Abstract

There has recently been a steady increase in the number of iterative approaches to density estimation. However, an accompanying burst of formal convergence guarantees has not followed; all results pay the price of heavy assumptions which are often unrealistic or hard to check. The Generative Adversarial Network (GAN) literature — seemingly orthogonal to the aforementioned pursuit — has had the side effect of a renewed interest in variational divergence minimisation (notably $f$-GAN). We show that by introducing a weak learning assumption (in the sense of the classical boosting framework) we are able to import some recent results from the GAN literature to develop an iterative boosted density estimation algorithm, including formal convergence results with rates, that does not suffer the shortcomings other approaches. We show that the density fit is an exponential family, and as part of our analysis obtain an improved variational characterization of $f$-GAN.

1 Introduction

In the emerging area of Generative Adversarial Networks (GAN’s) [Goodfellow et al., 2014] a binary classifier (called a discriminator in the parlance of the GAN literature) is used learn a highly efficient sampler for a data distribution $P$; combining what would traditionally be two steps — first learning the density function from a family of densities, then fine-tuning a sampler — into one. Interest in this field as sparked a series of formal inquiries and generalisations describing GAN’s in terms of (among other things) divergence minimisation [Nowozin et al., 2016, Arjovsky et al., 2017]. Using a similar framework to Nowozin et al. [2016], Grover and Ermon [2018] make a preliminary analysis of an algorithm that takes a series of iteratively trained discriminators to estimate a density’s function. The cost here, insofar as we have been able to devise, is that one forgoes learning an efficient sampler (as with a GAN), and must make do with classical sampling techniques to sample from the learned density. This we leave the issue of efficient sampling in large dimensions as an open problem, and instead focus on analysing the densities learned with formal convergence guarantees.

The rest of the paper and our contributions are as follows: in §2, to make explicit the connections between classification, density estimation, and divergence minimisation we re-introduce the variational $f$-divergence formulation, and in doing so are able to fully explain some of the underspecified components of $f$-GAN [Nowozin et al., 2016]; in §3, we relax a number of the assumptions of Grover and Ermon [2018], and then give both more...
general, and much stronger bounds for their algorithm; in §4, we apply our algorithm to several toy datasets in order to demonstrate convergence and compare directly with Tolstikhin et al. [2017]; and finally, a final section §5 concludes. The appendices that follow in the supplementary material are: §A, we compare our formal results with other related works; §B, a geometric account of the function class in the variational form of an $f$-divergence; §C, a further relaxation of the weak learning assumptions to some that could actually be estimated experimentally and a proof that the boosting rates are slightly worse but of essentially the same order; §D, proofs for the main formal results from the paper; and finally, §E, technical details for the settings of our experiments.

1.1 Related work

In learning a density — that is minimising a divergence $\min_Q I(P, Q)$ — it is remarkable that most previous approaches [Grover and Ermon, 2018, Guo et al., 2016, Li and Barron, 2000, Miller et al., 2017, Rosset and Segal, 2002, Tolstikhin et al., 2017, Zhang, 2003, and references therein] have investigated a single update rule, not unlike Frank–Wolfe optimisation:

$$Q_{t+1} = f(\alpha_t g(c_t) + (1 - \alpha_t)g(Q_t)),$$

where $g$ is in general (but not always) the identity. Grover and Ermon [2018] is one (recent) rare exception to (1) wherein alternative choices are explored. Few works in this area are accompanied by convergence proofs, and even less display convergence rates, which are mandatory in a boosting setting [Guo et al., 2016, Li and Barron, 2000, Rosset and Segal, 2002, Tolstikhin et al., 2017, Zhang, 2003].

To establish convergence and/or bound convergence by a rate, all approaches necessarily make structural assumptions or approximations on the parameters involved in (1). These can be on the (local) variation of $I$ [Guo et al., 2016, Naito and Eguchi, 2013, Zhang, 2003]; the true density $P$ or the updates $Q_t$ [Grover and Ermon, 2018, Guo et al., 2016, Li and Barron, 2000]; the mixing parameter $\alpha_t$ [Miller et al., 2017, Tolstikhin et al., 2017]; the weak learners $c_t$ [Grover and Ermon, 2018, Rosset and Segal, 2002, Tolstikhin et al., 2017, Zhang, 2003]; the previous updates, $(c_j)_{j \leq t}$ [Rosset and Segal, 2002]; and so on. The price to get the best geometric convergence bounds is in fact heavy considering that the update $c_t$ is in all cases required to be close to the optimal one [Tolstikhin et al., 2017, Corollaries 2, 3].

However, it must be kept in mind that for many of these works [viz. Tolstikhin et al., 2017] the primary objective is to develop an efficient black box sampler for $P$, in particular for large dimensions. Our objective however is to focus on furtive lack of formal results on the densities and convergence, instead leaving the problem of sampling from these densities as an open question.

2 Preliminaries

In the sequel $(X, \tau)$ is a topological space. Unnormalised Borel measures on $X$ are indicated by decorated capital letters, $\tilde{P}$, and Borel probability measures by capital letters without decoration, $P$. To a function $f : X \to (-\infty, +\infty]$ we associate another function $f^*$, called the *Fenchel conjugate* with $f^*(x^*) = \sup_{x \in X} (x^*, x) - f(x)$. If $f$ is convex, proper, and lower semi-continuous, $f = (f^*)^*$. If $f$ is strictly convex and differentiable on $\text{int}(\text{dom} f)$ then $(f^*)' = (f')^{-1}$. Theorem-like formal statements are numbered to be logically consistent with their appearance in the appendix (§D) to which we defer all proofs.

An important tool of ours are the $f$-divergences of information theory [Ali and Silvey, 1966, Csiszár, 1967]. The $f$-divergence of $P$ from $Q$ is

$$I_f(P, Q) = \int f\left(\frac{dP}{dQ}\right) dQ,$$
\[ \int_t^\infty \exp \left( \frac{x}{t} \right) dx = \int_t^\infty \frac{x}{t} \exp \left( \frac{x}{t} \right) dx = \int_t^\infty \frac{dx}{t} \exp \left( \frac{x}{t} \right) \]

where it is assumed that \( f : \mathbb{R} \rightarrow (-\infty, +\infty) \) is convex and lower semi-continuous, and \( Q \) dominates \( P \). Every \( f \)-divergence has a variational representation [Reid and Williamson, 2011] via the Fenchel conjugate:

\[ I_f(P, Q) = \sup_{u \in (\text{dom } f^*)^X} \left( E_P u - E_Q f^* u \right), \tag{2} \]

where the supremum is implicitly over all measurable real functions.

In contrast to the abstract family \((\text{dom } f^*)^X\), machine learning models tend to be specified in terms of density ratios, binary conditional distributions, and binary classifiers, these are respectively:

\[ \mathcal{R}(\mathcal{X}) \doteq \{ d : \mathcal{X} \rightarrow (0, \infty) \}, \quad \mathcal{D}(\mathcal{X}) \doteq \{ D : \mathcal{X} \rightarrow (0, 1) \}, \quad \mathcal{C}(\mathcal{X}) \doteq \{ c : \mathcal{X} \rightarrow \mathbb{R} \}. \]

It is easy to see that these sets are all isomorphic with the commonly used connections

\[ \varphi(D) = \frac{D}{1 - D}, \quad \sigma(c) = \frac{1}{1 + \exp(-c)}, \quad (\varphi \circ \sigma) = \exp, \]

which are illustrated in Figure 2.

It is a common result [Nguyen et al., 2010, Grover and Ermon, 2018, Nowozin et al., 2016] that the supremum in (2) is achieved for \( f^* \circ dP/dQ \). It’s convenient to define the reparameterised variational problem:

\[ \text{maximise} \quad J(u) = E_P f^* u - E_Q f^* f' \circ u \text{ subject to } u \in \mathcal{F}. \tag{V} \]

This reparameterisation can be justified in the case where \( f \) is strictly convex since \( f' \) a bijection.\(^5\)

**Example 1 (Neural Classifier).** When \( d \in \mathcal{R}(\mathcal{X}) \) is modelled using a neural network classifier \( D \in \mathcal{C}(\mathcal{X}) \), \( d \) can be efficiently calculated by substituting the softmax layer with

\[ \exp \left( \frac{c(x)}{1 - \exp(c(x))} \right) = \varphi D(x) = d(x), \]

\(^2\)Common divergence measures such as Kullback–Liebler (KL) and total variation can easily be shown to be members of this family by picking \( f \) accordingly [Reid and Williamson, 2011]. Several examples of these are listed in Table 1.

\(^3\)While it might seem like there are certain inclusions here (for example \( \mathcal{D}(\mathcal{X}) \subseteq \mathcal{R}(\mathcal{X}) \subseteq \mathcal{C}(\mathcal{X}) \)), these categories of functions really are distinct objects when thought of with respect to their corresponding binary classification decision rules (listed in Figure 3).

\(^4\)It is worth noting the selection of isomorphisms here is not unique and can be designed from principles involving loss functions [Reid and Williamson, 2010].

\(^5\)What one may lose with this reparameterisation is convexity—that is, \( J \) is not necessarily convex.

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Table 1: Some common \( f \)-divergences and their variational components.

| \( f \)                  | \( f(t) \) | \( f^*(t^*) \) | \( f'(t) \) | \( (f^* \circ f')(t) \) |
|--------------------------|------------|----------------|-------------|--------------------------|
| Kullback–Liebler KL      | \( t \log t \) | \( \exp(t^* - 1) \) | \( \log t + 1 \) | \( t \) |
| Reverse KL               | \( [t - 1] \) | \( - \log(-t^*) - 1 \) | \( -1/t \) | \( \log t - 1 \) |
| Hellinger                | \( (\sqrt{t} - 1)^2 \) | \( 3(t^* - 1)^4 - 1 \) | \( 1 - 1/t \) | \( \sqrt{t} - 1 \) |
| Pearson                  | \( \chi^2 \) | \( t^* (4 + t^* )/4 \) | \( 2(t - 1) \) | \( 2t^2 \) |
| GAN GAN reparameterised | \( t \log t - (t + 1) \log(t + 1) \) | \( - \log (1 - \exp(t^*)) \) | \( - \log (t) - \log(t + 1) \) | \( \log(1 + t) \) |

Table 3: Classification decision rules.

| Decision rule | \( \mathcal{R}(\mathcal{X}) \) | \( \mathcal{D}(\mathcal{X}) \) | \( \mathcal{C}(\mathcal{X}) \) |
|---------------|-------------------------------|-------------------------------|-----------------------------|
| \( d \geq 1 \) | \( D \geq 1 - D \) | \( c \geq 0 \) |
where \( c(x) \) is the neural network potential at \( x \in \mathcal{X} \). This is just the arrow \( \mathcal{C}(\mathcal{X}) \to \mathcal{R}(\mathcal{X}) \) in Figure 2.

**Example 2** (f-GAN). The GAN objective [Goodfellow et al., 2014] is an example of (V):

\[
\sup_{D \in \mathcal{D}(\mathcal{X})} (E_P \log(D) + E_Q \log(1 - D)) = \sup_{D \in \mathcal{D}(\mathcal{X})} (E_P(f' \circ \varphi) \circ D - E_Q(f' \circ \varphi) \circ D) = \text{GAN}(P, Q),
\]

where the function \( f \) is defined in Table 1 corresponding to the GAN f-divergence. In our derivation it’s clear that (V) together with the isomorphisms in Figure 2 give a simple, principled choice for the “output activation function”, \( g_f \), of Nowozin et al. [2016].

### 3 Boosted density estimation

We fit distributions \( Q_t \) for over the space \( \mathcal{X} \) of the following form

\[
(\forall t \in \mathbb{N}) \quad \text{d}Q_t = \frac{1}{\int \prod_{i=1}^{t} d_{\alpha_i}^* \text{d}Q_0} \prod_{i=1}^{t} d_{\alpha_i}^* \text{d}Q_0, \tag{3}
\]

where \( Q_0 \) is an initial reference distribution, \((\alpha_t)_{t \in \mathbb{N}} \subseteq [0, 1]\) are the step sizes (for reasons that will be clear shortly), and \( d_t : \mathcal{X} \to \mathbb{R}_+ \) are some positive functions. The previous density can be expressed recursively as follows:

\[
\text{d}Q_t = d_{\alpha_t}^* \cdot \text{d}Q_{t-1}, \quad Q_t = \frac{1}{Z_t} \tilde{Q}_t, \quad Z_t = \int \tilde{Q}_t. \tag{4}
\]

**Proposition 2.** The normalisation factors can be written recursively with \( Z_t = Z_{t-1} \cdot E_{Q_{t-1}} d_{\alpha_t}^* \).

