LOWER BOUNDING RATE-DISTORTION FROM SAMPLES

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ABSTRACT

The rate-distortion function $R(D)$ tells us the minimal number of bits on average to compress a random object within a given distortion tolerance. A lower bound on $R(D)$ therefore represents a fundamental limit on the best possible rate-distortion performance of any lossy compression algorithm, and can help us assess the potential room for improvement. We make a first attempt at an algorithm for computing such a lower bound, applicable to general memoryless data sources that we have samples of. Based on a dual characterization of $R(D)$ in terms of constrained maximization, our method approximates the exact constraint function by an asymptotically unbiased estimator, allowing for stochastic optimization. On a 2D Gaussian source, we obtain a lower bound within 1 bit of the analytical $R(D)$.

1 INTRODUCTION AND BACKGROUND

Let $X \in \mathcal{X}$ be a random variable with distribution P_X [1] that represents a memoryless data source, let $\mathcal{Y}$ be the set of lossy representations, and let $\rho : \mathcal{X} \times \mathcal{Y} \to [0, \infty)$ be a distortion cost function. The (information) rate-distortion function $R(D)$ is defined as the solution to the optimization problem,

$$R(D) = \inf_{P_{Y|X} : \mathbb{E}[\rho(X,Y)] \le D} I(X;Y), \tag{1}$$

where we consider all stochastic transforms $P_{Y|X}$ whose expected distortion is within the given threshold D, and minimize the mutual information between the source X and its reproduced representation Y. Rate-distortion theory (Shannon, 1959; Cover, 1999) gives operational meaning to the above definition as the asymptotic fundamental limit of lossy data compression. In essence, $R(D)$ delimits the minimal average number of bits (or nats, depending the base of $\log$) needed to convey i.i.d. samples of X within average distortion D, for any block code that is allowed arbitrarily long blocks or high complexity, regardless of its implementation technology. Therefore, the rate-distortion function, or a lower bound on it, can help analyze how close lossy compression algorithms are to their theoretical performance limits. If the operational rate and distortion of a compression algorithm lies far above the $R(D)$ curve (or its lower bound), then we may expect room for further improvement; otherwise, the algorithm's rate-distortion performance is already close to theoretically optimal, so we may better focus our attention on improving other aspects of the algorithm.

Although $R(D)$ has no analytical form in general, it can be computed in principle by solving the convex optimization problem Eq. 1. The mutual information $I(X;Y)$, however, is typically challenging to compute, so a tractable upper bound $I(X;Y) \le I(X;Y) + KL(P_Y \| \tilde{P}_Y) = \mathbb{E}_X[KL(P_{Y|X} \| \tilde{P}_Y)]$ is often used instead in the optimization problem. Solving the resulting minimization problem then leads to upper bounds on $R(D)$, and is the basis of the Blahut–Arimoto algorithm (Arimoto, 1972). The same mutual information upper bound has also made numerous appearances in machine learning (Alemi et al., 2017; Poole et al., 2019), notably as the aggregate KL-divergence regularizer in Variational-Autoencoders (VAEs) (Kingma & Welling, 2013). Traditionally, the set of lossy presentations $\mathcal{Y}$ is often a subset of the data space $\mathcal{X}$, in the form of quantization points, and distortion ρ is fixed. In VAEs and their recent application to learned data compression (Ballé et al., 2017), $\mathcal{Y}$ has the interpretation of a *latent space*, $\tilde{P}_Y$ is the *prior*, and $\rho(x, y) = \rho_0(x, f_\theta(y))$ corresponds

[1] Formally, $X : \Omega \to \mathcal{X}$ is a measurable function on an underlying probability space $(\Omega, \mathcal{A}, \mathbb{P})$, and P_X is the image measure of $\mathbb{P}$ under X.

to the negative log likelihood $\log p_\theta(x|y)$ parameterized by a *decoder* $f_\theta : \mathcal{Y} \to \mathcal{X}$ (e.g., $p_\theta(x|y)$ is a Gaussian density with mean $f_\theta(y)$, ρ_0 is a squared error), so the distortion ρ is learned. The Lagrangian $\mathbb{E}_X[KL(P_{Y|X}\|\tilde{P}_Y)] + \lambda\mathbb{E}[\rho(X,Y)]$ then corresponds to the negative ELBO (Kingma & Welling, 2013) for learning and inference. Using the analytical density of $P_{Y|X}$ that optimizes the Lagrangian (assumed to exist), Huang et al. (2020) sample from this optimal $P_{Y|X}$ to compute optimistic upper bounds on $R(D)$ of trained VAEs and other generative models, hinting at their *possible* compression performance. Our method is agnostic to the choice of representations $\mathcal{Y}$ or distortion ρ, and can also be extended to compute $R(D)$ lower bounds of trained decoder-based models. Unlike (Huang et al., 2020), however, we do not assume (or require) a prior distribution $\tilde{P}_Y$, and our lower bound establishes what kind of lossy compression performance is theoretically *impossible* to obtain.

