, and thus it appears open how to simultaneously give bounds for \( Lip(g^*) \) and \( R(g^*) \). Future investigations on the expressive power of restricted classes of neural networks would help refining our conservativeness results further.

**D Lower-Bound Efficiency Certificate and Estimators**

In Section 3, we described an approach that gives an estimator for the rare-event probability with an upper-bound relaxed efficiency certificate. Here we present analogous definitions and results on the lower-bound relaxed efficiency certificate. This lower-bound estimator gives an estimation gap for the upper-bound estimator. Moreover, by combining both of them, we can obtain an interval for the target rare-event probability.

The lower-bound relaxed efficiency certificate is defined as follows (compare with Definition 2).

**Definition 5.** We say an estimator \( \hat{\mu}_n \) satisfies an lower-bound relaxed efficiency certificate to estimate \( \mu \) if \( P(\hat{\mu}_n - \mu > \epsilon \mu) \leq \delta \) with \( n \geq \tilde{O}(\log(1/\mu)) \), for given \( 0 < \epsilon, \delta < 1 \).

This definition requires that, with high probability, \( \hat{\mu}_n \) is a lower bound of \( \mu \) up to an error of \( \epsilon \mu \). We have the following analog to Proposition 4.
Corollary 2. Suppose \( \hat{\mu}_n \) is downward biased, i.e., \( \overline{\mu} := E[\hat{\mu}_n] \leq \mu \). Moreover, suppose \( \hat{\mu}_n \) takes the form of an average of \( n \) i.i.d. simulation runs \( Z_i \), with \( RE = Var(Z_i)/\overline{\mu}^2 = \tilde{O}(\log(1/\overline{\mu})) \). Then \( \hat{\mu}_n \) possesses the lower-bound relaxed efficiency certificate.

This motivates us to learn an inner approximation of the rare-event set in Stage 1 and then in Stage 2, we use IS as in Theorem 1 to estimate the probability of this inner approximation set. For the inner approximation, like the outer approximation case, we draw \( \tilde{X}_1, \ldots, \tilde{X}_{n_1} \) from some sampling distribution that has sufficient presence throughout the space, and evaluate \( Y_i := I(\tilde{X}_i \in \mathcal{S}_\gamma) \). Based on these data, we construct an approximation set \( \widehat{\mathcal{S}}_\gamma \), that has zero false positive rate, i.e.,

\[
P(X \in \widehat{\mathcal{S}}_\gamma, Y = 0) = 0. \tag{9}
\]

To make sure of (9), we again exploit the knowledge that the rare event set \( \mathcal{S}_\gamma \) is orthogonally monotone. Indeed, denote \( T_1 := \{ \tilde{X}_1 : Y_1 = 1 \} \) as the rare-event sampled points and for each point \( x \in \mathbb{R}^d \), let \( Q(x) := \{ x' : x' \geq x \} \). We construct \( J(T_1) := \cup_{x \in T_1} Q(x) \) which serves as the "upper orthogonal monotone hull" of \( T_1 \). The orthogonal monotonicity property of \( \mathcal{S}_\gamma \) implies that \( J(T_1) \subset \mathcal{S}_\gamma \). Moreover, \( J(T_1) \) is the largest choice of \( \overline{\mathcal{S}}_\gamma \), such that (9) is guaranteed. Based on this observation, in parallel to Section 3 depending on how we construct the inner approximation to the rare-event set, we propose the following two approaches.

Lazy-Learner IS (Lower Bound). We now consider an estimator for \( \mu \) where in Stage 1, we sample a constant \( n_1 \) i.i.d. random points from some density, say \( q \). Then, we use the mixture IS depicted in Theorem 1 to estimate \( P(X \in J(T_1)) \) in Stage 2. Since \( J(T_1) \) takes the form \( \cup_{x \in T_1} Q(x) \), it has a finite number of dominant points, which can be found by a sequential algorithm. But as explained in Section 3 this leads to a large number of mixture components that degrades the IS efficiency.

Deep-Learning-Based IS (Lower Bound). We train a neural network classifier, say \( \hat{g} \), using all the Stage 1 samples \( \{(\tilde{X}_i, Y_i)\} \), and obtain an approximate rare-event region \( \overline{\mathcal{S}}_\gamma^k = \{ x : \hat{g}(x) \geq \kappa \} \), where \( \kappa \) is say \( 1/2 \). Then we adjust \( \kappa \) minimally away from 1/2, say to \( \hat{\kappa} \), so that \( \overline{\mathcal{S}}_\gamma^k \subset J(T_1) \), i.e.,

\[
\hat{\kappa} = \min \{ \kappa \in \mathbb{R} : \overline{\mathcal{S}}_\gamma^k \subset J(T_1) \}.
\]

Then \( \overline{\mathcal{S}}_\gamma^k \) is an inner approximation for \( \mathcal{S}_\gamma \) (see Figure 1(c), where \( \hat{\kappa} = 0.83 \)). Stage 1 in Algorithm 2 shows this procedure. With this, we can run mixture IS to estimate \( P(X \in \overline{\mathcal{S}}_\gamma^k) \) in Stage 2.

Algorithm 2: D-PrAE to estimate \( \mu = P(X \in \mathcal{S}_\gamma) \) (lower bound).

Input: Black-box evaluator \( I(\cdot \in \mathcal{S}_\gamma) \), sampling density \( q \), sample budgets \( n_1, n_2 \), input distribution \( N(\lambda, \Sigma) \).

Output: IS estimate \( \hat{\mu}_n \).