**Proposition 3.** Let \( Q_t \) be defined via (3) with a sequence of binary classifiers \( c_1, \ldots, c_t \in \mathcal{C}(\mathcal{X}) \), where \( c_i = \log d_i \) for \( i \in [t] \). Then \( Q_t \) is an exponential family distribution with natural parameter \( \alpha = (\alpha_1, \ldots, \alpha_t) \) and sufficient statistic \( c(x) = (c_1(x), \ldots, c_t(x)) \).

The sufficient statistic of our distributions are classifiers that would hence be learned, along with the appropriate fitting of natural parameters. As explained in the proof, the representation may not be minimal; however, without further constraints on \( \alpha \), the exponential family is regular [Barndorff-Nielsen, 1978]. A similar interpretation of a neural network in terms of parameterising the sufficient statistics of a *deformed exponential family* is given by Nock et al. [2017].

In the remainder of this section, we show how to learn the classifiers from \( c \) and fit the natural parameters \( \alpha \) from (observed) data to ensure a convergence \( Q_t \to P \) that fits to the boosting framework.

#### 3.1 General convergence results of \( Q_t \) to \( P \)

The updates \( d_t \) are chosen by taking the minimiser in (V). To make explicit the dependence of \( Q_t \) on \( \alpha_t \) we will sometimes write \( \text{d}Q_t|_{\alpha_t} = d_{\alpha_t}^* \cdot \text{d}Q_{t-1} \) and \( \text{d}Q_t|_{\alpha_t} = \frac{1}{Z_t} \cdot \text{d}Q_t|_{\alpha_t} \). Since \( Q_t \) is an exponential family (Proposition 3), we measure the divergence between \( P \) and \( Q_t \) using the KL divergence (Table 1), which is the canonical divergence of exponential families [Amari and Nagaoka, 2000]. Notice that we can write any solution to (V) as \( d_t = \text{d}P/\text{d}Q_{t-1} : \varepsilon_t \), where \( \varepsilon_t : \mathcal{X} \to \mathbb{R}_+ \) is called the *error term* due to the fact that it is parameterised by the difference between the constrained solution to (V) and the global solution. A more detailed analysis of the quantity \( \varepsilon_t \) is presented in §B.
**Theorem 5.** For any \( \alpha_t \in [0,1] \), letting \( Q_t, Q_{t-1} \) as in (4), we have:

\[
(\forall d_t \in \mathcal{R}(\mathcal{X})) \quad \text{KL}(P, Q_{t|\alpha_t}) \leq (1 - \alpha_t) \text{KL}(P, Q_{t-1}) + \alpha_t (\log E_P \varepsilon_t - E_P \log \varepsilon_t).
\]

(5)

where \( d_t = \frac{dP}{dQ_{t-1}} \cdot \varepsilon_t \).

We emphasize the fact that Theorem 5 holds for any update \( d_t \), but in fact for all possible functions \( \mathcal{X} \rightarrow \mathbb{R}_+ \), covering all ways — and thus applying to all related algorithms — for computing \( Q_t \) as in (3).

**Remark 3.** Grover and Ermon [2018] assume a uniform error term, \( \varepsilon_t \equiv 1 \). In this case Theorem 5 yields geometric convergence

\[
(\forall \alpha_t \in [0,1]) \quad \text{KL}(P, Q_{t|\alpha_t}) \leq (1 - \alpha_t) \text{KL}(P, Q_{t-1}).
\]

This result is significantly stronger than Grover and Ermon [2018, Theorem 2], who just show the non-increase of the KL divergence. If, in addition to achieving uniform error, we fix in this case \( \alpha_t = 1 \), then (5) guarantees \( Q_{t|\alpha_t=1} \) is immediately equal to \( P \).

We can express the update (3) and (5) in a way that more closely resembles Frank–Wolfe update (1). Since \( \varepsilon_t \) takes on positive values, we can identify it with a density ratio involving a (not necessarily normalised) measure \( \tilde{R}_t \), as follows

\[
d\tilde{R}_t = \varepsilon_t \cdot dP \quad \text{and} \quad R_t = \frac{1}{\int d\tilde{R}_t} \cdot \tilde{R}_t.
\]

(6)

Thus, in the case where \( d_t \) is an inexact solution to the variational problem, the update (4) becomes

\[
dQ_t \propto \left( \frac{dR_t}{dQ_{t-1}} \right)^{\alpha_t} dQ_{t-1} = (dR_t)^{\alpha_t} \cdot (dQ_{t-1})^{1-\alpha_t},
\]

which bears in disguise the Frank–Wolfe type update for iterate \( R_t \). We insist on the fact that this iterate is unknown in general — the parallel with Frank–Wolfe is therefore more superficial than for (1). Introducing \( \tilde{R}_t \) allows us to lend some interpretation to Theorem 5 in terms of the probability measure \( R_t \).

**Corollary 6.** For any \( \alpha_t \in [0,1] \) and \( \varepsilon_t \in [0, +\infty)^{\mathcal{X}} \), letting \( Q_t \) as in (3) and \( R_t \) from (6). If \( R_t \) satisfies

\[
\text{KL}(P, R_t) \leq \gamma \text{KL}(P, Q_{t-1})
\]

for \( \gamma \in [0,1] \), then

\[
\text{KL}(P, Q_{t|\alpha_t}) \leq (1 - \alpha_t(1 - \gamma)) \text{KL}(P, Q_{t-1}).
\]

We obtain the same geometric convergence result as in the best result of Tolstikhin et al. [2017, Corollary 2] for an update \( Q_t \) which is not a convex mixture, which, to our knowledge, is a new result. Corollary 6 is restricted to the KL divergence but we do not need the technical domination assumption of \( Q_t \) with respect to \( P \) that Tolstikhin et al. [2017, Corollary 2] requires. From the standpoint of weak versus strong learning, Tolstikhin et al. [2017, Corollary 2] requires an condition similar to (7) — iterate \( R_t \) has to be close enough to the optimal iterate with respect to \( P \), while we assume that it is close enough to \( P \). We insist on the fact that such assumptions are very strong. It is the objective of the following sections to relax them to a setting compatible with boosting.
The Weak Learning Assumption is in effect a separation condition of \( c_t \) and its decision rule \( \gamma \) originates from \( \mathcal{P} \). We note that classical boosting would rely on a single inequality for the weak learning assumption (involving the two edges) \([Schapire and Singer, 1999]\) instead of two as in our (WLA). The difference is however superficial as we can show that both assumptions are equivalent (Lemma 7 in §D). A boosting algorithm would ensure, for any given error \( \varrho > 0 \), that there exists a number of iterations \( T \) for which we do have \( \text{KL}(P, Q_T) \leq \varrho \), where \( T \) is required to be polynomial in all relevant parameters, in particular \( 1/\gamma_p, 1/\gamma_Q, c_t^*, \text{KL}(P, Q_0) \). Notice that we have to put \( \text{KL}(P, Q_0) \) in the complexity requirement since it can be arbitrarily large compared to the other parameters.

**Theorem 18.** Suppose WLA holds at each iteration. Then using \( Q_t \) as in (3) and \( \alpha_t \) as in §3.2, we are guaranteed that \( \text{KL}(P, Q_T) \leq \varrho \) after a number of iterations \( T \) satisfying:

\[
T \geq 2 \cdot \frac{\text{KL}(P, Q_0) - \varrho}{\gamma_p \gamma_Q}.
\]
There is more to boosting: the question naturally arises as to whether faster convergence is possible. A simple observation allows to conclude that it should require more than just WLA. Define
\[ \mu_{\varepsilon_t} = \frac{1}{c_t} \cdot E_P \log \varepsilon_t, \]
the normalized expected log-density estimation error. Then we have \( \mu_P = (1/c_{\star t}) \cdot \text{KL}(P, Q_{t-1}) + \mu_{\varepsilon_t}, \) so controlling \( \mu_P \) does not give substantial leverage on \( \text{KL}(P, Q_t) \) because of the unknown \( \mu_{\varepsilon_t}. \) We show that an additional weak assumption on \( \mu_{\varepsilon_t} \) is all that is needed with WLA, to obtain convergence rates that compete with Tolstikhin et al. [2017, Lemma 2] but using much weaker assumptions. We call this assumption the Weak Dominance Assumption (WDA).

**Assumption 2 (Weak Dominance Assumption).**
\[ (\exists \Gamma_\varepsilon > 0)(\forall t \geq 1) \quad \mu_{\varepsilon_t} \geq -\Gamma_\varepsilon \quad (\text{WDA}) \]

The assumption WDA takes its name from the observation that we have \( c_t = \log d_t = \log \left( \frac{dP}{dQ_{t-1}} \cdot \varepsilon_t \right) \) and \( |c_t| \leq c_{\star t}, \) so by ensuring that \( \varepsilon_t \) is going to be non-zero \( P \)-almost everywhere, WDA states that nowhere in the support do we have \( Q_t - 1 \) negligible against \( P. \) This also looks like a weak finite form of absolute continuity of \( P \) with respect to \( Q_{t-1}, \) which is not unreminiscent of the boundedness condition on the log-density ratio of Li and Barron [2000, Theorem 1]. Provided WLA and WDA hold, we are able to show geometric boosting convergence rates.

**Theorem 19.** Suppose WLA and WDA hold at each boosting iteration. Then we get after \( T \) boosting iterations:
\[ \text{KL}(P, Q_T) \leq \left( 1 - \frac{\min\{2,\gamma_Q/c_{\star t}\}\gamma_P}{2(1 + \Gamma_\varepsilon)} \right)^T \cdot \text{KL}(P, Q_0). \]

Hence, we get a boosting algorithm which guarantees \( \text{KL}(P, Q_T) \leq \varrho \) after a number of iterations \( T \) which is now logarithmic in relevant parameters: \( T \geq (1/\log K) \cdot \log(\text{KL}(P, Q_0)/\varrho), \) where \( K = 1/(1 - (\min\{2,\gamma_Q/c_{\star t}\}\gamma_P/(2(1 + \Gamma_\varepsilon)))). \)

4 Experiments

Let \( t \in \{0, \ldots, T\}. \) Our experiments take place in \( \mathcal{X} = \mathbb{R}^2, \) where we use a simple neural network classifier \( c_t \in \mathcal{C}^{\mathcal{X}}, \) which we train (in the usual way) using cross entropy error by post composing it with the logistic sigmoid: \( \sigma \circ c_t. \) After training \( c_t \) we transform it into a density ratio using an exponential function: \( d_t = \exp \circ c_t \) (cf. §2) which we use to update \( Q_{t-1}. \)

In most experiments we train for \( T > 1 \) rounds therefore we need to sample from \( Q_{t-1}. \) Our setting here is simple and so this is easily accomplished using random walk Metropolis–Hastings. As noted in the introduction, in more sophisticated domains it remains an open question how to sample effectively from a density of the form (3), in particular for a support having large dimensionality.

Since our classifiers \( c_t \) are the outputs of a neural network they are unbounded, this violates the assumptions of §3, therefore in most cases we use the naive choice \( \alpha_t = 1/2. \)

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\textsuperscript{6}The Julia-language code to run the subsequent experiments is made available at github.com/ZacCranko/BoostedDensities.jl, complete with details about the implementation of kernel density estimation.

\textsuperscript{7}It is easy to pick \( Q_0 \) to be convenient to sample from.
**Metrics** At each $t \in \{0, \ldots, T\}$ we estimate compute $\text{KL}(P, Q_t)$, Negative Log-Likelihood ($\text{NLL}$) $\frac{1}{n} \sum P \log P - Q_t$, and accuracy $E_P \left[ c_t > \frac{1}{2} \right]$. Note that we normalise NLL by its true value to make this quantity more interpretable. The KL divergence is computed using numerical integration, and as such it can be quite tricky to ensure stability when running stochastically varying experiments, and becomes very hard to compute in dimensions higher than $n = 2$. In these computationally difficult cases we use NLL, which is much more stable by comparison. We plot the mean and 95% confidence intervals for these quantities.

### 4.1 Results

Complete details about the experimental procedures including target data and network architectures are deferred to the supplementary material (§E).