Lower bounds of $R(D)$, by contrast, have received considerably less attention, potentially because of difficulty in obtaining them. A variational lower bound of $R(D)$ already appeared in Shannon's landmark paper (Shannon, 1948), which was later extended (Berger, 1971) and proved rigorously for X in a general abstract probability space by Csiszár (1974); we adopt the version in (Kostina, 2016). The special case of a discrete and known source P_X is considered by Chiang & Boyd (2004), who solve the corresponding (finite-dimensional) dual problem of $R(D)$ by geometric programming.

2 METHOD

2.1 DUAL CHARACTERIZATION OF $R(D)$

We use the below general characterization of $R(D)$ in terms of a constrained maximization problem:

Theorem 2.1. *(Kostina, 2016) Under basic regularity conditions (e.g., satisfied by a bounded ρ; see Appendix Sec. A.1), for any distortion tolerance $D > D_{min} := \inf\{D : R(D) \leq \infty\}$, it holds that*

$$R(D) = \max_{g(x),\lambda} \{\mathbb{E}[-\log g(X)] - \lambda D\} \tag{2}$$

where the maximization is over $g(x) \geq 0$ and $\lambda \geq 0$ satisfying the constraint

$$\mathbb{E}\left[\frac{\exp(-\lambda\rho(X,y))}{g(X)}\right] = \int \frac{\exp(-\lambda\rho(x,y))}{g(x)} dP_X(x) \leq 1, \forall y \in \mathcal{Y} \tag{3}$$

In other words, every pair of feasible (λ, g) satisfying Eq. 3 yields a lower bound of $R(D)$, i.e., $\mathbb{E}[-\log g(X)] - \lambda D \leq R(D)$, and we obtain $R(D)$ via the tightest such lower bound. This characterization of $R(D)$ can be derived from Lagrange duality (Chiang & Boyd, 2004) in the case of a finite alphabet $\mathcal{X}$; the extension to a general $\mathcal{X}$ requires a more involved argument (Csiszár, 1974).

2.2 LOWER BOUNDING $R(D)$ VIA NUMERICAL OPTIMIZATION

We rarely know P_X explicitly; e.g., when P_X is induced by natural images, characterizing the support of P_X (a low dimensional manifold of Euclidean space) alone is non-trivial. However, if we can compute the expectations in Eqs. 2 and 3, then we can still obtain a lower bound of $R(D)$ by numerically solving a constrained optimization problem. The main idea is to replace maximizing over functions $g \geq 0$ by a subset of functions $g_\theta \geq 0$ parameterized by a vector θ. Any feasible (g_θ, λ) would then give us a (possibly loose) lower bound on $R(D)$. We can use a flexible family of functions for g_θ, such as neural networks with a non-negative output activation to ensure $g_\theta \geq 0$ (or, we can parameterize $\log g$ instead). Noting that the constraint Eq. 3 is equivalent to the constraint function $c(g,\lambda) := \sup_y \mathbb{E}\left[\exp(-\lambda\rho(X,y))/g(X)\right] - 1$ being non-positive, we can then consider solving the following constrained maximization problem to obtain a $R(D)$ lower bound, $R_L(D)$:

$$R(D) \geq R_L(D) = \max_{\theta,\lambda\geq 0} f(\theta,\lambda), \quad \text{where } f(\theta,\lambda) := \mathbb{E}[-\log g_\theta(X)] - \lambda D \tag{4}$$

$$\text{subject to} \quad c(\theta,\lambda) = \sup_y \mathbb{E}\left[\frac{\exp(-\lambda\rho(X,y))}{g_\theta(X)}\right] - 1 \leq 0 \tag{5}$$

Assuming the supremum in Eq. 11 can be computed exactly, then a variety of algorithms can be used to find a local optimum of this problem. We consider a simple formulation based on exact penalty

method (Nocedal & Wright, 2006): we solve a sequence of unconstrained problems

$$\max_{\theta,\lambda\geq 0} f(\theta,\lambda) - \gamma_t[c(\theta,\lambda)]^+ \tag{6}$$

where $[c(\theta,\lambda)]^+ = \max\{0, c(\theta,\lambda)\}$ measures the amount of constraint violation, and the sequence of penalty coefficients γ_t is gradually increased. Under fairly general conditions, a feasible solution $\{(\theta_t^*, \lambda_t^*)\}$ to Eq. 6 is also a local optimum of the original constrained optimization problem in Eqs. 10, 11 (Theorem 17.4 of Nocedal & Wright (2006)). Then we can estimate $R_L = f(\theta_t^*, \lambda_t^*)$.