1 Stage 1 (Set Learning):
2 Sample \( \tilde{X}_1, \ldots, \tilde{X}_{n_1} \) from \( q \) and evaluate \( Y_i := I(\tilde{X}_i \in \mathcal{S}_\gamma) \) for \( i = 1, \ldots, n_1 \);
3 Train classifier with positive decision region \( \overline{\mathcal{S}}_\gamma^k = \{ x : \hat{g}(x) \geq \kappa \} \) using \( \{(\tilde{X}_i, Y_i)\}_{i=1,\ldots,n_1} \);
4 Replace \( \kappa \) by \( \hat{\kappa} = \min \{ \kappa \in \mathbb{R} : \overline{\mathcal{S}}_\gamma^k \subset J(T_1) \} \);

5 Stage 2 (Mixture IS based on Searched Dominant Points):
6 The same as Stage 2 of Algorithm 1.

As we can see, compared with Algorithm 1, the only difference is how we adjust \( \kappa \) in Stage 1. And similar to Theorem 3 we also have that Algorithm 2 attains the lower-bound relaxed efficiency certificate:

Theorem 8 (Lower-bound relaxed efficiency certificate for deep-learning-based mixture IS). Suppose \( \mathcal{S}_\gamma \) is orthogonally monotone, and \( \overline{\mathcal{S}}_\gamma^k \) satisfies the same conditions for \( \mathcal{S}_\gamma \) in Theorem 7. Then Algorithm 2 attains the lower-bound relaxed efficiency certificate by using a constant number of Stage 1 samples.

Finally, we investigate the conservativeness of this bound, which is measured by the false negative rate \( P(X \notin \overline{\mathcal{S}}_\gamma^k, Y = 1) \). Like in Section 3, we use ERM to train \( \hat{g} \), i.e., \( \hat{g} := \arg\min_{g \in \mathcal{G}} \{ R_{n_1}(g) := \frac{1}{n_1} \sum_{i=1}^{n_1} \ell(g(\tilde{X}_i), Y_i) \} \) where \( \ell \) is a loss function and \( \mathcal{G} \) is the considered hypothesis class. Let
While flexible and easy to use, the efficiency of IS estimator from the cross-entropy method depends on the selection of the parametric class of IS distributions. We provide some details on the cross-entropy method and adaptive multilevel splitting (or subset simulation). Here, Lip\(g^\cdot\) is the Lipschitz parameter of \(g^\cdot\), and the zero-variance IS distribution (the latter is only theoretically known but unimplementable).

\[ P_{X \sim q}(X \in \mathcal{S}_\gamma^\cdot \setminus \mathcal{S}_\gamma) \leq \frac{R(g^\cdot) + 2 \sup_{g \in \mathcal{G}} |R_{n_1}(g) - R(g)|}{h(\kappa^* + t(\delta, n_1)\sqrt{d\text{Lip}(g^\cdot)} + \|\hat{g} - g^\cdot\|_\infty)}. \]

Here, Lip\(g^\cdot\) is the Lipshitz parameter of \(g^\cdot\), and \(t(\delta, n_1) = 3 \left( \log(n_1 q_1) + d \log M + \log \frac{1}{\delta} \right) \frac{1}{n_1 q_1} \).

### E Cross Entropy and Adaptive Multilevel Splitting

We provide some details on the cross-entropy method and adaptive multilevel splitting (or subset simulation), and also discuss their challenges in black-box problems.

**Cross Entropy.** The cross-entropy method \([24, 25]\) uses a sequential optimization approach to iteratively solve for the optimal parameter in a parametric class of IS distributions. The objective in this optimization sequence is to minimize the Kullback–Leibler divergence between the IS distribution and the zero-variance IS distribution (the latter is only theoretically known but unimplementable). Specifically, assume we are interested in estimating \(P(g(X) > \gamma)\) and a parametric class \(p_\theta\) is considered. The cross-entropy method adaptively chooses \(\gamma_1 < \gamma_2 < \ldots < \gamma\). At each intermediate level \(k\), we use the updated IS distribution \(p_{\theta_1}\), designed for simulating \(P(g(X) > \gamma_k)\), as the sampling distribution to draw samples of \(X\) that sets up an empirical optimization, from which the next \(\theta_1\) is obtained.

While flexible and easy to use, the efficiency of IS estimator from the cross-entropy method depends crucially on the selection of the parametric class \(p_\theta\). A poor selection of \(p_\theta\) may lead to the underestimation issue (e.g., as in Theorem\([2]\)). Besides, cross-entropy can suffer from two possible issues in practice. We again use the rare-event set \(\{x : g(x) > \gamma\}\) for explanation. First, the adaptive threshold sequence might fail to reach \(\gamma\), if there exists a \(\gamma < \gamma\) such that the set \(\{x : g(x) > \gamma\}\) is “significantly different” from \(\{x : g(x) > \gamma\} - \delta\) for any \(\delta > 0\). That is, \(P_{\theta_1}(\{x : g(x) > \gamma\})\) is extremely small for any \(\delta > 0\), where \(\theta_1\) denotes the optimal parameter for the set \(\{x : g(x) > \gamma\}\). Since the number of samples used in each intermediate level is limited, such a significant difference would cause the algorithm to stagnate around \(\gamma\) (see an example in Figure\([4]\)). Second, \(\theta_1\) might fail to converge to the true \(\theta^*\). Since that exist a \(\gamma\) such that using \(p_{\theta_1}\) results in under-estimation. The failure of convergence would occur when the “missed” portion of the rare-event set (with relatively low density) in \(p_{\theta_1}\) has a larger density in \(p_{\theta_2}\) than those “targeted” rare-events (with relatively high density). The subsequent counter-example in this section shows such a phenomenon.