#### 4.1.1 Error and convergence

In order to minimise the divergence of $Q_t$ from $P$ we need to train a sufficiently good classifier $c_t$ such that we can build a good approximation to $dP/dQ_{t-1}$. Naturally as $Q_t \rightarrow P$ it should become harder and harder to tell the difference between a sample from $P$ and $Q_t$ with high probability.

This is exactly what we observe. In Figure 5 we train a classifier with the same neural network topology as in §4.1.2. The test accuracy over the course of training before each $t$ is plotted. As $\text{KL}(P, Q_t) \rightarrow 0$ samples from $P$ and $Q_t$ become harder and harder to tell apart and the best accuracy we can achieve over the course of training decreases, approaching $1/2$. Dually, the higher the training accuracy achieved by $c_t$, the greater the reduction from $\text{KL}(P, Q_{t-1})$ to $\text{KL}(P, Q_t)$, thus the decreasing saw-tooth shape in Figure 5 is characteristic of convergence.

#### 4.1.2 Activation functions

To look at the effect of the choice of activation function $a$ we train the same network topology, for a set of activation functions: Numerical results trained to fit a ring of Gaussians are plotted in Figure 7a, contour plots of some of the resulting densities are presented Figure 6. All activation functions except for Softplus performed about the same by the end of six round, with ReLU and SELU being the marginal winners. It is also interesting to note the narrow error ribbons on tanh compared to the other functions indicating more consistent training.

#### 4.1.3 Network topology

To compare the effect of the choice of network architecture we fix activation function and try a variety of combinations of network architecture, varying both the depth and the number nodes per layer. For this experiment the target distribution $P$ is a mixture of 8 Gaussians that are randomly positioned at the beginning of each run of training. Let $m \times n$ denote a fully connected neural network $c_t$ with $m$ hidden layers and $n$ nodes per layer. After each hidden layer we apply the SELU activation function.

Numerical results are plotted in Figure 7b. Interestingly doubling the nodes per layer has little benefit, showing only moderate advantage. By comparison, increasing the network depth allows us to achieve over a 70% reduction in the minimal divergence we are able to achieve.
Figure 6: The effect of different activation functions, modelling a ring of Gaussians. The “petals” in the ReLU condition are likely due to the linear hyperplane sections the final network layer being shaped by the final exponential layer.

Figure 7: KL divergence for a variety of activation functions and architectures over six iterations of boosting.

4.1.4 Convergence across dimensions
For this experiment we vary the dimension $n \in \{2, 4, 6\}$ of the space $X = \mathbb{R}^n$ using a neural classifier $c_t$ that is trained without regard for overfitting and look at the convergence of NLL (Figure 8). After we achieve the optimal NLL of 1, we observe that NLL becomes quite variable as we begin to overfit. Secondly overfitting the likelihood becomes harder as we increase the dimensionality, taking roughly two times the number of iterations to pass NLL = 1 in the $n = 4$ condition as the $n = 2$ condition. We conjecture that not overfitting is a matter of early stopping boosting, in a similar way as it was proven for the consistency of boosting algorithms [Bartlett and Traskin, 2006].

4.1.5 Comparison with kernel density estimation
In this experiment we compare our boosted densities with Kernel Density Estimation (KDE). For this experiment we train a deep neural network with three hidden layers. The step size $\alpha$ is selected to minimise NLL by evaluating the training set at 10 equally spaced points over $[0, 1]$. We compare the resultant density after $T = 2$ rounds with a variety of kernel density estimators, with bandwidth selected via the Scott/Silverman rule.\(^8\)

\(^8\)The Scott and Silverman rules yield identical bandwidth selection criteria in the two-dimensional case.
| Condition  | Mean NLL ±95% CI |
|------------|------------------|
| \(Q_0\)   | 1.5131 ± 0.0459  |
| \(\text{COSINE}\) | 0.7734 ± 0.0112  |
| \(Q_2\)   | 0.8685 ± 0.0946  |
| \(\text{TRIANGULAR}\) | 0.8898 ± 0.0089  |
| \(\text{EXPONENTIAL}\) | 0.9154 ± 0.0088  |
| \(Q_1\)   | 1.0492 ± 0.0437  |
| \(\text{GAUSSIAN}\) | 1.0333 ± 0.0118  |
| \(\text{EPANECHNIKOV}\) | 0.9675 ± 0.0105  |
| \(\text{TOPHAT}\) | 0.9983 ± 0.0117  |

Figure 9: KDE comparison results. The conditions are in decreasing order with respect to the absolute difference of mean NLL and 1.

Results from this experiment are displayed in Figure 9. On average \(Q_1\) fits the target distribution \(P\) better than all but the most efficient kernels, and at \(Q_2\) we begin overfitting, which aligns with the observations made in §4.1.4. We note that his performance is with a model with around 200 parameters, while the kernel estimators each have 2000 — i.e. we achieve KDE’s performances with models whose size is the tenth of KDE’s. Also, in this experiment \(\alpha_t\) is selected to minimise NLL, however it is not hard to imagine that a different selection criteria for \(\alpha_t\) would yield better properties with respect to overfitting.

4.1.6 Comparison with Tolstikhin et al. [2017]

To compare the performance of our model (here called DISCRIM) with AdaGAN we replicate their Gaussian mixture toy experiment, fitting a randomly located eight component isotropic Gaussian mixture where each component has constant variance. These are sampled using the code provided by Tolstikhin et al. [2017].

We compute the coverage metric\(^{10}\) of Tolstikhin et al. [2017]: \(C_\kappa(P, Q) = P(\text{lev}_{> \beta} dQ)\), where \(Q(\text{lev}_{> \beta} dQ) = \kappa\), and \(\kappa \in [0, 1]\). That is, we first find \(\beta\) to determine a set where most of the mass of \(Q\) lies, \(\text{lev}_{> \beta} dQ\), then look at how much of the mass of \(P\) resides there.

Results from the experiment are plotted in Figure 10. Both DISCRIM and AdaGAN converge closely to the true NLL, and then we observe the same characteristic overfitting in previous experiments after iteration 4 (Figure 10a). It is also interesting that this also reveals itself in a degradation of the coverage metric Figure 10b. Notably AdaGAN converges tightly, with NLL centered around its mean, while DISCRIM begins to vary wildly. However the AdaGAN procedure includes a step size that decreases with \(1/t\) — thereby preventing to some extent overfitting with \(t\) —, whereas DISCRIM uses a constant step size \(1/2\). Suggesting that a similarly decreasing procedure for \(\alpha_t\) may have desirable properties.

4.2 Summary

We summarize here some key experimental observations:

- both the activation functions and network topology have a large effect on the ease of training and the quality of the learned density \(Q_T\) with deeper networks with fewer nodes per layer yielding the best results (§4.1.2, §4.1.3).
When the networks $c_t$ are trained long enough we observe overfitting in the resulting densities $Q_T$ and instability in the training procedure after the point of overfitting (§4.1.4 §4.1.5, §4.1.6), indicating that a procedure to take $\alpha_t \to 0$ should be optimal.

We were able to match the performance of kernel density estimation with a naive procedure to select $\alpha_t$. With a better selection procedure we may very well be able to do much better, but this is beyond the scope of our preliminary investigation here (§4.1.5).

We were able to at least match the performance of AdaGAN with respect to density estimation (§4.1.6).

Finally, while we have used KDE as a point of comparison of algorithm, there is no reason why the two techniques could not be combined. Since KDE is a closed form mixture distribution that’s quite easy sampled, there is no reason why one couldn’t build some kind of kernel density distribution and use this for $Q_0$ which one could refine with a neural network.

5 Conclusion

The idea of learning a density in an iterative, “boosting”-type combination of proposal densities has recently met with significant attention. Typically, approaches use a subroutine oracle to fit the coefficients in the combination of densities. In all cases that have significant convergence rates, such an oracle is required to satisfy very strong constraints.

In this paper, we have shown that all it takes to learn a density iteratively in a boosting fashion is a weak learner in the original sense of the Probably Approximately Correct learning model of Kearns [1988], leading to comparable or better convergence bounds than previous approaches at comparatively very reduced price in assumptions. We derive this result through a series of related contributions, including (i) a finer characterization of the solution to the $f$-GAN problem and (ii) a full characterization of the distribution we learn in exponential families.

Experimentally, our approach shows very promising results for an early capture of modes, and significantly outperforms AdaGAN during the early boosting iterations using a comparatively very small architecture. Our experiments leave however open the challenge to obtain a black box sampler for domains with moderate to large dimension. We conjecture that the full characterization that we get of the distribution learned might be of significant help to tackle this challenge.
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A Epilogue

Results in the area of iterative approaches to density estimation, including boosting approaches which are iterative by nature, can be characterized according to three features: how the convergence is characterized, what kind of assumptions it does rely upon and finally, whether it is of direct relevance to current empirical settings for machine learning.

Regarding convergence, there are three kinds of formal results that are traditionally proven. Some are convergence without rates [Grover and Ermon, 2018, Dudık et al., 2004], and others give rates that are negligible with regard to recent results (including ours) [Rosset and Segal, 2002]. In the third and final category are explicit convergence rates. Some of the related approaches have an explicit intractable objective and they rather optimize a tractable surrogate bound. This is the case for variational inference, where the surrogate is the evidence lower-bound [Guo et al., 2016, Khan et al., 2016, Locatello et al., 2017, Miller et al., 2017]. Because of the explicit gap to the intractable optimum, we do not mean to compare such approaches to ours, but can summarize most of the formal results in those papers as showing sublinear convergence, that is, of the form $I(P,Q_T) \leq \inf_Q I(P,Q) + J/T$ for $J > 0$ parameter dependent and $I$ defining a suitable divergence.

In the rest of the related approaches, it is quite remarkable that all of them exploit the same Frank–Wolfe-type update (1) [Li and Barron, 2000, Naito and Eguchi, 2013, Tolstikhin et al., 2017, Zhang, 2003] — even when the connection to Frank–Wolfe is explicit in few of them [Locatello et al., 2017]. Until recently [Tolstikhin et al., 2017], all these other approaches essentially displayed sublinear convergence rates [Li and Barron, 2000, Naito and Eguchi, 2013, Zhang, 2003]. This can be compared to our rates from Theorem 15 and Theorem 18. We compare favorably with them from three standpoints. First, all these algorithms integrate calls to an oracle/subroutine that needs to solve a nested optimization problem for its optimum — the contraint put on our oracle, the weak learner, appears much weaker. Second, all these algorithms integrate parameters whose computation would require the full knowledge of distributions [Naito and Eguchi, 2013, Zhang, 2003] or their parameterized space [Li and Barron, 2000]. It is unclear how approximations would impact convergence [Miller et al., 2017]. In our case, Theorem 18 just operates on estimated parameters, straightforward to compute. Third and last, previous works make more stringent structural assumptions restricting the form of the optimum [Li and Barron, 2000, Naito and Eguchi, 2013, Zhang, 2003], while we just assume that $c^*_t$ is bounded, which puts a constraint — easily enforceable — on the proposals of the weak learner and not on the optimum.

To drill down further in the assumptions required, the very few previous approaches that manage to beat sublinear convergence to reach geometric convergence — that we reach in Theorem 19 — require very strong assumptions, such as the constraint that iterates are close enough to the optimum sought [Tolstikhin et al., 2017, Corollaries 1, 2]. In fact, in this latter work, the parameterization of the weight $\alpha$ in (1) chosen for their experiments implicitly imposes the convergence of iterates to this optimum [Tolstikhin et al., 2017, §4]. In our case, we have shown that equivalent convergence rates can be obtained without boosting (Corollary 6) but with an assumption which is used in [Tolstikhin et al., 2017, Corollary 1, Eq. 10], and is thus very strong. Even when this is not our main result, Corollary 6 is new and interesting in the light of [Tolstikhin et al., 2017]’s results because (i) it does not make use of their convex mixture model and (ii) we do not have the additional technical
requirement that \( P(dQ_{t-1}/dP = 0) < \alpha_t \), that is, roughly the mass where \( dQ_{t-1} = 0 \) is bounded by the leveraging coefficient. Our main result on geometric convergence shows that such convergence is within reach with much weaker assumptions than [Tolstikhin et al., 2017, Corollary 1, Eq. 10], in fact as weak as the weak learning assumption. To get our result, we need an additional assumption on the lower-boundedness of the log-errors \( \varepsilon_t \). For example, via the WDA, but this is still very weak considering that we fit an exponential family and in interesting applications like image processing, \( \mathcal{X} \) is closed so unless \( dP \) is allowed to peak arbitrarily, we essentially get WDA for reasonable \( \Gamma_t \).