2.3 An Approximate Algorithm using stochastic estimators

In most practical problems, the expectations in the optimization problem can only be approximated by Monte-Carlo averaging over samples of X. Let's focus on the constraint function c for now, and denote $\psi(x,y) := \frac{\exp(-\lambda\rho(x,y))}{g(x)} - 1$, suppressing its dependence on (g,λ) for brevity. Note, however, that $c = \sup_y \mathbb{E}[\psi(X,y)]$ does not have the form of an expectation due to the maximization over y. Still, we may try to estimate c by maximizing the sampled approximation of $\mathbb{E}[\psi(X,y)]$, i.e., compute the k-sample estimator $C_k := \sup_y \frac{1}{k}\sum_{i=1}^k \psi(X_i,y)$, with $X_i \sim P_X$. What's the relation between C_k and c? Given a candidate (g,λ), can we verify its feasibility using C_k, instead of the intractable c? We answer these questions in the following theorem (proved in Appendix Sec. A.2):

Theorem 2.2. *Let $X_1, X_2, ...$ be a sequence of i.i.d. random variables with the shared data distribution $X_k \sim P_X$. Define the sequence of random variables $C_k := \sup_y \frac{1}{k}\sum_i \psi(X_i,y)$. Then*

1. $\mathbb{E}[C_k] = \mathbb{E}_{X_1,...,X_k}[\sup_y \frac{1}{k}\sum_i \psi(X_i,y)] \geq \sup_y \mathbb{E}[\psi(X,y)] =: c$;
2. $\mathbb{E}[C_1] \geq \mathbb{E}[C_2] \geq ... \geq \mathbb{E}[C_k] \geq \mathbb{E}[C_{k+1}] \geq ... \sup_y \mathbb{E}[\psi(X,y)] = c$;
3. *If $\psi(x,y)$ is bounded and continuous in y, and if $\mathcal{Y}$ is compact, then C_k converges to c almost surely (as well as in probability, i.e., $\lim_{k\to\infty}\mathbb{P}(|C_k - c| > \epsilon) = 0, \forall\epsilon > 0$), and $\lim_{k\to\infty}\mathbb{E}[C_k] = c$.*

Theorem 2.2 tells us that C_k is on average an over-estimator of the value of the constraint function c; and like the Importance-Weighted ELBO (Burda et al., 2015), the bias of the estimator decreases monotonically as $k \to \infty$, and that under continuity assumptions, C_k is asymptotically unbiased and converges to c. This means that we can form an empirical estimate of the constraint function c by computing $\hat{C}_k := \sup_y \frac{1}{k}\sum_i \psi(x_i,y)$ from a large batch of samples $\{x_1, x_2, ..., x_k\}$ (or, to be more precise, we average many such $\hat{C}_k$ computed from multiple batches to estimate $\mathbb{E}[C_k]$); if the empirical estimate of c is satisfied, then we can be confident so is the true constraint c satisfied.

In light of this, we can replace the original constraint $c \leq 0$ by the more conservative constraint $\mathbb{E}[C_k] \leq 0$. Using the unbiased estimator $\hat{C}_k$ for $\mathbb{E}[C_k]$, and similarly the sample-mean $\hat{f} := \frac{1}{m}\sum_{j=1}^m -\log g(x_j) - \lambda D$ for f, our algorithm solves the following sequence of penalty problems,

$$\max_{\theta,\lambda\geq 0} \hat{\ell}(\theta,\lambda), \quad \text{with } \hat{\ell}(\theta,\lambda) := \hat{f}(\theta,\lambda) - \gamma_t[\hat{C}_k(\theta,\lambda)]^+ \tag{7}$$

where given a penalty coefficient γ_t, we perform stochastic gradient ascent on the unconstrained objective $\hat{\ell}(\theta,\lambda)$ till convergence; we then increase the penalty e.g., $\gamma_{t+1} := \beta\gamma_t$ with $\beta > 1$, and solve the maximization problem w.r.t. (θ,λ) again, until we can verify feasibility of resulting (θ,λ) (e.g., $\hat{C}_k \leq 0$) with high confidence. We specify Algorithm 1 in full detail in Appendix Sec. A.3.

2.4 Inner optimization with respect to y

So far we have assumed that we can exactly compute the supremum $\hat{C}_k = \sup_y \frac{1}{k}\sum_i \psi(x_i,y)$. In practice, $\frac{1}{k}\sum_i \psi(x_i,y)$ is rarely concave in y, and we can only find a local optimum, e.g., with a gradient-based method. This is less problematic during training, as long as (g,λ) receive the appropriate training signal to eventually arrive at a feasible solution. However, once the training terminates with some candidate solution (g^*,λ^*), we need to compute $\hat{C}_k$ exactly (ideally with as large k as possible), in order to verify that the solution (g^*,λ^*) is feasible (with