**Adaptive Multilevel Splitting.** Adaptive multilevel splitting (AMS) (or subset simulation) \([27, 26]\) decomposes the rare-event estimation into estimating a sequence of conditional probabilities. We adaptively choose a threshold sequence \(\gamma_1 < \gamma_2 < \ldots < \gamma_K = \gamma\). Then \(P(g(x) > \gamma)\) can be rewritten as \(P(g(x) > \gamma) = P(g(x) > \gamma_1) \prod_{k=2}^K P(g(x) > \gamma_k | g(x) > \gamma_{k-1})\). AMS then aims to estimate \(P(g(x) > \gamma_1)\) and \(P(g(x) > \gamma_k | g(x) > \gamma_{k-1})\) for each intermediate level \(k = 2, \ldots, K\). In standard implementations, these conditional probabilities are estimated using samples from \(P(g(x) > \gamma_k | g(x) > \gamma_{k-1})\) though variants of Metropolis-Hasting (MH) algorithms.

The performance of AMS largely depends on the mixing property of the proposal distribution in the MH steps \([48]\). Ideally, AMS requires a proposal distribution that can efficiently generate samples with low correlations. The theoretical convergence rate of MH algorithms can be studied through the ergodicity properties of the underlying Markov chain \([49]\) that indicate exploration “globally”. However, since \(\{x : g(x) > \gamma_k\}\) shrinks as \(k\) increases, such “global” proposal distributions might
have large rejection rates as $k$ increases, which in turn leads to long mixing time. On the other hand, focusing on “local” exploration would reduce the rejection rate, but we might encounter similar under-estimation issues as in the cross-entropy method caused by significant shifting of the level sets (see the counter-example next). Such issues are also observed in “deterministic” multilevel splitting.

**Counterexample for CE and AMS** We consider an experiment where we observe under-estimation issues for CE and AMS. Our objective is to estimate $P(g(X) < 0)$ where $X \sim N(0, \sigma^2 I_{2 \times 2})$. For both CE and AMS, we adaptively choose $\gamma_1 < \gamma_2 < ... < 0$ and deal with the level sets $\{g(X) < \gamma_k\}$. In the experiment, we consider a function $g(x) = \min\{\|x - (0.5)\| - 1/s_1, \|x - (5, 0)\| - 0.5/s_2\}$ where $s_1, s_2$ are sensitivity parameters (with regard to $\gamma_k$) for the two rare-event region, a circle centered at $(0, 5)$ and a circle centered at $(5, 0)$ respectively. More specifically, we have $s_1 = 1$ and $s_2 = 100$, which represents that the more “important” rare-event region is much less sensitive to $\gamma_k$. In Figure 5, we show that CE and AMS significantly under-estimate the target probability with different value of $\sigma^2$.
Further Details for Numerical Experiments

This section provides more details on the two experimental examples in Section 4.

F.1 2D example

In the 2D example, the rarity parameter \( \gamma \) governs the shape of the rare-event set \( \mathcal{S}_\gamma = \{ x : g(x) \geq \gamma \} \). We consider a linear combination of sigmoid functions \( g(x) = \| \theta_1 \psi(x-c_1-\gamma) + \theta_2 \psi(x-c_2-\gamma) + \theta_3 \psi(x-c_3-\gamma) + \theta_4 \psi(x-c_4-\gamma) \| \) where \( \theta, c \) are some constant vectors and \( \psi(x) = \frac{\exp(x)}{1+\exp(x)} \). A point \( x \) is a rare-event if \( g(x) > \gamma \), where we take \( \gamma = 1.8 \) in Section 4. We use \( p = N([5,5]^T, 0.25I_{2\times2}) \).

Figure 6 shows the rare-event set and its approximations for various \( \gamma \)'s. The D-PrAE boundaries seem tight in most cases, attributed to both the sufficiently-trained NN classifier and the bisection algorithm implemented for tuning \( \hat{\kappa} \) after the NN training.

![Figure 6](image)

Figure 6: The contour of \( p \), rare-event set \( \mathcal{S}_\gamma \) (reddish region), outer- and inner- approximation boundaries (black lines) and D-PrAE UB and LB decision boundaries (white lines) for some \( \gamma \) values in the 2D example.

F.2 Self-Driving Example

We provide more details about the self-driving example, which simulates the interaction of an autonomous vehicle (AV) model that follows a human-driven lead vehicle (LV). The AV is controlled by the Intelligent Driver Model (IDM), widely used for autonomy evaluation and microscopic transportation simulation, that maintains a safety distance while ensuring smooth ride and maximum efficiency. The states of the AV are \( s_t = [x_{\text{follow}}, x_{\text{lead}}, v_{\text{follow}}, v_{\text{lead}}, a_{\text{follow}}, a_{\text{lead}}, t] \) which are the position, velocity and acceleration of the AV and LV respectively. The throttle input to the AV is defined as \( u_t \) which has an affine relationship with the acceleration of the vehicle. Similarly, the randomized throttle of the LV is represented by \( w_t \). With a car length of \( L \), the distance between the LV and AV at time \( t \) is given by \( r_t = x_{\text{lead},t} - x_{\text{follow},t} - L \), which has to remain below the crash threshold for safety.