Now, why is the assessment of all assumptions important in the light of experimental settings? Because it brings them to a trial by fire, as to whether results survive to experimental machine learning, with available information which is in general a partial estimated snapshot of the theory. It should be clear at this point that, with the sole exception of a subset of variational approaches — which, again, settle for an explicitly tractable surrogate of the objective —, all previous approaches would fail at this test, [Grover and Ermon, 2018, Guo et al., 2016, Li and Barron, 2000, Locatello et al., 2017, Naito and Eguchi, 2013, Tolstikhin et al., 2017, Zhang, 2003]. They would all fail essentially because in practice, we obviously would not have access to \( P \) to test assumptions nor carry out fine-grained optimisation involving \( P \). To our knowledge, our result in §C is the first attempt to provide an algorithm fully executable on current experimental learning settings and whose convergence relies on assumptions that would also easily be testable or enforceable empirically.

We must insist however on the fact that all previous approaches that investigate variational inference or GANs get a black box sampler which may be hard to train but it always easy to sample from, in particular high dimensions [Guo et al., 2016, Khan et al., 2016, Locatello et al., 2017, Miller et al., 2017, Tolstikhin et al., 2017] — this is clearly where the bottleneck of our theory lies currently, even when our experiments display that efficient sampling is available up to moderate dimensions. We conjecture that it is much further scalable.

## B The error term

Recall the reparameterised variational problem from §2

\[
\text{minimize } \quad J(u) = \mathbb{E}_Q f^* \circ f' \circ u - \mathbb{E}_P f' \circ u \quad \text{subject to } \quad u \in \mathcal{F}. \tag{V}
\]

The solution to (V) easily follows when \( \mathcal{F} \) is a large enough set of measurable functions [Nowozin et al., 2016, Nguyen et al., 2010, Grover and Ermon, 2018]. However when \( \mathcal{F} \) is a more constrained class, a stronger result is necessary. Assume \( \mathcal{F} \) is a subset of the normed space, \((\mathcal{F}, | \cdot |)\). Let \( \mathcal{F}^* \) be its continuous dual. The Fréchet normal cone (also called prenormal cone) of \( \mathcal{F} \subseteq \mathcal{F} \) at \( u \in \mathcal{F} \) is

\[
N_{\mathcal{F}}(u) \doteq \left\{ u^* \in \mathcal{F}^* : \limsup_{F \ni v \rightarrow u} \frac{(u^*, v - u)}{|v - u|} \leq 0 \right\}.
\]

When \( \mathcal{F} \) is convex, \( N_{\mathcal{F}}(u) \) is the ordinary normal cone.

**Theorem 1.** Assume \( f : \mathbb{R}_+ \rightarrow \mathbb{R}_+ \) is strictly convex and twice differentiable, and \( \mathcal{F} \) is a normed space of functions \( \mathcal{X} \rightarrow \text{int(dom} f) \). Let \( \mathcal{F} \subseteq \mathcal{F} \) and \( \bar{u} \in \text{arg min}_{u \in \mathcal{F}} J(u) \). If \( J \) is finite on a neighbourhood of \( \bar{u} \), then

\[
\bar{u} \in \frac{dP}{dQ} - N_{\mathcal{F}}(\bar{u}).
\]

If, in addition, \( \mathcal{F} \) is convex with \( dP/dQ \in \text{int} \mathcal{F} \), then \( \bar{u} = dP/dQ \).

**Proof.** Because \( f \) is twice differentiable on \( \text{int(dom} f) \), and \( J \) is finite on a neighbourhood of \( \bar{u} \), \( J \) is Fréchet differentiable at \( \bar{u} \) with

\[
J'(\bar{u}) = \left( (f^*)' \circ f' \circ \bar{u} \right) \cdot \left( f'' \circ \bar{u} \right) \cdot dQ - \left( f'' \circ \bar{u} \right) \cdot dP.
\]

\[
= \bar{u} \cdot \left( f'' \circ \bar{u} \right) \cdot dQ - \left( f'' \circ \bar{u} \right) \cdot dP.
\]
where \((f^*)' = (f')^{-1}\) since \(f\) is strictly convex. By hypothesis \(J\) attains its minimum on \(\mathcal{F}\) at \(\bar{u}\), thus Fermat’s rule [Penot, 2012, Theorem 2.97, p. 170] yields

\[
0 \in J'(\bar{u}) + N_{\mathcal{F}}(\bar{u}) \iff 0 \in \bar{u} \cdot (f'' \circ \bar{u}) \cdot dQ - (f'' \circ \bar{u}) \cdot dP + N_{\mathcal{F}}(\bar{u})
\]

\[
\iff 0 \in \bar{u} \cdot \frac{dP}{dQ} + \frac{1}{(f'' \circ \bar{u}) \cdot dQ} \cdot N_{\mathcal{F}}(\bar{u})
\]

\[
\iff \bar{u} \in \frac{dP}{dQ} - N_{\mathcal{F}}(\bar{u}),
\]

where the final biconditional follows since \(N_{\mathcal{F}}(\bar{u})\) is a cone.

Now, suppose \(\frac{dP}{dQ} \in \text{int} \mathcal{F}\) with \(\mathcal{F}\) convex. Then the Fréchet cone becomes usual normal cone [Penot, 2012, Ex. 6, p. 174],

\[
N_{\mathcal{F}}(\bar{u}) = \{u^* \in \mathcal{F}^* : (\forall v \in \mathcal{F}) \langle u^*, v - \bar{u} \rangle \leq 0\}.
\]

It’s immediate from the definition that \(N_{\mathcal{F}}\) always contains 0. We use a contradiction to show that \(N_{\mathcal{F}}(\bar{u}) \subseteq \{0\}\). Take \(z^* \neq 0 \in N_{\mathcal{F}}(\bar{u})\). Let \(\mathcal{F}_\bar{u} = \mathcal{F} - \bar{u}\). First note that \(\bar{u} \in \text{int} \mathcal{F}\) implies \(0 \in \text{int} \mathcal{F}_\bar{u}\). Thus there is a closed symmetric neighbourhood \(U\) with \(0 \in U \subseteq \text{int} \mathcal{F}_\bar{u}\).

The Hahn–Banach strong separation theorem [Penot, 2012, Theorem 1.79, p. 55] guarantees the existence of a vector \(u \in U\) such that

\[
\langle z^*, u \rangle > 0 \iff (\exists v \in \mathcal{F}) \langle z^*, v - \bar{u} \rangle > 0,
\]

contradicting the assumption \(z^* \in N_{\mathcal{F}}\). Thus \(N_{\mathcal{F}}(dP/dQ) = \{0\}\).

The set \(N_{\mathcal{F}}(\bar{u})\) can be thought of as containing a direction \(v\) that pulls \(dP/dQ\) to the constrained minimiser \(\bar{u}\). This is illustrated in Figure 11.

Figure 11: Illustration of Theorem 1 wherein there exists \(v \in N_{\mathcal{F}}(\bar{u})\) which pulls the unconstrained minimiser, \(\frac{dP}{dQ}\), onto the constrained minimiser, \(\bar{u}\).

Theorem 1 also gives us give a more explicit characterisation of the error term in §3 since

\[
(\exists v_t \in N_{\mathcal{F}}(d_t)) \quad d_t = \frac{dP}{dQ_t} \cdot \varepsilon_t = \frac{dP}{dQ_t} - v_t, \iff \varepsilon_t = 1 - \frac{dQ_t - 1}{dP} \cdot v_t.
\]

C Boosting with estimates

In practice, we do not have access to \(P\) and we rather sample from \(Q\). We thus assume the possibility to sample \(P\) and \(Q\) to compute all needed estimates of \(\mu_P\) and \(\nu_Q\). So let us assume that the weak learner has access to a sampler of \(P\) and a sampler of \(Q\), “SAMPL”. SAMPL takes as input a distribution and a natural \(m\); it samples from the distribution and returns an i.i.d. sample of size \(m\). It does so separately for \(P\) and \(Q\), with separate sizes \(m_P\) and \(m_Q\) for the respective samples. The full Algorithm 2 is very similar to Algorithm 1

\(^{11}\)We could also assume the availability of training samples, in particular for \(P\) as is usually carried out.
that the following holds: at each iteration $m$ with $\alpha$ in the clamped regime for $\nu_{Q_{t-1}}$ and get a classifier $c_t$ that empirically satisfies WLA. Since we still focus on the decrease of $\text{KL}(P,Q)$, one might expect this to weaken our results, which is indeed the case, but we can show that only constants are slightly affected, thereby not changing significantly convergence rates. We provide in one theorem the reframing of both Theorem 15 and Theorem 17. In the same way as we did for Theorem 17, whenever we are in the clamped regime for $\alpha_t$, we let $\delta_{t-1} \geq 0$ be defined from $\tilde{\nu}_{Q_{t-1}} = (1 + \tilde{\delta}_{t-1})\nu_{c_t}$.

**Theorem 23.** Suppose $\text{EWLA}_{\delta,T}$ holds. Then with probability of at least $1 - \delta$, 

$$\forall t = 1, 2, \ldots, T \quad \text{KL}(P,Q_t) \leq \text{KL}(P,Q_{t-1}) - \Delta_t,$$ 

where 

$$\Delta_t = \begin{cases} \frac{\mu_P \log(1+\nu_{Q_{t-1}})}{16} & \text{in the non-clamped regime,} \\ \frac{\mu_P \nu_{c_t}^2}{2} + \nu_{c_t}^2 \left( \frac{1}{4} + \frac{\delta_{t-1}}{1-\nu_{c_t}} \right) & \text{otherwise.} \end{cases}$$

**D Proofs of formal results**

**Proposition 2.** The normalisation factors can be written recursively with $Z_t = Z_{t-1} \cdot E_{Q_{t-1}} d_t^{c_t}$.
Proof. We just need to write
\[
\frac{Z_t}{Z_{t-1}} = \frac{1}{Z_{t-1}} \int d\tilde{Q}_t = \frac{1}{Z_{t-1}} \int d_{t}^{\alpha_i} \tilde{d}Q_{t-1} = \int d_{t}^{\alpha_i} dQ_{t-1} = E_{Q_{t-1}} d_{t}^{\alpha_i}\tag{9}
\]
thus \(Z_t = Z_{t-1} \cdot E_{Q_{t-1}} d_{t}^{\alpha_i}\).

\begin{proposition}
Let \(Q_t\) be defined via (3) with a sequence of binary classifiers \(c_1, \ldots, c_t \in \mathcal{C}(X)\). Then \(Q_t\) is an exponential family distribution with natural parameter \(\alpha = (\alpha_1, \ldots, \alpha_t)\) and sufficient statistic \(c(x) = (c_1(x), \ldots, c_t(x))\).
\end{proposition}

Proof. We can convert the binary classifiers \(c_1, \ldots, c_t \in \mathcal{C}(X)\) to a sequence of density ratios \((d_i)\) using the connections in \(\S2\), which yields
\[
d_{t}^{\alpha_i} = (\varphi \circ \sigma \circ c_i)^{\alpha_i} = \exp(\alpha_i c_i).
\]
In this setting, the multiplicative density at round \(t\) is
\[
dQ_t(x) = \frac{1}{\prod_{i=1}^{t} d_{t}^{\alpha_i}} \prod_{i=1}^{t} d_{t}^{\alpha_i} dQ_t(x)
= \exp \left( \sum_{i=1}^{t} \alpha_i c_i(x) - C(\alpha) \right) dQ_0(x),
\]
with \(\alpha = (\alpha_1, \ldots, \alpha_t)\) and \(C(\alpha) = \log \int \exp (\sum_{i=1}^{t} \alpha_i c_i) dQ_0\), which is an exponential family distribution with natural parameter \(\alpha\), sufficient statistic \(c(x) = (c_1(x), \ldots, c_t(x))\), cumulant function \(C(\alpha)\), reference measure \(Q_0\). We note that in the general case, it may be the case that for some non-all-zero constants \(z_0, z_1, \ldots, z_t \in \mathbb{R}\), we have \(z_0 = \sum_{i=1}^{t} z_i c_i(x)\), that is, the representation is not minimal.

\begin{lemma}
For any \(\alpha_t \in [0, 1]\) and \(\epsilon_t \in [0, +\infty)^X\) we have:
\[
\exp \left( \alpha_t (E_{Q_{t-1}} \log \epsilon_t - r_{KL}(P, Q_{t-1})) \right) \leq \frac{Z_t}{Z_{t-1}} \leq (E_P \epsilon_t)^{\alpha_t}.
\]
\end{lemma}

Proof. Since \(\alpha_t \in [0, 1]\), by Jensen’s inequality it follows that
\[
E_{Q_{t-1}} d_{t}^{\alpha_i} = \left( \int \frac{dP}{dQ_{t-1}} \cdot \epsilon_t dQ_{t-1} \right)^{\alpha_i} = (E_P \epsilon_t)^{\alpha_i}.	ag{10}
\]

The upper bound on \(Z_t/Z_{t-1}\) follows:
\[
\frac{Z_t}{Z_{t-1}} \overset{(9)}{=} E_{Q_{t-1}} d_{t}^{\alpha_i} \overset{(10)}{=} (E_P \epsilon_t)^{\alpha_i}.
\]

For the lower bound on \(Z_t/Z_{t-1}\), note that
\[
\log \left( \frac{Z_t}{Z_{t-1}} \right) \overset{(9)}{=} \log E_{Q_{t-1}} d_{t}^{\alpha_i} \\
\geq \alpha_t E_{Q_{t-1}} \log d_t \\
= \alpha_t E_{Q_{t-1}} \left[ \log \epsilon_t + \log \left( \frac{dP}{dQ_{t-1}} \right) \right],
\]
which implies the lemma.