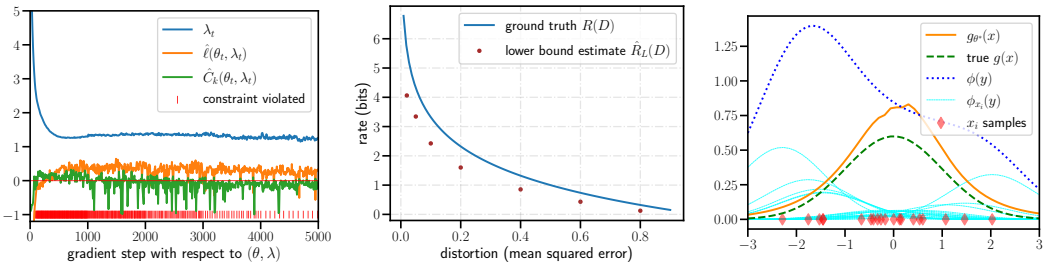

Figure 1: **Left**: trajectories of various quantities across training steps, for the $D = 0.6$ experiment; **Middle**: the final lower bound estimate $\hat{R}_L(D)$, plotted against the true $R(D)$; **Right**: visualizing (along the y-axis of $\mathbb{R}^2$) a converged neural network solution $g_{\theta^*}(x)$, the theoretically optimal $g(x)$, and the optimization objective of the constraint estimator $\hat{C}_k$, $\phi(y) := \sum_{i=1}^{k} \phi_{x_i}(y)$, with $\phi_{x_i}(y) := \exp\{-\lambda^* \|x_i - y\|^2\}/\{k g_{\theta^*}(x_i)\}$, computed from $k = 20$ samples, in the $D = 0.6$ experiment.

high probability) and that $\hat{f}(g^*, \lambda^*)$ gives a valid estimate of a $R(D)$ lower bound. This requirement makes it computationally expensive (if not infeasible) to verify a solution, and indeed poses an open challenge for our method; techniques from global optimization might offer useful tools. We note that in the simple case $\mathcal{X} = \mathcal{Y} = \mathbb{R}^n$ and ρ is the (mean) squared error, maximizing $\phi(y) := \frac{1}{k}\sum_i \psi(x_i, y) + 1 = \alpha \sum_i \alpha_i \exp(-\lambda \|x_i - y\|^2)$ is equivalent to finding the mode of a k-component Gaussian mixture density. Global optimization algorithms for the latter problem exist with (partial) optimality guarantees (Carreira-Perpinan, 2000); e.g., we can run k gradient ascent procedures separately from each of the component modes $x_1, ..., x_k$, and take the largest result.

3 Results

We apply our algorithm to a 2D standard Gaussian source, using mean-squared error as distortion ρ. We parameterize $\log g$ by a two-layer fully connected neural network. During training, we use $k = 100$ for the constraint estimator $\hat{C}_k$, and run a simple gradient ascent procedure in the inner optimization w.r.t. y for computational efficiency. We start with a penalty parameter $\gamma_0 = 1$, and double it every 1000 training steps (which seemed sufficient for convergence). We stop training after 4000 steps, at which point our simple estimate of constraint $\hat{C}_k$ is frequently satisfied across training steps; see Fig. 1 (Left) for example training curves. To certify the resulting solution (g^*, λ^*) as valid, we then compute $\hat{C}_k$ with the global optimization algorithm described in Section 2.4, using a large number of samples ($k = 10000$); in all our experiments, $\hat{C}_{10000}(g^*, \lambda^*) < 0$, so we conclude the solutions are feasible, and $\hat{f}(g^*, \lambda^*)$ gives a valid lower bound of $R(D)$ with very high probability.

We repeat the above with D ranging from 0.02 to 0.8, and plot the corresponding $\hat{R}_L(D) = \hat{f}(g^*, \lambda^*)$ to trace out an $R(D)$ lower bound. As shown in Fig. 1 (Middle), our lower bound shows good agreement with the true $R(D)$, with an average gap of 0.74 bit. Fig. 1 (Right) visualizes the optimization problem for $D = 0.6$, where we take a vertical slice of $\mathbb{R}^2$ and show the learned $g_{\theta^*}(x)$, the theoretically derived optimal $g(x)$ (a scaled Gaussian density), and the $\hat{C}_k$ optimization objective $\phi(y)$ and its component functions $\phi_{x_i}(y)$ centered on $k = 20$ random samples, plugging in the learned $(g_{\theta^*}, \lambda^*)$. Note that the component functions have the form of a Gaussian kernel, whose steepness is controlled by λ. When λ is large or k is small, the resulting $\hat{C}_k = \max_y \phi(y) - 1$ more severely overestimates the true constraint c. With a smaller λ, or by increasing k, the landscape of $\phi(y)$ is more smoothed out, so the overestimating effect is reduced. Indeed, in this figure we see $\max_y \phi(y) > 1.25$; by increasing the sample size k from 20 to 10000, $\max_y \phi(y)$ would decrease to around 0.93 instead (so that $\hat{C}_k \approx -0.07 < 0$), as predicted by Theorem 2.2. In the low distortion (small D) regime, λ is driven to large values, so that $\hat{C}_k$ exhibits higher bias, and constraint violations $\max\{0, \hat{C}_k\}$ are often penalized overly harshly (as $\hat{C}_k$ tends to overestimate c); this likely explains why our lower bound has a larger gap to the true $R(D)$ as we decrease D. We expect the bound can be improved by more accurately estimating the gradient of the penalty/constraint function (we elaborate this point in Appendix Sec. A.3), and/or training with a larger k especially in the lower distortion regime. We provide more experimental details and visualizations in Appendix Sec. A.4.