We describe the dynamics in more detail below. Figure 7 gives a pictorial overview of the interaction.
Figure 7: The states $s_t$ and input $u_t$ of the self-driving safety-testing simulation. $w_t$ denotes the throttle input of the AV from the IDM.

| Parameters                                      | Value     |
|------------------------------------------------|-----------|
| Safety distance, $s_0$                          | 2 m       |
| Speed of AV in free traffic, $v_0$              | 30 m/s    |
| Maximum acceleration of AV, $a$                 | $2\gamma$ m/s$^2$ |
| Comfortable deceleration of AV, $b$             | 1.67 m/s$^2$ |
| Maximum deceleration of AV, $d$                 | $2\gamma$ m/s$^2$ |
| Safe time headway, $\bar{T}$                    | 1.5 s     |
| Acceleration exponent parameter, $\delta$     | 4         |
| Car length, $L$                                 | 4 m       |

LV actions. The LV action contains human-driving uncertainty in decision-making modeled as Gaussian increments. For every $\Delta t$ time-steps, a Gaussian random variable is generated with the mean centered at the previous action $u_{t-\Delta t}$. We initialize $u_0 = 10$ (unitless) and $\Delta t = 4$ sec, which corresponds to zero initial acceleration and an acceleration change in the LV once every 4 seconds.

Intelligent Driver Model (IDM) for AV. The IDM is governed by the following equations (the subscripts “follow” and “lead” defined in Figure 7 is abbreviated to “f” and “l” for conciseness):

$$
\dot{x}_f = v_f \\
\dot{v}_f = \text{max} \left( a \left( 1 - \left( \frac{v_f}{v_0} \right)^\delta \right) - \left( \frac{s^*(v_f, \Delta v_f)}{s_f} \right)^2, -d \right) \\
\Delta v_f = v_f - v_l \\
s_f = x_l - x_f - L \\
s^*(v_f, \Delta v_f) = s_0 + v_f \bar{T} + \frac{v_f \Delta v_f}{2\sqrt{ab}}
$$

The parameters are presented in Table 1, and $v_l \propto u_t$ and $v_f \propto w_t$. The randomness of LV actions $u_t$'s propagates into the system and affects all the simulation states $s_t$. The IDM is governed by simple first-order kinematic equations for the position and velocity of the vehicles. The acceleration of the AV is the decision variable where it is defined by a sum of non-linear terms which dictate the “free-road” and “interaction” behaviors of the AV and LV. The acceleration of the AV is constructed in such a way that certain terms of the equations dominate when the LV is far away from the AV to influence its actions and other terms dominate when the LV is in close proximity to the AV.

Rarity parameter $\gamma$. Parameter $\gamma$ signifies the range invoked by the AV acceleration and deceleration pedals. Increasing $\gamma$ implies that the AV can have sudden high deceleration and hence avoid crash scenarios better and making crashes rarer. In contrast, decreasing $\gamma$ reduces the braking capability of the AV and more easily leads to crashes. For instance, $\gamma = 1.0$ corresponds to AV actions in the range $[5, 15]$ or correspondingly $a_{\text{follow}, t} \in [-2, 2]$, and $\gamma = 2.0$ corresponds to $a_{\text{follow}, t} \in [-4, 4]$. Figure 8 shows the approximate rare-event set by randomly sampling points and evaluating the inclusion in the set, for the two cases of $\gamma = 1.0$ and $\gamma = 2.0$. In particular, we slice the 15-dimensional space onto pairs from five of the dimensions. In all plots, we see that the crash set (red) are monotone, thus supporting the use of our D-PrAE framework. Although the crash set is not located in the “upper-right corner”, we can implement D-PrAE framework for such problems by simple re-orientation.
Figure 8: Slice of pairs of the first 5 dimensions of LV action space. For any \((u_i, u_{i'})\) shown, \(u_j, j \not\in \{i, i'\}\) is fixed at a constant value. Blue dots = non-crash cases, red dots = crash cases.

**Sample trajectories.** Figure 9 shows two examples of sample trajectories, one successfully maintaining a safe distance, and the other leading to a crash. In Figure 9(e)-(h) where we show the crash case, the AV maintains a safe distance behind the LV until the latter starts rapidly decelerating (Figure 9(h)). Here the action corresponds to the throttle input that has a linear relationship with the acceleration of the vehicle. The LV ultimately decelerates at a rate that the AV cannot attain and its deceleration saturates after a point which leads to the crash.

Figure 9: Autonomous Car Following Experiment Trajectories. Figures (a) - (d) represent a simulation episode without a crash occurring where the AV follows the LV successfully at a safe distance. Figures (e) - (h) represents a simulation episode where crash occurs at \(t = 23\) seconds due to the repeated deceleration of the LV.

**F.3 Code**

The code and environment settings for the experiments is available at [https://github.com/safeai-lab/D-PrAE/](https://github.com/safeai-lab/D-PrAE/).
G Proofs

G.1 Proofs for the Dominant Point Methodologies

Proof of Proposition[2] Since \( \mu \) is exponentially decaying in \( \gamma \) while \( n \) is polynomially growing in \( \gamma \), we know that \( \lim_{\gamma \to \infty} n \mu = 0 \). Since \( n\tilde{\mu}_n \) takes values in \( \{0, 1, \ldots, n\} \), we get that \( \tilde{P}(|n\tilde{\mu}_n - n\mu| > \varepsilon n\mu) \to 1 \) as \( \gamma \to \infty \).