The error term allows us to bound the KL divergence of \(P\) from \(Q_t\) as follows.
Theorem 5. For any $\alpha_t \in [0, 1]$, letting $Q_t, Q_{t-1}$ as in (4), we have:

\[(\forall d_t \in \mathbb{R}(X)) \quad \text{KL}(P, Q_t|_{\alpha_t}) \leq (1 - \alpha_t) \text{KL}(P, Q_{t-1}) + \alpha_t (\log E_P \varepsilon_t - E_P \log \varepsilon_t). \quad (11)\]

where $d_t = dP/dQ_{t-1} \cdot \varepsilon_t$.

Proof. First note that

\[dQ_t = \frac{1}{Z_t} d\tilde{Q}_t = \frac{1}{Z_t} d\tilde{Q}_{t-1} \frac{1}{Z_t} = \frac{Z_{t-1}}{Z_t} d\tilde{Q}_{t-1}. \quad (12)\]

Now consider the following two identities:

\[\alpha_t \log E_P \varepsilon_t \leq \log \left( \frac{Z_{t-1}}{Z_t} \right), \quad (13)\]

which follows from Lemma 4, and

\[
\int \left( \log \left( \frac{dP}{dQ_{t-1}} \right) - \alpha_t \log d_t \right) dP \\
= \int \left( \log \left( \frac{dP}{dQ_{t-1}} \right) - \alpha_t \log \left( \frac{dP}{dQ_{t-1}} \right) - \alpha_t \log \varepsilon_t \right) dP \\
= (1 - \alpha_t) \int \log \left( \frac{dP}{dQ_{t-1}} \right) dP - \alpha_t \int \log \varepsilon_t dP \\
= (1 - \alpha_t) \text{KL}(P, Q_{t-1}) - \alpha_t E_P \log \varepsilon_t. \quad (14)
\]

Then

\[
\text{KL}(P, Q_t) = \int \log \left( \frac{dP}{dQ_t} \right) dP \\
\overset{(12)}{=} \int \left( \log \left( \frac{dP}{dQ_{t-1}} \right) - \log \left( \frac{Z_{t-1}d\tilde{Q}_t}{Z_t} \right) \right) dP \\
= \int \left( \log \left( \frac{dP}{dQ_{t-1}} \right) - \alpha_t \log d_t \right) dP - \log \left( \frac{Z_{t-1}}{Z_t} \right) \overset{(14)}{=} \overset{(13)}{=}
\leq (1 - \alpha_t) \text{KL}(P, Q_{t-1}) + \alpha_t (\log E_P \varepsilon_t - E_P \log \varepsilon_t),
\]

as claimed. $\blacksquare$

Corollary 6. For any $\alpha_t \in [0, 1]$ and $\varepsilon_t \in [0, +\infty)^X$, letting $Q_t$ as in (3) and $R_t$ from (6). If $R_t$ satisfies

\[\text{KL}(P, R_t) \leq \gamma \text{KL}(P, Q_{t-1}) \]

for $\gamma \in [0, 1]$, then

\[\text{KL}(P, Q_t|_{\alpha_t}) \leq (1 - \alpha_t(1 - \gamma)) \text{KL}(P, Q_{t-1}). \quad (15)\]

Proof. We first show

\[\text{KL}(P, Q_t|_{\alpha_t}) \leq (1 - \alpha_t) \text{KL}(P, Q_{t-1}) + \alpha_t \text{KL}(P, R_t). \quad (16)\]
By definition $\varepsilon_t = dR_t/dP$. The rightmost term in (11) reduces as follows
\[
\log E_P \varepsilon_t - E_P \log \varepsilon_t = \log \int \frac{d\tilde{R}_t}{dP} dP - \int \log \left( \frac{d\tilde{R}_t}{dP} \right) dP \\
= \log \int d\tilde{R}_t + \int \log \left( \frac{dP}{d\tilde{R}_t} \right) dP \\
= \int \log \left( \frac{dP}{d\tilde{R}_t} \right) + \log \int d\tilde{R}_t dP \\
= \int \log \left( \frac{dP}{\int_{\tilde{R}_t} dR_t} \right) dP,
\]
which completes the proof of (16). The proof of (15) is then immediate.  

Define WeakLearn the weak learner which, taking $P$ and $Q_{t-1}$ as input, delivers $c_t$ satisfying the conditions of WLA. In the boosting theory, which involves a supervised learning problem, there is one condition instead of two as in WLA: given a distribution $D$ over $X \times \{-1, +1\}$, we rather require from the weak learner, WeakLearn*, that
\[
(\exists \gamma \in (0, 1]) \frac{1}{c_t^*} E_D y \cdot c_t \geq \gamma,
\]
where $y$ denotes the class, mapping $X \to \{-1, +1\}$. While it seems rather intuitive that we can craft WeakLearn* from WeakLearn, it is perhaps less intuitive as to whether the same can be done for the reverse direction. We now show that it is indeed the case and WLA and WLA* are in fact equivalent.

**Lemma 7.** Suppose $\gamma_P = \gamma_Q = \gamma$ in WLA and WLA*, without loss of generality. Then there exists WeakLearn satisfying WLA iff there exists WeakLearn* satisfying WLA*.

**Proof.** To simplify notations, we suppose without loss of generality that $C(X) \subseteq \{-1, 1\}^X$.

($\Rightarrow$) Let $D$ be a distribution on $X \times \{-1, +1\}$. It can be factored as a triple $(\pi, P, N)$ where $P$ is a distribution over the positive examples, $N$ is a distribution over negative examples and $\pi$ is the mixing probability, $\pi = Pr_D[y = +1]$. Now, feed $P$ and $N$ in lieu of $P$ and $Q_t$, respectively. We get $c_t$ which, from WLA, satisfies $E_N[-c_t] \geq \gamma$ and $E_P[c_t] \geq \gamma$, which implies
\[
E_D[yc_t] = \pi E_P[c_t] + (1 - \pi) E_N[-c_t] \geq \pi \gamma + (1 - \pi) \gamma = \gamma
\]
and we get our weak learner WeakLearn* satisfying WLA*.

($\Leftarrow$) We create a two-class classification problem in which observations from $P$ have positive class $y = +1$, observations from $Q_t$ have negative class $y = -1$ and there is a special observation $x^* \in X$ which is equally present with probability $1 - 2\pi$ in both the positive and negative class. Hence, we are artificially increasing the difficulty of the problem by making its Bayes optimum worse. Obviously, WLA* having to hold under any distribution, it will have to hold under the distribution $D$ that we create. To explicit $D$, consider $\pi \in [0, 1/2]$ and the following sampler for $D$:

- sample $z \in [0, 1]$ uniformly;
  - if $z \leq (1 - 2\pi)/2$ return $(x^*, +1)$;
  - else if $z \leq 1 - 2\pi$ return $(x^*, -1)$;
  - else if $z \leq 1 - \pi$, return $(x \sim P, +1)$;
– else return \((x \sim Q_t, -1)\);

Let \(D\) denote the distribution induced on \(X \times \{-1, +1\}\). Remark that the error of Bayes optimum is at least \(1/2 - \pi\). Let \(c_t\) returned by \textsc{WeakLearn}*. We have because of \textsc{WLA}*,

\[
E_D[yc_t] = \pi(\mu_P + \nu_{Q_{t-1}}) + \left(\frac{1 - 2\pi}{2} - \frac{1 - 2\pi}{2}\right) c_t(x^*) = \pi(\mu_P + \nu_{Q_{t-1}}) \geq \gamma
\]

Consider

\[
\pi = \frac{\gamma}{1 + \gamma}
\]

Which makes

\[
\mu_P + \nu_{Q_{t-1}} \geq 1 + \gamma.
\]

It easily comes that if \(\mu_P < \gamma\), then we must have \(\nu_{Q_{t-1}} > 1\), which is not possible, and similarly if \(\nu_{Q_{t-1}} < \gamma\), then we must have \(\mu_P > 1\), which is also impossible. Therefore we have both \(\mu_P \geq \gamma\) and \(\nu_{Q_{t-1}} \geq \gamma\), and we get our weak learner \textsc{WeakLearn} meeting \textsc{WLA}, as claimed. ■

\section*{D.0.1 Proof of Theorem 15}

The proof of Theorem 15 is achieved in two steps: (i) any \(c_t\) meeting \textsc{WLA} can be transformed through scaling into a classifier that we call \textsc{Properly Scaled} without changing it satisfying \textsc{WLA} (for the same parameters \(\gamma_P, \gamma_Q\)), (ii) Theorem 15 holds for such \textsc{Properly Scaled} classifiers.

\textbf{Definition 4.} The classifier \(c_t\) is said to be \textsc{Properly Scaled (PS)} if it meets:

\[
\exp(2c_t^*) \leq 2 + \mu_P c_t^* \quad \text{(PS.1)}
\]

\[
E_{Q_{t-1}} \exp(c_t) \leq \exp\left(\frac{\mu_P c_t^*}{4}\right). \quad \text{(PS.2)}
\]

Hence, we first show how any classifier meeting \textsc{WLA} can be made \textsc{PS} without changing \(\mu_P\) nor \(\nu_{Q_{t-1}}\) (hence, still meeting \textsc{WLA}), modulo a simple positive scaling. The proof involves a reverse of Jensen’s inequality which is much simpler than previous bounds [Simić, 2009a,b] and of independent interest.

Our proof will equivalently give upper bounds on \(c_t^*\) that make \(c_t\) \textsc{PS}. We note that our proof is constructive, that is, we give eligible upper bounds for \(c_t^*\). The proof of Theorem 12 is split in several lemmata, the first of which is straightforward since \(\mu_P \geq 0\) under \textsc{WLA}.

\textbf{Lemma 8.} Suppose \(c_t\) meets \textsc{WLA}. Then, (PS.1) holds for any \(c_t^* \leq \log(2)/2\).

To prove how to satisfy (PS.2), we use the notions of Bregman divergences and Bregman information. For \(\varphi : \mathbb{R} \to \mathbb{R}\) convex differentiable with derivative \(\varphi'\), we define the Bregman divergence with generator \(\varphi\) as \(D_\varphi(z \| z') = \varphi(z) - \varphi(z') - (z - z')\varphi'(z')\). Following [Banerjee et al., 2005], we define the minimal Bregman information of \((c_t, Q_{t-1})\) (or just Bregman information for short) relative to \(\varphi\) as

\[
I_\varphi(c_t; Q_{t-1}) = E_{Q_{t-1}}[D_\varphi(c_t \| E_{Q_{t-1}} c_t)].
\]

The Bregman information is a generalization of the variance for which \(\varphi(z) = z^2\). Jensen’s inequality would give us a lowerbound, but we need an upperbound. We devise for this objective a reverse of Jensen’s inequality. We suppose that \(c_t\) takes values in \([a, b]\), where we would thus have \(|a|\) or \(|b|\) which would be \(c_t^*\).
Lemma 9. (Reverse of Jensen’s inequality) Suppose \( \varphi \) strictly convex differentiable and \( c_t(x) \in [a, b] \) for all \( x \in X \). Then,
\[
I_{\varphi}(c_t; Q_{t-1}) \leq D_{\varphi}(u \left\| (\varphi^*)'(\frac{\varphi(a) - \varphi(b)}{a-b}) \right\|),
\]
(18)
where \( u \) can be chosen to be \( a \) or \( b \).