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A APPENDIX

A.1 FULL VERSION OF THEOREM 2.1

Theorem A.1. *(Kostina, 2016) Suppose that the following basic assumptions are satisfied.*

1. *$R(D)$ is finite for some D, i.e., $D_{min} := \inf\{D : R(D) \leq \infty\} < \infty$;*
2. *The distortion metric ρ is such that there exists a finite set $E \subset \mathcal{Y}$ such that*
$$\mathbb{E}[\min_{y \in E} \rho(X, y)] < \infty$$

Then, for each $D > D_{min}$, it holds that

$$R(D) = \max_{g(x), \lambda} \{\mathbb{E}[-\log g(X)] - \lambda D\} \tag{8}$$

where the maximization is over $g(x) \geq 0$ and $\lambda \geq 0$ satisfying the constraint

$$\mathbb{E}\left[\frac{\exp(-\lambda\rho(X, y))}{g(X)}\right] = \int \frac{\exp(-\lambda\rho(x, y))}{g(x)} dP_X(x) \leq 1, \forall y \in \mathcal{Y} \tag{9}$$

Note: the basic assumption 2 is trivially satisfied when the distortion ρ is bounded from above; the maximization over $g(x) \geq 0$ can be restricted to only $1 \geq g(x) \geq 0$. Unless stated otherwise, we use $\log$ base e in this work, so the $R(D)$ above is in terms of nats.

A.2 PROOF OF THEOREM 2.2

Theorem A.2. *(We restate the theorem for completeness). Let $X_1, X_2, ...$ be a sequence of i.i.d. random variables with the shared data distribution $X_k \sim P_X$. Define the sequence of random variables $C_k := \sup_y \frac{1}{k} \sum_i \psi(X_i, y)$. Then*

1. *$\mathbb{E}[C_k] = \mathbb{E}[\sup_y \frac{1}{k} \sum_i \psi(X_i, y)] \geq \sup_y \mathbb{E}[\psi(X, y)] =: c$;*
2. *$\mathbb{E}[C_1] \geq \mathbb{E}[C_2] \geq ... \geq \mathbb{E}[C_k] \geq \mathbb{E}[C_{k+1}] \geq ... \sup_y \mathbb{E}[\psi(X, y)] = c$;*
3. *If $\psi(x, y)$ is bounded and is continuous in y, and if $\mathcal{Y}$ is compact , then C_k converges to $c = \sup_y \mathbb{E}[\psi(X, y)]$ almost surely (as well as in probability), and we have $\lim_{k\to\infty} \mathbb{E}[C_k] = c$.*

Proof. We prove each in turn:

1. $\mathbb{E}[C_k] = \mathbb{E}[\sup_y \frac{1}{k} \sum_i \psi(X_i, y)] \geq \sup_y \mathbb{E}[\frac{1}{k} \sum_i \psi(X_i, y)] = \sup_y \mathbb{E}[\psi(X, y)] = c$
2. First, note that $\mathbb{E}[C_1] \geq \mathbb{E}[C_k]$ since
$$\mathbb{E}[C_1] = \mathbb{E}[\sup_y \psi(X_1, y)] = \mathbb{E}[\frac{1}{k} \sum_i \sup_y \psi(X_i, y)] \geq \mathbb{E}[\sup_y \frac{1}{k} \sum_i \psi(X_i, y)] = \mathbb{E}[C_k]$$
We therefore have
$$\begin{aligned}
\mathbb{E}[C_{k+1}] &= \mathbb{E}[\sup_y \frac{1}{k+1} \sum_{i=1}^{k+1} \psi(X_i, y)] \\
&= \mathbb{E}[\sup_y \{\frac{1}{k+1} \sum_{i=1}^{k} \psi(X_i, y) + \frac{1}{k+1} \psi(X_{k+1}, y)\}] \\
&\leq \mathbb{E}[\sup_y \{\frac{1}{k+1} \sum_{i=1}^{k} \psi(X_i, y)\} + \sup_y \{\frac{1}{k+1} \psi(X_{k+1}, y)\}] \\
&= \frac{k}{k+1} \mathbb{E}[C_k] + \frac{1}{k+1} \mathbb{E}[C_1] \\
&\leq \mathbb{E}[C_k]
\end{aligned}$$