Proof of Theorem[3] We know that
\[
\tilde{E}[Z^2] = \sum_j \tilde{E}[I(X \in S_j) L^2(X)] \leq \sum_j e^{-(a_j - \lambda_j)'\Sigma_{-1}^{-1}(a_j - \lambda_j)/\alpha_j} \sim e^{-(a^* - \lambda)'\Sigma_{-1}^{-1}(a^* - \lambda)}.
\]
Denote \( Y = B(X - \lambda) \sim N(0, BSB') \) and \( s = B(a^* - \lambda) \). Define \( \tilde{\varepsilon} = \varepsilon \min_{u \neq 0} (BSB')^{-1} u \|u\|_{\infty} \). Then we also know that
\[
\tilde{E}[I(X \in S_j)L(X)] \\
\leq P(B(X - a^*) \geq 0, (X - a^)'\Sigma_{-1}(X - a^*) \leq \tilde{\varepsilon}^2) \\
= P(Y \geq s, (Y - s)'(BSB')^{-1}(Y - s) \leq \tilde{\varepsilon}^2) \\
\int_{y \geq s, (y - s)'(BSB')^{-1}(y - s) \leq \tilde{\varepsilon}^2} (2\pi)^{-d/2} |B \Sigma B'|^{-1/2} e^{-y'(B \Sigma B')^{-1}y/2} dy \\
\geq (2\pi)^{-d/2} |B \Sigma B'|^{-1/2} e^{-\varepsilon^2/2} e^{-(a^* - \lambda)'\Sigma_{-1}(a^* - \lambda)/2} \\
\int_{y \geq s, (y - s)'(BSB')^{-1}(y - s) \leq \tilde{\varepsilon}^2} e^{-s'(B \Sigma B')^{-1}(y - s)} dy \\
\geq (2\pi)^{-d/2} |B \Sigma B'|^{-1/2} e^{-\varepsilon^2/2} e^{-(a^* - \lambda)'\Sigma_{-1}(a^* - \lambda)/2} \prod_{i=1}^{d} \int_0^{\tilde{\varepsilon}} e^{-s_i'(B \Sigma B')^{-1}s_i} ds_i \\
= (2\pi)^{-d/2} |B \Sigma B'|^{-1/2} e^{-\varepsilon^2/2} e^{-(a^* - \lambda)'\Sigma_{-1}(a^* - \lambda)/2} \prod_{i=1}^{d} \frac{1 - e^{-s_i'(B \Sigma B')^{-1}s_i}}{s_i'(B \Sigma B')^{-1}s_i}.
\]
Note that it is easy to verify that \( s_i'(B \Sigma B')^{-1}s_i \geq 0 \). If \( s_i'(B \Sigma B')^{-1}s_i = 0 \), then we naturally use \( \tilde{\varepsilon} \) to substitute \( \frac{1 - e^{-s_i'(B \Sigma B')^{-1}s_i}}{s_i'(B \Sigma B')^{-1}s_i} \). Since we have assumed that the components of \( a^* \) are at most polynomially growing in \( \gamma \), finally we get that
\[
\tilde{E}[I(X \in S_j)L(X)] \sim e^{-(a^* - \lambda)'\Sigma_{-1}(a^* - \lambda)/2}
\]
and hence \( \tilde{E}[Z^2]/\tilde{E}[Z]^2 \) is at most polynomially growing in \( \gamma \).

Proof of Theorem[3] We know that \( E[Z] = \tilde{\Phi}(\gamma) + \tilde{\Phi}(k\gamma) \). Moreover,
\[
\tilde{E}[Z^2] = e^{\gamma^2}(\tilde{\Phi}(2\gamma) + \tilde{\Phi}((k - 1)\gamma)).
\]
If \( 0 < k \leq 1 \), then \( \tilde{E}[Z] \sim e^{-k^2\gamma^2/2} \) and \( \tilde{E}[Z^2] \sim e^{\gamma^2} \) as \( \gamma \to \infty \). If \( 1 < k < 3 \), then \( \tilde{E}[Z] \sim e^{-\gamma^2/2} \) and \( \tilde{E}[Z^2] \sim e^{(1-(k-1)^2/2)\gamma^2} \) as \( \gamma \to \infty \). In both cases, we get that \( \tilde{E}[Z^2]/\tilde{E}[Z]^2 \) grows exponentially in \( \gamma \). On the other hand, we know that
\[
\tilde{P} \left( \left| \frac{1}{n} \sum_{i} Z_i - \tilde{\Phi}(\gamma) \right| > \varepsilon \tilde{\Phi}(\gamma) \right) \\
\leq \tilde{P}(\exists i : X_i \leq -k\gamma) + \tilde{P} \left( \left| \frac{1}{n} \sum_{i} I(X_i \geq \gamma)e^{\gamma^2/2-\gamma X_i} - \tilde{\Phi}(\gamma) \right| > \varepsilon \tilde{\Phi}(\gamma) \right).
\]
Clearly $\bar{\Phi}(\gamma) = 1 - (1 - \Phi((k + 1)\gamma))n \sim n\Phi((k + 1)\gamma)$, which is exponentially decreasing in $\gamma$ as $n$ is polynomial in $\gamma$. Moreover, by Chebyshev’s inequality,

$$
\bar{\Phi} \left( \left\{ \frac{1}{n} \sum_i I(X_i \geq \gamma) e^{\gamma^2/2 - \gamma X_i} - \Phi(\gamma) \right\} > \varepsilon \Phi(\gamma) \right)
\leq \frac{\bar{\Phi}[I(X_i \geq \gamma) e^{\gamma^2 - 2\gamma X_i}]}{n\varepsilon^2 \Phi^2(\gamma)} = \frac{e^{\gamma^2} \Phi(2\gamma)}{n\varepsilon^2 \Phi^2(\gamma)} \sim \frac{\gamma}{n\varepsilon^2}.
$$