Proof. The proof is in fact straightforward, as illustrated in Figure 12.

We now show how to satisfy (PS.2).

Lemma 10. Suppose \( c_t \) meets WLA and
\[
c_t^* \leq \left( \frac{\gamma P}{4} + \frac{1 - \exp(-2\gamma Q)}{2} \right).
\]
Then
\[
E_{Q_{t-1}} \exp(c_t) \leq \exp\left(\frac{\mu P c_t^*}{4}\right),
\]
that is, (PS.2) holds.

Proof. Consider \( \varphi(z) = \exp(z) \) and so \( \varphi^*(z) = z \log z - z \) in Lemma 9. Suppose without loss of generality that \( a = -c_t^*, b = c_t^* \). We get
\[
I_{\exp}(c_t; Q_{t-1}) = E_{Q_{t-1}} \exp(c_t) - \exp E_{Q_{t-1}} c_t
\leq D_{\varphi}(c_t^* \left\| (\varphi^*)'(\frac{\varphi(c_t^*) - \varphi(-c_t^*)}{2c_t^*}) \right\|).
\]
Now, we just need to ensure that
\[ D_{\varphi} \left( c_1 \left\| (\varphi^\ast)' \left( \frac{\varphi(c_1^*) - \varphi(-c_1^*)}{2c_1^*} \right) \right\| \right) \leq \exp \left( \frac{\mu_P c_1^*}{4} \right) - \exp(-\nu_{Q_{i-1}} c_1^*), \] (19)
as indeed we shall then have, because of WLA,
\[ E_{Q_{i-1}} \exp(c_1) \leq \exp \left( \frac{\gamma_P c_1^*}{4} \right) - \exp(-\gamma_Q c_1^*) + \exp E_{Q_{i-1}}, \]
\[ = \exp \left( \frac{\mu_P c_1^*}{4} \right) - \exp(-\nu_{Q_{i-1}} c_1^*) + \exp(-\nu_{Q_{i-1}} c_1^*) \]
\[ = \exp \left( \frac{\mu_P c_1^*}{4} \right) , \]
which is the statement of the lemma.

**Proposition 11.** Pick \( \varphi = \exp \). If \( |z| \leq 2 \), then
\[ D_{\varphi} \left( z \left\| (\varphi^\ast)' \left( \frac{\varphi(z) - \varphi(-z)}{2z} \right) \right\| \right) \leq z^2. \]

**Proof.** Equivalently, we need to show
\[ z^2 \geq \exp(z) \left( \frac{1}{2} - \frac{1}{2z} \right) + \exp(-z) \left( \frac{1}{2} + \frac{1}{2z} \right) \]
\[ + \left( \frac{\exp(z) - \exp(-z)}{2z} \right) \log \left( \frac{\exp(z) - \exp(-z)}{2z} \right). \]
We split the proof in two. First, let us fix
\[ g_1(z) = 2(\exp(z) \left( \frac{1}{2} - \frac{1}{2z} \right) + \exp(-z) \left( \frac{1}{2} + \frac{1}{2z} \right)) \]
\[ = \frac{\exp(-z)(-z^2 - 3z - 3 + \exp(2z)(z^2 - 3z + 3))}{2z^4}. \]
We remark that
\[ g_1'(z) = \frac{\exp(-z)(-z^2 - 3z - 3 + \exp(2z)(z^2 - 3z + 3))}{2z^4}. \]
We then remark that, letting \( g_2(z) = -z^2 - 3z - 3 + \exp(2z)(z^2 - 3z + 3), \)
\[ g_2(z) = \sum_{k \geq 2} \frac{2k^{k+2}}{k!} - \sum_{k \geq 0} \frac{3 \cdot 2k^{k+1}}{k!} + \sum_{k \geq 0} \frac{2 \cdot 2k^k}{k!} \]
\[ = \sum_{k \geq 2} \left( \frac{2k^2}{(k-2)!} - \frac{3 \cdot 2k^{k-1}}{(k-1)!} + \frac{3 \cdot 2^k}{k!} \right) z^k \]
\[ = \sum_{k \geq 5} \left( \frac{2k^2}{(k-2)!} - \frac{3 \cdot 2k^{k-1}}{(k-1)!} + \frac{3 \cdot 2^k}{k!} \right) z^k \]
\[ = \sum_{k \geq 5} \left( k^2 - 7k + 12 \right) \frac{2k^{k-2}}{k!} \cdot \]
We then check that \( z \mapsto z^2 - 7z + 12 < 0 \) only for \( z \in (3, 4). \) That is, it is never negative over naturals so \( g_2(z) \geq 0, \forall z \geq 0. \) We also check that \( \lim_0 g_1'(z) = 0 \) and so \( g_1(z) \) is increasing for \( z \geq 0. \) Finally,
\[ g_1(2) = \frac{1}{2} \cdot \left( \frac{\exp(2)}{4} + \frac{3}{4 \exp(2)} \right) < \frac{7.81}{8} < 1, \]
The analysis for \( z < 1 \) which shows that \( \sum \) completes the proof.

Putting it together with (20), we now have

\[
\text{convex for } z \geq 1
\]

\[
\text{But } \sum_{k \geq 1} \frac{z^k}{k!} \geq 1 + \frac{z^2}{2}
\]

\[
\text{Hence, we want to show that } \exp(z) \leq \exp(-z) + 2z + z^3/2 \text{ for } z \in [-2, 2]. \text{ We now have } \exp(-z) \geq 1 - z + z^2/2 - z^3/6 + z^4/24 - z^5/120 \text{ for } z \geq 0, \text{ so we just need to show } \exp(z) \leq 1 - z + z^2/2 - z^3/6 + z^4/24 - z^5/120 + 2z + z^3/2 = 1 + z + z^2/2 + z^3/3 + z^4/24 - z^5/120 + 2z + z^3/2 \text{ for } z \in [0, 2] \text{ (we will then use the fact that both functions in (21) are even), which simplifies, using Taylor series for } \exp, \text{ in showing}
\]

\[
(\forall z \in [0, 2]) \frac{\sum z^k}{k!} \leq \frac{z^3}{6} - \frac{z^5}{60},
\]

or after dividing both sides by \( z^3 > 0 \) (the inequality is obviously true for \( z = 0 \)),

\[
(\forall z \in (0, 2]) \sum_{k \geq 6} \frac{1}{k(k-1)(k-2)} \frac{z^k-3}{(k-3)!} \leq \frac{8 - z^2}{60}.
\]

Since \( k(k-1)(k-2) \geq 120 \text{ for } k \geq 6 \), it is enough to show that \( \sum_{k \geq 6} \frac{z^{k-3}}{(k-3)!} \leq 20 - 2z^2 \).

But \( \sum_{k \geq 6} \frac{z^k}{(k-3)!} = \sum_{k \geq 3} \frac{z^k}{k!} = \exp(z) - 1 - z - z^2/2 \), so we just need to show that \( \exp(z) \leq 21 + z - 3z^2/2 \text{ for } z \in (0, 2], \) which is easy to show as the rhs is concave, decreasing for \( z \geq 1/3 \) and intersecting \( \exp \) for \( z \geq 5/2 \). So (21) holds. Since \( \log(z) \leq z - 1 \), we get

\[
\frac{\exp(z) - \exp(-z)}{2z} \log \left( \frac{\exp(z) - \exp(-z)}{2z} \right) \leq \frac{z \exp(z) - z \exp(-z)}{8}.
\]

Now, we have \( \exp(z) - \exp(-z) - 4z \leq 0 \text{ for } z \in [0, 2], \) since the function is strictly convex for \( z \geq 0 \) with two roots at \( z = 0 \) and \( z > 2 \). Reorganising, this shows that \( (\exp(z) - z \exp(-z))/8 \leq z^2/2 \text{ for } z \in [0, 2], \) and so

\[
(\forall z \in [0, 2]) \frac{\exp(z) - \exp(-z)}{2z} \log \left( \frac{\exp(z) - \exp(-z)}{2z} \right) \leq \frac{z^2}{2}.
\]

Putting it together with (20), we now have

\[
D_\varphi \left( z \parallel (\varphi^*)' \left( \frac{\varphi(z) - \varphi(-z)}{2z} \right) \right)
= \exp(z) \left( \frac{1}{2} - \frac{1}{2z} \right) + \exp(-z) \left( \frac{1}{2} + \frac{1}{2z} \right)
+ \left( \exp(z) - \exp(-z) \right) \log \left( \frac{\exp(z) - \exp(-z)}{2z} \right)
= \frac{z^2}{2} + z^2
= \frac{z^2}{2}
\]

for \( z \in [0, 2], \) and therefore, since both functions are even, the same holds for \( z \in [-2, 0] \) and completes the proof. □
To show (19), we therefore just need to ensure \( c_t^* \) small enough so that
\[
c_t^* \leq \exp \left( \frac{\mu PC_t^*}{4} \right) - \exp(-\nu_{Q_t-1} c_t^*). \tag{22}
\]
Because \( \exp(-\nu_{Q_t-1} c_t^*) \) is convex, it is upper-bounded over the interval \([0, 2]\) by its chord between its two points in abscissae 0 and 2,
\[
(\forall c_t^* \in [0, 2]) \quad \exp(-\nu_{Q_t-1} c_t^*) \leq 1 - \frac{1 - \exp(-2\nu_{Q_t-1})}{2} c_t^*,
\]
and we also have, since \( \exp(z) \geq 1 + z \),
\[
\exp \left( \frac{\mu PC_t^*}{4} \right) \geq 1 + \frac{\mu PC_t^*}{4}.
\]
To ensure (22), it is therefore sufficient, as long as \( c_t^* \leq 2 \). The maximal value of the rhs in (23), taking into account that \( \gamma_P, \gamma_Q \leq 1 \), is \( 1/4 + (1 - \exp(-2))/2 \approx 0.57 < 2 \), which shows that the condition of Proposition 11 indeed applies and proves Lemma 10.

**Theorem 12.** Suppose \( c_t \) satisfies WLA. Then there exists a constant \( \eta > 0 \) such that \( \eta \cdot c_t \) satisfies WLA and is PS.

**Proof.** Even when better bounds are possible, the combination of Lemma 8 and Lemma 10 show that any \( c_t \) satisfying the WLA, positively scaled so that \( c_t^* \leq \log(2)/2 \), still satisfies WLA and is PS, as claimed.

We shall now prove Theorem 15. The proof mainly consists of two lemmata, one showing that \( E_{Q_t-1} \exp(\alpha_t c_t) \) is small, the second one showing, under conditions on \( c_t \), that \( E_{Q_t-1} \exp(c_t) \) is conveniently upper-bounded by \( E_{Q_t-1} \exp(\alpha_t c_t) \), leading to the theorem.