3. The proof for this resembles that of Theorem 1 in (Burda et al., 2015). We use standard arguments from probability theory and real analysis. Fix $y \in \mathcal{Y}$, and consider the random variable $M_k = \frac{1}{k}\sum_{i=1}^{k} \psi(X_i, y)$. If ψ is bounded, then it follows from the Strong Law of Large Numbers that M_k converges to $\mathbb{E}[M_1] = \mathbb{E}[\psi(X, y)]$ almost surely; in other words, for every ω outside a set of measure zero,

$$\lim_{k\to\infty} \frac{1}{k}\sum_{i=1}^{k} \psi(X_i(\omega)), y) = \mathbb{E}[\psi(X(\omega), y)],$$

Then, for every such ω

$$\lim_{k\to\infty} \sup_y \frac{1}{k}\sum_{i=1}^{k} \psi(X_i(\omega)), y) = \sup_y \lim_{k\to\infty} \frac{1}{k}\sum_{i=1}^{k} \psi(X_i(\omega)), y) = \sup_y \mathbb{E}[\psi(X(\omega), y)],$$

where we used the fact that the sequence of continuous functions $s_k(y) := \frac{1}{k}\sum_{i=1}^{k} \psi(X_i(\omega)), y)$ converges pointwise to $s(y) := \mathbb{E}[\psi(X(\omega), y)]$ on a compact set $\mathcal{Y}$, so s_k converges to s also uniformly, so we are allowed to exchange limit and supremum, i.e., $\lim_{k\to\infty} \sup_y s_k(y) = \sup_y \lim_{k\to\infty} s_k(y) = \sup_y s(y)$. But the above equation precisely means that C_k converges to $c = \sup_y \mathbb{E}[\psi(X, y)]$ almost surely. Therefore C_k also converges to c in probability, and $\lim_{k\to\infty} \mathbb{E}[C_k] = c$.

□

Corollary A.2.1. *Under the conditions of Theorem 2.1, if any pair of non-negative (g, λ) satisfies $\mathbb{E}[C_k] \leq 0$, where $C_k := \sup_y \frac{1}{k}\sum_i \psi(X_i, y) = \sup_y \frac{1}{k}\sum_i \psi(X_i, y)$ and $\psi(x, y) := \frac{\exp(-\lambda\rho(x,y))}{g(x)} - 1$ as before, then for every $D > D_{min}$, it holds that $\mathbb{E}[-\log g_\theta(X)] - \lambda D \leq R(D)$.*

Proof. The feasibility of such (g, λ) trivially follows from the fact that $c \leq \mathbb{E}[C_k] \leq 0$ by Theorem 2.2. The fact that the resulting function $\mathbb{E}[-\log g_\theta(X)] - \lambda D$ underestimates $R(D)$ for *every* $D > D_{\text{min}}$ follows from the variational characterization of $R(D)$ as the upper envelope of tangent linear underestimators (see, e.g., lemma 1.2 of Csiszár (1974)). □

A.3 Proposed Stochastic Optimization Algorithm

Our algorithm aims to find a solution to the following constrained optimization problem:

$$\max_{\theta,\lambda\geq 0} f(\theta, \lambda), \quad \text{where } f(\theta, \lambda) := \mathbb{E}[-\log g_\theta(X)] - \lambda D \tag{10}$$

$$\text{subject to} \quad \mathbb{E}[C_k(\theta, \lambda)] = \mathbb{E}\left[\sup_y \frac{1}{k}\sum_i \frac{\exp(-\lambda\rho(X_i, y))}{g_\theta(X_i)}\right] - 1 \leq 0 \tag{11}$$

which, by Theorem 2.2 and Corollary A.2.1, would guarantee a feasible solution to the original problem and yield a valid lower bound on $R(D)$.

We apply the penalty method and solve the following sequence of unconstrained problems:

$$\max_{\theta,\lambda\geq 0} f(\theta, \lambda) - \gamma_t[\mathbb{E}[C_k(\theta, \lambda)]]^+$$

where we have essentially replaced $c(\theta, \lambda)$ in Eq. 6 by its overestimator $\mathbb{E}[C_k(\theta, \lambda)]$.

We estimate $\mathbb{E}[C_k(\theta, \lambda)]]^+$ by the plug-in estimator:

$$[\mathbb{E}[C_k]]^+ \approx \left[\frac{1}{s}\sum_{j=1}^{s} \hat{C}_k^j\right]^+ = \left[\frac{1}{s}\sum_{j=1}^{s} \sup_y \frac{1}{k}\sum_{i=1}^{k} \psi(x_{s[i]}, y)\right]^+$$

where we draw s mini-batches of data samples, each mini-batch containing k samples. Since computing each $\hat{C}_k$ requires solving a global optimization problem with respect to y, we simply use $s = 1$ for computational efficiency, i.e.,

$$[\mathbb{E}[C_k]]^+ \approx \left[\hat{C}_k\right]^+ = \left[\sup_y \frac{1}{k}\sum_{i=1}^{k} \psi(x_i, y)\right]^+$$

Algorithm 1: Proposed algorithm for estimating rate-distortion lower bound $R_L(D)$.