Thus $P(|\hat{\mu}_n - \Phi(\gamma)| > \varepsilon \Phi(\gamma)) = O(\frac{1}{n\varepsilon^2})$. Moreover, we know that $P(\exists i : Z_i > 0) \geq 1 - 1/2^n$ and if $Z_i > 0$ for some $i$, then we have that

$$
\frac{\sum_i Z_i^2 / n}{(\sum_i Z_i/n)^2} \leq n^2.
$$

\[ \square \]

### G.2 Proofs for the Relaxed Efficiency Certificate

**Proof of Proposition 1** We have

$$
P(\hat{\mu}_n - \mu < -\epsilon \mu) \leq P(\hat{\mu}_n - \bar{\mu} < -\epsilon \bar{\mu})
$$

since $\bar{\mu} \geq \mu$ and $1 - \epsilon > 0$. Note that the Markov inequality gives

$$
P(\hat{\mu}_n - \bar{\mu} < -\epsilon \bar{\mu}) \leq \frac{\text{Var}(Z_i)}{n\epsilon^2 \bar{\mu}^2}
$$

so that

$$
n \geq \frac{\text{Var}(Z_i)}{\delta^2 \epsilon^2 \bar{\mu}^2} = \frac{RE}{\delta^2} = \tilde{O} \left( \log \frac{1}{\bar{\mu}} \right) = \tilde{O} \left( \log \frac{1}{\mu} \right)
$$

achieves the relaxed efficiency certificate. \[ \square \]

**Proof of Proposition 3** The proof follows from that of Proposition 1 with a conditioning on $D_{n1}$. We have

$$
P(\hat{\mu}_n - \mu < -\epsilon \mu|D_{n1}) \leq P(\hat{\mu}_n - \bar{\mu}(D_{n1}) < -\epsilon \bar{\mu}(D_{n1})|D_{n1})
$$

since $\bar{\mu}(D_{n1}) \geq \mu$ almost surely and $1 - \epsilon > 0$. Note that the Markov inequality gives

$$
P(\hat{\mu}_n - \bar{\mu}(D_{n1}) < -\epsilon \bar{\mu}(D_{n1})|D_{n1}) \leq \frac{\text{Var}(Z_i|D_{n1})}{n_2 \epsilon^2 \bar{\mu}(D_{n1})^2}
$$

so that

$$
n_2 \geq \frac{\text{Var}(Z_i|D_{n1})}{\delta^2 \epsilon^2 \bar{\mu}(D_{n1})^2} = \frac{RE(D_{n1})}{\delta^2} = \tilde{O} \left( \log \left( \frac{1}{\bar{\mu}(D_{n1})} \right) \right) = \tilde{O} \left( \log \frac{1}{\mu} \right)
$$

almost surely. Thus,

$$
n = n_1 + n_2 \geq \tilde{O} \left( \log \frac{1}{\mu} \right)
$$

achieves the relaxed efficiency certificate. \[ \square \]

**Proof of Corollary 1** Follows directly from Proposition 3 since $\mathbb{S}_\gamma \supset \mathbb{S}_\gamma$ implies $\bar{\mu}(D_{n1}) \geq \mu$ almost surely. \[ \square \]

**Proof of Theorem 3** We have assumed that $\mathbb{S}_\gamma$ satisfies the assumptions for $\mathbb{S}_\gamma$ in Theorem 5. Then following the proof of Theorem 5, we obtain the efficiency certificate for the IS estimator in estimating its mean. Theorem 3 is then proved by directly applying Corollary 1. \[ \square \]
G.3 Proofs for Conservativeness

Recall that \( T_0 = \{ \tilde{X}_i : Y_i = 0 \} \) where the samples are generated as in Algorithm 1. By some combinatorial argument, we can prove the following lemma which says that with high probability, each point in \( S_{\gamma} \) that has sufficient distance to its boundary could be covered by \( \mathcal{H}(T_0) \).

**Lemma 1.** Suppose that the density \( q \) has bounded support \( K \subset [0, M]^d \), and for any \( x \in K \), suppose that \( 0 < q_i(x) \leq q \). Define \( B_{d}: = \{ x \in S_{\gamma}: x + t1_{d 	imes 1} \in S_{\gamma}^c \} \). Then with probability at least \( 1 - \delta \), we have that \( B_{d} \in \mathcal{H}(T_0) \). Here \( \delta = \left( \frac{\log(nq_{i}) + d \log M + \log \frac{1}{\delta}}{nq_{i}} \right)^{2} \). 

**Proof.** The basic idea is to construct a finite number of regions, such that when there are at least one sample point in each of these regions, we would have that \( B_{d} \subset \mathcal{H}(T_0) \). Then we could give a lower bound to the probability of \( B_{d} \subset \mathcal{H}(T_0) \) in terms of the number of regions and the volume of each of these regions.

By dividing the first \( d - 1 \) coordinates into \( \frac{d-1}{d} \) equal parts, we partition the region \([0, M]^d\) into rectangles, each with side length \( \delta \), except for the \( d \)-th dimension (the \( \delta \) here is not exactly the \( \delta \) in the statement of the lemma, since we will do a change of variable in the last step). To be more precise, the rectangles are given by

\[
Z_j = \left( \prod_{i=1}^{d-1} (j_i - 1)\delta, j_i \delta \right] \times [0, M].
\]

Here the index \( j \in J \) and \( J \) is defined by \( J := \{ j = (j_1, \ldots, j_{d-1}), j_i = 1, 2, \ldots, \frac{M}{\delta} \} \).