**Lemma 13.** Let \( \alpha_t = \frac{1}{2c_t^*} \log \left( \frac{1 + \nu_{Q_t-1}}{1 - \nu_{Q_t-1}} \right) \). Then
\[
E_{Q_t-1} \exp(\alpha_t c_t) \leq \sqrt{1 - \nu_{Q_t-1}^2}.
\]

**Proof.** We know [Nock and Nielsen, 2007] that
\[
(\forall a, b \in [-1, 1]) \quad 1 - ab \geq \sqrt{1 - a^2} \exp \left( -\frac{b}{2} \log \left( \frac{1 + a}{1 - a} \right) \right). \tag{24}
\]
Let \( a = \nu_{Q_t-1} \) and \( b = -c_t/c_t^* \), for short. Then we obtain
\[
\begin{align*}
\exp(\alpha_t c_t) &= \exp \left( -\left( -c_t \cdot \frac{1}{2c_t^*} \log \left( \frac{1 + \nu_{Q_t-1}}{1 - \nu_{Q_t-1}} \right) \right) \right) \\
&\leq \frac{1 + \nu_{Q_t-1} c_t^*}{\sqrt{1 - \nu_{Q_t-1}^2}} \\
&= \frac{1 - \nu_{Q_t-1} \cdot \left( -\frac{c_t}{c_t^*} \right)}{\sqrt{1 - \nu_{Q_t-1}^2}}, \tag{25}
\end{align*}
\]
which implies the lemma.
Lemma 14. Fix any $J \geq 0$. Suppose that the two conditions hold:

\[ E_{Q_{t-1}} \exp(c_t) \leq \exp \left( \frac{J}{2} \right) \tag{26} \]

\[ \nu_{Q_{t-1}} \leq \frac{J}{1+J}. \tag{27} \]

Then,

\[ E_{Q_{t-1}} \exp(c_t) \leq \frac{1}{\sqrt{1 - \nu^2_{Q_{t-1}}}} \cdot E_{Q_{t-1}} \exp(\alpha_t c_t + J). \]

Proof. Jensen’s inequality yields

\[ E_{Q_{t-1}} \exp(\alpha_t c_t) \geq \exp(E_{Q_{t-1}} \alpha_t c_t) = \exp(-\alpha_t c_t^t \nu_{Q_{t-1}}), \]

hence we rather show the stronger statement

\[ E_{Q_{t-1}} \exp(c_t) \leq \frac{1}{\sqrt{1 - \nu^2_{Q_{t-1}}}} \cdot \exp(-\alpha_t c_t^t \nu_{Q_{t-1}} + J). \]

We use two inequalities:

\[ (\forall z \in [0, 1]) \quad \frac{2z^2}{1-z} \geq 4 \log \frac{1}{\sqrt{1-z^2}} \geq z \log \left( \frac{1+z}{1-z} \right). \tag{28} \]

Let us summarize these as $A \geq B \geq C$. To first check these inequalities, we remark:

- to check $A \geq B$, we simplify it: it yields equivalently $g_1(z) = z^2(1+z) \geq -(1-z^2) \log(1-z^2) = g_2(z)$. We then check that $g_2'(z) = 2z(1+\log(1-z^2))$ while $g_1'(z) = 2z(1+3z/2)$. Both derivatives are continuous with the same limit in 0 and it is easy to check that for $z \geq 0$, $g_2'(z) \leq g_1'(z)$. Since $g_1(0) = g_2(0)$, we get $A \geq B$;

- to check $B \geq C$, we simplify it, which yields equivalently $g_3(z) = (z-2) \log(1-z) - (z+2) \log(1+z) \geq 0$. We have $g_3'(z) = 4z^2/(z^2-1)^2 \geq 0$, which shows the strict convexity of the function. We also have $g_3'(0) = g_3(0) = 0$, which gives $g_3(z) \geq 0$ for all $z$ and shows $B \geq C$.

With the latter ineq. (28) and the expression of $\alpha_t$ for the regular boosting regime, we get

\[
\frac{1}{\sqrt{1 - \nu^2_{Q_{t-1}}}} \cdot \exp(-\alpha_t c_t^t \nu_{Q_{t-1}} + J)
\]

\[ = \exp \left( J + \log \left( \frac{1}{\sqrt{1 - \nu^2_{Q_{t-1}}}} \right) - \frac{\nu_{Q_{t-1}}}{2} \log \left( \frac{1+\nu_{Q_{t-1}}}{1-\nu_{Q_{t-1}}} \right) \right) \tag{29} \]

\[ \geq \exp \left( J - \frac{\nu_{Q_{t-1}}}{4} \log \left( \frac{1+\nu_{Q_{t-1}}}{1-\nu_{Q_{t-1}}} \right) \right) \]

\[ \geq \exp \left( J - \frac{1}{4} \cdot \frac{2\nu^2_{Q_{t-1}}}{1-\nu_{Q_{t-1}}} \right). \tag{30} \]

The last inequality follows from the former ineq. (28). Suppose now that we can ensure

\[ \frac{2\nu^2_{Q_{t-1}}}{1-\nu_{Q_{t-1}}} \leq 2J. \tag{31} \]
It would follow from (30) that
\[
\frac{1}{\sqrt{1 - \nu_{Q,t-1}^2}} \cdot \exp(-\alpha_t c_t^2 \nu_{Q,t-1} + J) \geq \exp\left(J - \frac{1}{4} \cdot 2J\right) = \exp\left(\frac{J}{2}\right),
\]
and so to prove the lemma, we would just need
\[
E_{Q,t-1} \exp(c_t) \leq \exp\left(\frac{J}{2}\right),
\]
which is precisely (26). To get (31), we equivalently need \(\nu_{Q,t-1}^2 + J \nu_{Q,t-1} - J \leq 0\), that is,
\[
\nu_{Q,t-1} \leq \frac{1}{2} \cdot (-J + \sqrt{J^2 + 4J}) \quad (32)
\]
To prove a simpler equivalent condition, we let \(g_4(z) = (1 + z)\sqrt{z^2 + 4z}/(z(3 + z))\). We easily get \(\lim_{z \to 0} g_4(z) = +\infty\), \(\lim_{z \to \infty} g_4(z) = 1\) and \(g_4'(z) = -6(z + 4)/N\) with \(N = (z^2 + 4z)^{3/2}(3 + z)^2 \geq 0\), so \(g_4(z) \geq 1\) for all \(z \geq 0\), and reordering this inequality yields equivalently \(z/(1 + z) \leq (1/2) \cdot (-z + \sqrt{z^2 + 4z})\) for \(z \geq 0\), so to get (32), we just require \(\nu_{Q,t-1} \leq J/(1 + J)\), which is (27), and ends the proof of Lemma 14.

Let \(\alpha_t = \min\left\{1, \frac{1}{2\pi} \log\left(\frac{1 + \nu_{Q,t-1}}{1 - \nu_{Q,t-1}}\right)\right\}\). Because there are two regimes for \(\alpha_t\), we define two boosting regimes, a high boosting regime, \(\alpha_t = 1\) (“clamped”), and a regular boosting regime, \(\alpha_t < 1\) (“not clamped”). We show two rates of decrease for the KL divergence, one for each regime.

**Convergence in the regular boosting regime**  The WLA alone is sufficient to guarantee a significant decrease of the KL divergence of \(P\) from \(Q_{t-1}\) at each boosting iteration. The proof of the theorem uses a simple reverse of Jensen’s inequality which may be of independent interest. Note that even when we require that \(c_t\) meet WLA, the decrease of the KL divergence uses its actual values for \(\mu_P, \nu_{Q,t-1}\), which can yield a substantially larger KL decrease.

**Theorem 15.** In the regular boosting regime and under WLA,
\[
\text{KL}(P, Q_{t|\alpha_t}) \leq \text{KL}(P, Q_{t-1}) - \frac{\mu_P}{4} \log\left(\frac{1 + \nu_{Q,t-1}}{1 - \nu_{Q,t-1}}\right).
\]

**Proof.** We have
\[
E_P \varepsilon_t = E_{Q,t-1} \left[\frac{dP}{dQ_{t-1}} \cdot \varepsilon_t\right] = E_{Q,t-1} \exp(c_t).
\]
Hence, combining successively the statements of Lemma 14 (we check below that the conditions of the lemma are indeed satisfied) and Lemma 13, we get:
\[
\log E_P \varepsilon_t = \log E_{Q,t-1} \exp(c_t)
\]
\[
\leq \log \left(\frac{1}{\sqrt{1 - \nu_{Q,t-1}^2}} \cdot E_{Q,t-1} \exp(\alpha_t c_t + J)\right)
\]
\[
= \log \left(\frac{E_{Q,t-1} \exp(\alpha_t c_t)}{\sqrt{1 - \nu_{Q,t-1}^2}} \cdot \exp(J)\right)
\]
\[
\leq \log \exp(J)
\]
\[
= J.
\]
On the other hand, WLA yields
\[ \mu P c^* = E_P c_t = E_P \log \left( \frac{dP}{dQ_{t-1}} \cdot \varepsilon_t \right) = \text{KL}(P, Q_{t-1}) + E_P \log \varepsilon_t. \] (36)

Since \( \alpha_t \geq 0 \), it follows from Theorem 5 and (36), (35) in this order that
\[ \text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \alpha_t(\mu P c^* + J) \]
\[ = \text{KL}(P, Q_{t-1}) - \alpha_t(\mu P c^* - J). \] (38)

It remains to fix \( J = \mu P c^*/2 \), and we get
\[ \text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \frac{\alpha_t \mu P c^*}{2} \]
\[ = \text{KL}(P, Q_{t-1}) - \frac{\mu P}{4} \log \left( \frac{1 + \nu_{Q_{t-1}}}{1 - \nu_{Q_{t-1}}} \right), \] (39)

which is the statement of the theorem. We end up the proof of Theorem 15 by showing that the PS property for \( c_t \) implies that the conditions of Lemma 14 are satisfied — hence, Theorem 15 is shown for \( c_t \) being PS, which we recall is always possible from Theorem 12 when \( c_t \) satisfies the WLA. While it is clear that (26) is one of the PS properties for \( c_t \), we still need to show that the PS ensures (27) with \( J = \mu P c^*/2 \), that is, we need to show that
\[ \nu_{Q_{t-1}} \leq \frac{\mu P c^*}{2 + \mu P c^*}. \] (40)

Recall that we are in the regular boosting regime where we do not clamp \( \alpha_t \), and therefore, if we let
\[ \nu_{c_t} = \frac{\exp(2c^*_t) - 1}{\exp(2c^*_t) + 1} \in (0, 1), \] (41)

then we know that \( \nu_{Q_{t-1}} \leq \nu_{c_t} \), so to have (40), it suffices to ensure \( \nu_{c_t} \leq \mu P c^*/(2 + \mu P c^*) \), which equivalently yields
\[ \exp(2c^*_t) \leq 2 + \mu P c^*, \]

which is the first PS property. This ends the proof of Theorem 15. \( \blacksquare \)

**D.0.2 Proof of Theorem 17**

**Convergence in the high boosting regime** This is where things get interesting; when \( \alpha_t \) is clamped to 1, the decrease in the KL divergence at each iteration is *guaranteed* to be of order \( c^*_t \), and can even be significantly larger depending on the actual values of \( \nu_{Q_{t-1}} \) and \( \nu_{c_t} \), defined as
\[ \nu_{c_t} = \frac{\exp(2c^*_t) - 1}{\exp(2c^*_t) + 1} \in (0, 1). \] (42)

Because \( \alpha_t = 1 \), we have \( \nu_{Q_{t-1}} \geq \nu_{c_t} \), so let us write \( \nu_{Q_{t-1}} = (1 + \delta_{t-1})\nu_{c_t} \) for some \( \delta_{t-1} \geq 0 \). Note that Theorem 17 does not assume WLA. It is worthwhile remarking that Theorem 18 is a direct consequence of Theorem 15 above.

We follow some of the same steps as for Theorem 15.
Lemma 16. Let $\alpha_t \equiv 1$. Then
\[
E_{Q_{t-1}} \exp(c_t) \leq \frac{1 - \nu_{Q_{t-1}} \nu_{c_t^*}}{\sqrt{1 - \nu_{c_t^*}^2}},
\]
where $\nu_{c_t^*}$ is defined in (41).