Requires: Model g_θ (e.g., a neural network), initial parameters $(g_{\theta_0}, \lambda_0)$, initial penalty parameter $\gamma_0 = 1$, batch sizes k, m, gradient ascent step size η, step counter $t = 0$
while *True* **do**
  `// Find a local maximum of` $\hat{\ell}(\theta, \lambda)$ `given the current` γ_t
  while (θ_t, λ_t) *not converged* **do**
    Draw two batches of data samples $\{x_1, ..., x_k\}$ and $\{x_1, ..., x_m\}$
    $y^*, \hat{C}_k =$ `estimate_constraint` $(\theta_t, \lambda_t, \{x_1, ..., x_k\})$
    Update parameters by $(\theta_{t+1}, \lambda_{t+1}) = (\theta_t, \lambda_t) +$
    $\eta \nabla_{(\theta,\lambda)} \left(\frac{1}{m} \sum_{j=1}^{m} -\log g_{\theta_t}(x_j) - \gamma_t \max\{0, \frac{1}{k} \sum_{i=1}^{k} \frac{\exp\{-\lambda_t \rho(x_i, y^*)\}}{g_{\theta_t}(x_i)} - 1\} \right)$
    Update training step counter $t := t + 1$
  end
  $y^*, \hat{C}_k =$ `estimate_constraint_global_opt` $(\theta_t, \lambda_t, \{x_1, ..., x_k\})$
  if $\hat{C}_k \leq 0$ **then**
    `// True constraint` c `is likely satisfied`
    Return solution (θ_t, λ_t), and lower bound estimate $\hat{R}_L = \sum_{j=1}^{m} -\log g_{\theta_t}(x_j)$
  else
    Increase penalty parameter, $\gamma_t := \beta \gamma_t$, with e.g., $\beta = 2$ or 10
  end
end
Subroutine `estimate_constraint` $(\theta, \lambda, \{x_1, ..., x_k\})$:
  Run gradient ascent on $\phi(y) := \sum_{i=1}^{k} \exp\{-\lambda \rho(x_i, y)\} / g_\theta(x_i)$, until converging to y^*
  Compute $\hat{C}_k = \phi(y^*) - 1$
  Return $(y^*, \hat{C}_k)$
Subroutine `estimate_constraint_global_opt` $(\theta, \lambda, \{x_1, ..., x_k\})$:
  Find global maximizer $y^* = \arg\max_y \phi(y)$
  Compute $\hat{C}_k = \phi(y^*) - 1$
  Return $(y^*, \hat{C}_k)$

The sampled loss function of the unconstrained penalty (sub)problem is then

$$\max_{\theta, \lambda \geq 0} \hat{f}_m(\theta, \lambda) - \gamma_t [\hat{C}_k(\theta, \lambda)]^+$$

To apply stochastic gradient ascent, we derive the gradient for each of the two terms with respect to θ (the gradient with respect to λ is similar). The gradient of $\hat{f}$ is simply a sample average:

$$\nabla_\theta \hat{f}_m = \nabla_\theta \left(\frac{1}{m} \sum_{j=1}^{m} -\log g_\theta(x_j) - \lambda D \right) = \frac{1}{m} \sum_{j=1}^{m} -\nabla_\theta \log g_\theta(x_j) - \lambda D$$

The gradient with respect to the penalty term requires more work. First we need to compute $\hat{C}_k$ by solving a global optimization problem, finding a y^* such that

$$\hat{C}_k = \sup_y \frac{1}{k} \sum_{i=1}^{k} \psi_\theta(x_i, y) = \frac{1}{k} \sum_{i=1}^{k} \psi_\theta(x_i, y^*),$$

and then we have

$$\nabla_\theta [\hat{C}_k]^+ = \begin{cases} 0, & \text{if } \hat{C}_k \leq 0 \\ \nabla_\theta \hat{C}_k = \nabla_\theta \frac{1}{k} \sum_{i=1}^{k} \psi_\theta(x_i, y^*) = \frac{1}{k} \sum_{i=1}^{k} \nabla_\theta \psi_\theta(x_i, y^*), & \text{if } \hat{C}_k > 0 \end{cases}$$

where in the case $\hat{C}_k > 0$, we plug in y^* and remove the dependence of the gradient on y by appealing to an envelope theorem (Milgrom & Segal, 2002).

We give a pseudocode implementation of our proposed stochastic optimization procedure in Algorithm 1. We follow a simple exact penalty method (Nocedal & Wright, 2006), but other constrained optimization methods like augmented Lagrangian can also be used instead.

The subroutine `estimate_constraint` in the inner loop is intended as a computationally cheaper alternative to the exact (but expensive) `estimate_constraint_global_opt` procedure, which we reserve for verifying the feasibility of a candidate solution. We give an example implementation of `estimate_constraint` that simply performs a single gradient ascent run on $\phi(y)$ to estimate $\hat{C}_k$ (and its gradient), which proved sufficient for training in our experiments; however, since gradient ascent only gives us a local maximum of $\phi(y)$ in general, this naive implementation of the algorithm may run into convergence issues.