Denote by \( J_0 \) the set which consists of \( j \in J \) such that there exist a point in \( B_{d}\) whose first \( d - 1 \) coordinates are \( j_1\delta, j_2\delta, \ldots, j_{d-1}\delta \) respectively, i.e., \( J_0 = \{ j \in J : B_{d} \cap \left( \prod_{i=1}^{d-1} (j_i \delta) \right) \neq \emptyset \} \). For all \( j \in J_0 \), let \( p_j \) be the point such that

i) \( p_j \in B_{d}\)

ii) The first \( d - 1 \) coordinates of \( p_j \) are \( j_1\delta, j_2\delta, \ldots, j_{d-1}\delta \) respectively

iii) \( p_j \) has \( d \)-th coordinate larger than \(-\delta + \sup_{x} \gamma(x) \) (\( d \)-th coordinate of \( p \)).

From the definition of \( J_0 \) and the fact that \( B_{d} \supset B_{d}\), \( p_j \) is guaranteed to exist. We claim that \( B_{d} \cap Z_j \subset R(p_j) \), where \( R(p_j) \) is the rectangle that contains \( 0 \) and \( p_j \) as two of its corners. Clearly, from the definition of \( Z_j \), for all point in \( B_{d} \cap Z_j \), their first \( d - 1 \) coordinates are smaller than \( j_1\delta, j_2\delta, \ldots, j_{d-1}\delta \) respectively. For the \( d \)-th coordinate, suppose on the contrary that there exists \( x \in B_{d} \cap Z_j \) with \( d \)-th coordinate greater than the \( d \)-th coordinate of \( p_j \). Since \( x \in Z_j \), the first \( d - 1 \) coordinates of \( x \) are at least \( (j_1 - 1)\delta, (j_2 - 1)\delta, \ldots, (j_{d-1} - 1)\delta \), so we have that \( x + \delta 1_{d 	imes 1} \geq p_j + \delta e_\delta \). Since \( x \in B_{d}\), we know that \( x + 2\delta 1_{d 	imes 1} \in S_{\gamma}^c \). Hence by the previous inequality and the orthogonal monotonicity of \( S_{\gamma}, p_j + \delta e_d + \delta 1_{d 	imes 1} \in S_{\gamma}^c \). By definition of \( B_{d} \), this implies \( p_j + \delta e_d \in B_{d} \). This contradicts i) in the definition of \( p_j \). By contradiction, we have shown that each point in \( B_{d} \cap Z_j \) has \( d \)-th coordinate smaller than the \( d \)-th coordinate of \( p_j \). So the claim that \( B_{d} \cap Z_j \subset R(p_j) \) for any \( j \in J_0 \) is proved.

Then we consider those \( j \) such that \( j \in J - J_0 \). Since \( j \notin J_0 \), for any point in \( x \in Z_j \), since the first \( d - 1 \) coordinates of \( x + \delta 1_{d 	imes 1} \) are at least \( j_1\delta, j_2\delta, \ldots, j_{d-1}\delta \) respectively, we have that \( x + \delta 1_{d 	imes 1} \notin B_{d}\). This implies \( x + 3\delta 1_{d 	imes 1} \notin S_{\gamma}^c \), or \( x \notin B_{3\delta} \). So we have shown that for any \( j \notin J_0, B_{3\delta} \cap Z_j = \emptyset \). This implies \( B_{3\delta} \) has a partition given by \( B_{3\delta} = \cup_{j \notin J_0} (B_{3\delta} \cap Z_j) = \cup_{j \notin J_0} (B_{3\delta} \cap Z_j) \). Notice that \( B_{3\delta} \subset B_{d} \), from the result in the preceding paragraph, we conclude that \( B_{3\delta} \subset \cup_{j \notin J_0} R(p_j) \).

For each \( j \in J_0 \) and the constructed \( p_j \), consider the region

\[
G_j := \{ x \in S_{\gamma}^c : x \geq p_j \}.
\]

Observe that, if there exists a sample point in \( T_0 \) that lies in \( G_j \), then we have \( p_j \subset \mathcal{H}(T_0) \) which implies \( R(p_j) \subset \mathcal{H}(T_0) \). Since \( p_j \in B_{d} \) and \( S_{\gamma} \) is orthogonally monotone, we have that \( G_j \) contains
the rectangle which contains $p_j$ and $p_j + \delta \mathbf{1}_{d \times 1}$ as two of its corners, so $\text{Vol}(G_j) \geq \delta^d$. Hence the probability that $R(p_j) \subset \mathcal{H}(T_0)$ has a lower bound given by

$$P(R(p_j) \subset \mathcal{H}(T_0)) \geq P(T_0 \cap G_j \neq \emptyset) \geq 1 - (1 - \delta^d q_t)^n \geq 1 - e^{-n q_t \delta^d}.$$  

Notice that $|J_0| \leq \left(\frac{M}{d}\right)^{d-1}$, by union bound we have that

$$P(\bigcup_{j \in J_0} R(p_j) \subset \mathcal{H}(T_0)) \geq 1 - \frac{M^{d-1}}{d^{d-1}} e^{-n q_t \delta^d}.$$  

Since we have shown that $B_{3\delta} \subset \bigcup_{j \in J_0} R(p_j)$, this implies

$$P(B_{3\delta} \subset \mathcal{H}(T_0)) \geq 1 - \frac{M^{d-1}}{d^{d-1}} e^{-n q_t \delta^d}.$$  

Based on this inequality, it is not hard to check that for $t(\delta, n_1) = 3 \left( \frac{\log(n_1 q_t) + d \log M + \log q_t}{n_1 q_t} \right)^\frac{1}{2}$, we have that $P(B_t(\delta) \subset \mathcal{H}(T_0)) \geq 1 - \delta$. \hfill \Box