A.4 MORE EXPERIMENTAL DETAILS AND RESULTS

We used a simple 2 layer fully connected network with a scalar output for $\log g$, with 8 hidden units in each layer. We parameterized λ as $\lambda = \exp \tilde{\lambda}$ using an unconstrained variable $\tilde{\lambda}$. We used the Adam optimizer for all gradient based optimization. During training, we set batch size $k = m = 100$, and implement `estimate_constraint` by a single gradient ascent run, initializing y to the data sample in the batch that achieves the highest value of $\phi(\cdot)$ (we find that initializing y to the batch mean $\frac{1}{k}\sum_{i=1}^{k} x_i$ also works well).

We used the (g^*, λ^*) trained after 3500 steps for estimating the final $R(D)$ lower bound. We first verified their feasibility by running the global optimization procedure of Carreira-Perpinan (2000) with $k = 10000$, as assured by the negative values of the resulting $\hat{C}_{10000}$, which were $-0.199, -0.106, -0.254, -0.202, -0.115, -0.068, -0.052$, for $D = 0.02, 0.05, 0.1, 0.2, 0.4, 0.6, 0.8$. Then we compute $\hat{f}_m$ from $m = 10000$ samples, repeat for 10 different batches, and plot the mean $\hat{f}_m$ as the lower bound $\hat{R}_L(D)$ in Figure 1 (Middle), corresponding to the (D, R) points $(0.02, 4.062), (0.05, 3.343), (0.1, 2.424), (0.2, 1.600), (0.4, 0.853), (0.6, 0.432), (0.8, 0.125)$, in terms of (MSE, bits). The standard deviations of $\hat{f}$ from the 10 different batches are between 0.005 and 0.007, so the error bars do not appear noticeable in the figure.

In our problem setting, the optimal $g(x)$ can be found analytically as $g(x) = f_X(x)(2\pi D)^{n/2}$, where $n = 2$ and f_X is the density of the source X (2D standard Gaussian). The Shannon lower bound coincides with the true $R(D)$ (Cover, 1999), giving $R(D) = h(X) - h(D)$, where $h(X), h(D)$ are the differential entropy of X, and an isotropic n-dimensional Gaussian distribution with diagonal covariances equal to D, respectively.

In the next figure, we visualize the evolution of g_θ during training for a few experiments.

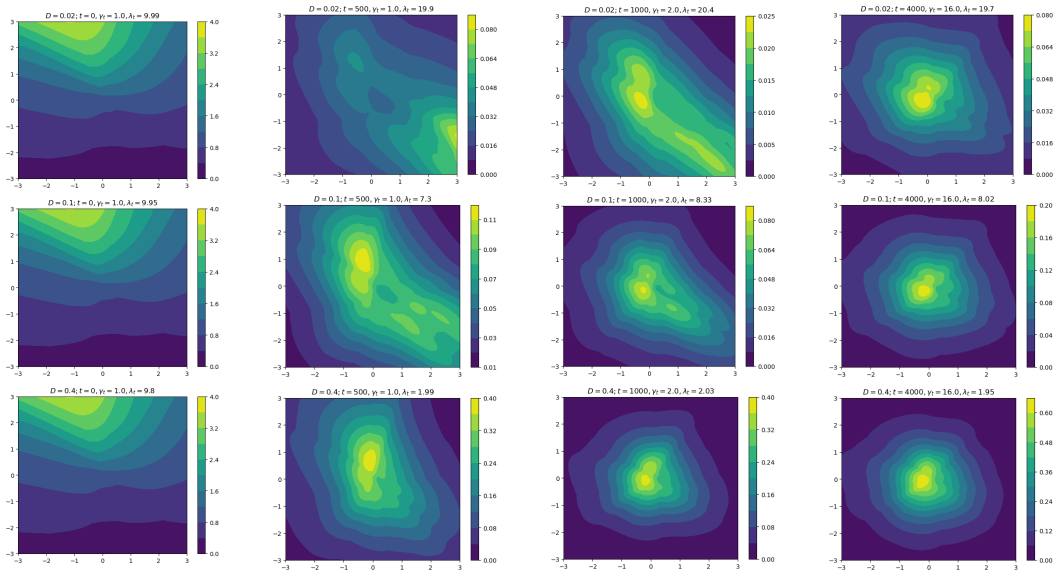

Figure 2: Example contour plots of g_θ during training. The columns correspond to the situation after step 0, 500, 1000, and 4000. Each row corresponds to a different setting of D, with $D = 0.02, 0.1, 0.4$; the training configuration (including initialization) is otherwise kept identical. In each case, the ground truth optimal g is a scaled Gaussian density with spherical contour lines, which attains its maximum value equal to D at the origin. The shape of the learned g_θ generally resembles the ground truth g, but in the lower distortion regime (e.g., when $D = 0.02$), the agreement is worse and g_θ more severely overestimates g.