Proof of Theorem \[1\] First, we show the inequality in the theorem, i.e., $P_{X \sim q}(X \in \mathcal{H}(T_0)^c \setminus S_\gamma) \leq M^{d-1} q_t \left( \frac{\sqrt{d}}{2} \right)^{d-1} w_{d-1}(\delta, n_1)$. It suffices to show that with probability at least $1 - \delta$, $\text{Vol} \left( \mathcal{H}(T_0)^c \setminus S_\gamma \right) \leq M^{d-1} \left( \frac{\sqrt{d}}{2} \right)^{d-1} w_{d-1}(\delta, n_1)$, or equivalently $\text{Vol}(S_\gamma^{c} \setminus \mathcal{H}(T_0)) \leq M^{d-1} \left( \frac{\sqrt{d}}{2} \right)^{d-1} w_{d-1}(\delta, n_1)$. Since by lemma \[1\] we have that $B_t(\delta, n_1) \subset \mathcal{H}(T_0)$ with probability at least $1 - \delta$, it suffices to show that $\text{Vol}(S_\gamma^{c} \setminus B_t(\delta, n_1)) \leq M^{d-1} \left( \frac{\sqrt{d}}{2} \right)^{d-1} w_{d-1}(\delta, n_1)$. This latter inequality actually follows from the definition of $B_t(\delta, n_1)$ and some geometric argument. Indeed, by definition of $B_t(\delta, n_1)$, for each $x \in S_\gamma^{c} \setminus B_t(\delta, n_1)$, $x$ belongs to the area which is obtained by moving the boundary of $S_\gamma$ in direction $-\frac{1}{\sqrt{d}} \gamma$ for a distance of $t(\delta, n_1) \sqrt{d}$. So the volume of $S_\gamma^{c} \setminus B_t(\delta, n_1)$ is bounded by

$$t(\delta, n_1) \sqrt{d} \times \text{Vol}_{d-1}(\text{projection of the boundary of } S_0 \text{ in direction } \mathbf{1}_{d \times 1})$$

$$\leq t(\delta, n_1) \sqrt{d} \times \text{Vol}_{d-1}(\text{projection of } [0, M]^d \text{ in direction } \mathbf{1}_{d \times 1})$$

Here $\text{Vol}_{d-1}$ means computing volume in the $d - 1$ dimensional space. Notice that $[0, M]^d$ is contained in a ball with radius $\frac{M \sqrt{d}}{2}$, we have that

$$\text{Vol}_{d-1}(\text{projection of } [0, M]^d \text{ in direction } \mathbf{1}_{d \times 1}) \leq M^{d-1} \left( \frac{\sqrt{d}}{2} \right)^{d-1} w_{d-1}.$$

Combining the preceding two inequalities, we have proved the inequality in the theorem. Next we show the equality in the theorem. Indeed, when $d$ is large, we have asymptotic formula $w_d = \frac{1}{\sqrt{d \pi}} \left( \frac{2 \pi}{d} \right)^\frac{d}{2} \left( 1 + O(d^{-1}) \right)$. Plugging this into the RHS above, we will obtain the asymptotic bound as stated in the theorem. \hfill \Box

Proof of Theorem \[2\] By Markov inequality and the definition of $h_S$, we know that

$$P_{X \sim q}(X \in \hat{S}_\gamma, X \in S_\gamma^{c}) = P_{X \sim q}(\hat{g}(X) \geq \hat{h}, X \in S_\gamma^{c}) \leq \frac{R(\hat{g})}{h(\hat{h})}.$$  

(10)

We will compare the numerator and denominator of the RHS of (10) with their counterparts for the true minimizer $g^\ast$. For the numerator, since $\hat{g}$ is the empirical risk minimizer, we have that

$$R(\hat{g}) \leq R_{n_1}(g) + \sup_{g_0 \in \mathcal{V}} |R_{n_1}(g_0) - R(g_0)| \leq R_{n_1}(g^\ast) + \sup_{g_0 \in \mathcal{V}} |R_{n_1}(g_0) - R(g_0)|$$

$$\leq R(g^\ast) + 2 \sup_{g_0 \in \mathcal{V}} |R_{n_1}(g_0) - R(g_0)|.$$
For the denominator, from the definition of $\tilde{S}^\kappa$, it is not hard to verify that, in Algorithm [1] our choice of $\hat{\kappa}$ is given by $\hat{\kappa} = \min\{\hat{g}(x) : x \in \mathcal{H}(T_0)^c\}$. By lemma [1] we have that with probability at least $1 - \delta$, $B_{t(\delta, n_1)} \subset \mathcal{H}(T_0)$, which implies that with probability at least $1 - \delta$,

$$
\hat{\kappa} \geq \min\{\hat{g}(x) : x \in B_{t(\delta, n_1)}^c\} \geq \min\{g^*(x) : x \in B_{t(\delta, n_1)}^c\} - \|\hat{g} - g^*\|_\infty
$$

$$
\geq \min\{g^*(x) : x \in S_\gamma\} - t(\delta, n_1) \sqrt{d \text{Lip}(g^*)} - \|\hat{g} - g^*\|_\infty
$$

$$
= \kappa^* - t(\delta, n_1) \sqrt{d \text{Lip}(g^*)} - \|\hat{g} - g^*\|_\infty.
$$

Putting the preceding two inequalities into the Markov inequality [10], and notice that $h$ is non decreasing by its definition, the theorem is proved. \qed