Proof. We have this time $E_{Q_{t-1}} \exp(c_t) = E_{Q_{t-1}} \exp(\alpha_t c_t)$. We use again (24) with $a = \nu_{c_t^*}$ and get, instead of (25):
\[
\exp(\alpha_t c_t) \leq \frac{1 - \nu_{c_t^*} \cdot \left(-\frac{2}{\nu_{c_t^*}^2}\right)}{\sqrt{1 - \nu_{c_t^*}^2}},
\]
which implies the lemma after taking the expectation and remarking that for the choice $a = \nu_{c_t^*}, \alpha_t = 1$. \qed

Theorem 17. In the high boosting regime,
\[
KL(P, Q_t|\alpha_t) \leq KL(P, Q_{t-1}) - \mu P c_t^* - \nu_{c_t^*}^2 \cdot \left(\frac{1}{2} + \frac{\delta_{t-1}}{1 - \nu_{c_t^*}^2}\right).
\]

Proof. Since we get a direct bound on $E_{Q_{t-1}} \exp(c_t)$, we can achieve the proof of Theorem 17 via (33) and (37) as
\[
KL(P, Q_t) \leq KL(P, Q_{t-1}) - \alpha_t(KL(P, Q_{t-1}) + E_P \log \epsilon_t) + \alpha_t \log E_P \epsilon_t
\]
\[
\leq KL(P, Q_{t-1}) - \mu P c_t^* + \log 1 - \frac{\nu_{Q_{t-1}} \nu_{c_t^*}}{\sqrt{1 - \nu_{c_t^*}^2}}
\]
\[
= KL(P, Q_{t-1}) - \mu P c_t^*
\]
\[
+ \log \left(\frac{1 - \nu_{c_t^*}^2}{\sqrt{1 - \nu_{c_t^*}^2}} - (\nu_{Q_{t-1}} - \nu_{c_t^*}) \cdot \frac{\nu_{c_t^*}}{\sqrt{1 - \nu_{c_t^*}^2}}\right)
\]
\[
= KL(P, Q_{t-1}) - \mu P c_t^* + \frac{1}{2} \cdot \log(1 - \nu_{c_t^*}^2)
\]
\[
+ \log \left(1 - (\nu_{Q_{t-1}} - \nu_{c_t^*}) \cdot \frac{\nu_{c_t^*}}{1 - \nu_{c_t^*}}\right)
\]
\[
\leq KL(P, Q_{t-1}) - \mu P c_t^* - \frac{\nu_{c_t^*}^2}{2} - (\nu_{Q_{t-1}} - \nu_{c_t^*}) \cdot \frac{\nu_{c_t^*}}{1 - \nu_{c_t^*}}
\]
\[
\leq KL(P, Q_{t-1}) - \mu P c_t^* - \nu_{c_t^*}^2 \cdot \left(\frac{1}{2} + \frac{\delta_{t-1}}{1 - \nu_{c_t^*}^2}\right),
\]
where we have let $\nu_{Q_{t-1}} = (1 + \delta_{t-1})\nu_{c_t^*}$. In (43), we have used $\log(1 - x) \leq -x$. \qed

I

Theorem 18. Suppose WLA holds at each iteration. Then using $Q_t$ as in (3) and $\alpha_t$ as in §3.2, we are guaranteed that $KL(P, Q_T) \leq \varrho$ after a number of iterations $T$ satisfying:
\[
T \geq 2 \cdot \frac{KL(P, Q_0) - \varrho}{\gamma_P \gamma_Q}.
\]
Proof. The proof stems from the regular boosting regime, using \( \frac{\log((1 + z)/(1 - z))}{2} \geq 2z \) for \( z \geq 0 \). Better rates are possible using the high boosting regime, and in any case, \( Q_t \) as in (3) and \( \alpha_t \) as in §3.2 define a simple boosting algorithm to come up with an analytical expression for \( Q_T \) that provably converges to \( P \). ■

D.1 Proof of Theorem 19

We reformulate the theorem involving a new notation for readability purpose in the proof.

**Theorem 19.** Suppose WLA holds with \( \gamma_Q = \gamma_r \cdot c_t^* \) for some \( \gamma_r > 0 \) and WDA hold at each boosting iteration. Then we get after \( T \) boosting iterations:

\[
\text{KL}(P, Q_T) \leq \left( 1 - \frac{\min\{2, \gamma_r\} \gamma_p}{2(1 + \Gamma_e)} \right)^T \cdot \text{KL}(P, Q_0).
\]

**Proof.** We proceed in two steps, first showing how WDA bounds KL\((P, Q_{t-1})\). We have by definition \( \log(dP/dQ_{t-1}) + \log \varepsilon_t = c_t \leq c_t^* \), and so, taking expectations, we get

\[
\text{KL}(P, Q_{t-1}) \leq c_t^* - c_t^* \mu \varepsilon_t \leq (1 + \Gamma_e) c_t^*.
\]

We now show the statement of the theorem. Suppose we are in the low-boosting regime where \( \alpha_t \) is not clamped. In this case, since \( \log((1 + z)/(1 - z)) \geq 2z \), we have

\[
\alpha_t \geq \frac{\nu_{Q_{t-1}}}{c_t^*} \geq \gamma_r,
\]

and it comes from (39)

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \frac{\gamma_r \gamma_p c_t^*}{2}.
\]

In the high-boosting regime, we have immediately \( \text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \gamma_r c_t^* \). So, letting \( \rho = \min\{1, \gamma_r/2\} \), we get under the assumptions of the theorem \( \text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \rho \gamma_p c_t^* \), and WDA yields in addition through D.1,

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \frac{\rho \gamma_p c_t^*}{1 + \Gamma_e} \cdot \text{KL}(P, Q_{t-1})
\]

\[
= \left( 1 - \frac{\min\{2, \gamma_r/2\} \gamma_p}{2(1 + \Gamma_e)} \right) \cdot \text{KL}(P, Q_{t-1})
\]

and we get the statement of the theorem by replacing \( \gamma_r \) by its expression. This ends the proof of ??.

D.1.1 Proof of Theorem 23

The proof of Theorem 23 is essentially a rewriting of the proof of Theorem 15 and Theorem 17, taking into account that we have just samples from distributions to compute the estimates of edges and WLA. We split the proof in three steps, one that provides an additional Lemma we shall need for the next steps, one for the non-clamped regime for \( \alpha_t \), one for the clamped regime for \( \alpha_t \).

**Step 1.** We need the additional simple Lemma, which is an exploitation of basic concentration inequalities [McDiarmid, 1998, Section 3.1].

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**Lemma 20.** For any $0 < \delta \leq 1$ and $0 < \kappa \leq 1$, suppose the weak learner samples at each iteration $t = 1, 2, \ldots, T$, $m_P$ times $P$ and $m_Q$ times $Q_t$, such that the following constraints hold:

$$m_P \geq \frac{1}{\kappa^2 \gamma P^2} \log \frac{4T}{\delta} \quad \text{and} \quad m_Q \geq \frac{1}{\kappa^2 \gamma Q^2} \log \frac{4T}{\delta}.$$ 

Then there is probability $1 - \delta$ that for any $t = 1, 2, \ldots, T$, the current estimators $\hat{\mu}_P$ of $\mu_P$ and $\hat{\nu}_{Q_{t-1}}$ of $\nu_{Q_{t-1}}$ satisfy:

$$|\hat{\mu}_P - \mu_P| \leq \kappa \gamma_P,$$ \hspace{1cm} (44)

$$|\hat{\nu}_{Q_{t-1}} - \nu_{Q_{t-1}}| \leq \kappa \gamma_Q.$$ \hspace{1cm} (45)

From now on, we denote as $E$ the proposition that both (44) and (45) hold for all $T$ iterations, for some $0 < \kappa \leq 1$ that will be computed later.

We have a slightly weaker version of Lemma 13, straightforward to prove from Lemma 13.

**Lemma 21.** Let $\alpha_t = \frac{1}{2\sigma} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right)$. Then we have under $E$,

$$E_{Q_{t-1}} \exp(\alpha_t c_t) \leq \sqrt{1 - \hat{\nu}_{Q_{t-1}}^2} + \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{\sqrt{1 - \hat{\nu}_{Q_{t-1}}^2}}.$$ 

**Lemma 22.** Fix any $J \geq 0$. Suppose that the two conditions hold:

$$E_{Q_{t-1}} \exp(c_t) \leq \exp \left( \frac{J}{2} \right),$$ \hspace{1cm} (46)

$$\hat{\nu}_{Q_{t-1}} \leq \frac{J}{1 + J}.$$ \hspace{1cm} (47)

Then we have under $E$,

$$E_{Q_{t-1}} \exp(c_t) \leq \frac{1}{\sqrt{1 - \hat{\nu}_{Q_{t-1}}^2}} \cdot E_{Q_{t-1}} \exp(c_t + J) \cdot \exp \left( \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \right).$$

**Proof.** Because the proof mixes the use of $\hat{\nu}_{Q_{t-1}}$ and $\nu_{Q_{t-1}}$, we re-sketch the major lines of the proof from Lemma 14. First, Jensen’s inequality still yields $E_{Q_{t-1}} \exp(\alpha_t c_t) \geq \exp(-\alpha_t c_t^2 \nu_{Q_{t-1}})$, so we in fact prove

$$\frac{1}{\sqrt{1 - \hat{\nu}_{Q_{t-1}}^2}} \cdot \exp(-\alpha_t c_t^2 \nu_{Q_{t-1}} + J) \geq E_{Q_{t-1}} \exp(c_t).$$

The chain of (in)equalities in (29)-(30) now becomes with the use of $E$:

$$\frac{1}{\sqrt{1 - \hat{\nu}_{Q_{t-1}}^2}} \cdot \exp(-\alpha_t c_t^2 \nu_{Q_{t-1}} + J)$$

$$= \exp \left( J + \log \left( \frac{1}{\sqrt{1 - \hat{\nu}_{Q_{t-1}}}} \right) - \frac{\nu_{Q_{t-1}}}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \right)$$

$$\geq \exp \left( J + \log \left( \frac{1}{\sqrt{1 - \hat{\nu}_{Q_{t-1}}}} \right) - \frac{\nu_{Q_{t-1}}}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \right)$$

$$- \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right)$$

$$\geq \exp \left( J - \frac{1}{4} \cdot \frac{2\nu_{Q_{t-1}}^2}{1 - \hat{\nu}_{Q_{t-1}}^2} - \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \right).$$
Provided we have \( \hat{\nu}_{Q_{t-1}} \leq J/(1 + J) \), which is (47), we have similarly to Lemma 14,
\[
\frac{2\hat{\nu}_Q^2}{1 - \hat{\nu}_{Q_{t-1}}} \leq 2J.
\]
Hence, it follows that
\[
\exp \left( \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \right) \cdot \frac{1}{\sqrt{1 - \hat{\nu}_Q^2}} \cdot \exp \left( -\alpha_t c_t^* + J \right) \\
\geq \exp \left( J - \frac{1}{4} \cdot 2J \right) \\
= \exp \left( \frac{J}{2} \right),
\]
and so to prove the lemma, we would just need
\[
E_{Q_{t-1}} \exp(c_t) \leq \exp \left( \frac{J}{2} \right),
\]
which is (46).

Now, instead of (34)–(35), we get
\[
\log E_P \varepsilon_t \leq \log \left( \frac{\nu Q}{1 - \nu^2_{Q_{t-1}}} \cdot E_{Q_{t-1}} \exp(\alpha_t c_t + J) \right) + \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \\
= \log \left( \frac{E_{Q_{t-1}} \exp(\alpha_t c_t) \exp(J)}{\sqrt{1 - \hat{\nu}_Q^2}} \right) + \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \\
\leq \log \left( \frac{1 + \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_Q^2}}{\sqrt{1 - \hat{\nu}_Q^2}} \right) + \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \\
= J + \log \left( 1 + \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_Q^2} \right) + \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right).
\]

We get from (38)
\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \alpha_t (\mu_P c_t^* - J - J')
\]
with, because \( \log(1 + x) \leq x \),
\[
J' = \log \left( 1 + \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_Q^2} \right) + \frac{\kappa \gamma Q}{2} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \\
= \log \left( 1 + \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_Q^2} \right) + \frac{\kappa \gamma Q}{2} \log \left( 1 + \frac{2\hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) \\
\leq \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_Q^2} + \frac{\kappa \gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \\
\leq \kappa \cdot \frac{2\gamma Q \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}}
\]
Now, we would like from the PS property and (40) that we have:
\[
\hat{\nu}_{Q_{t-1}} \leq \frac{\mu_P c_t^*}{2 + \mu_P c_t^*},
\]
so

\[ J' \leq \kappa \gamma Q \mu P \mu_P^*, \]

and we get from (48),

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \alpha_t (1 - \kappa \gamma Q) \mu_P \mu_P^* - J,
\]

and if we fix again \( J = \mu_P \mu_P^* / 2 \), we get this time

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \alpha_t \left( \frac{1}{2} - \kappa \gamma Q \right) \cdot \mu_P \mu_P^*.
\]

If we pick \( \kappa \) satisfying

\[
\kappa \leq \min \left\{ 1, \frac{1}{4 \gamma Q} \right\}, \tag{50}
\]

then we are guaranteed \( 1/2 - \kappa \gamma Q \geq 1/4 \) and so

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \frac{\hat{\mu}_P}{8} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right), \tag{51}
\]

In the same way as for Theorem 15, we ensure (49) by noting that, since we are in the case where we do not clamp \( \alpha_t \), letting

\[
\hat{\mu}_P^* = \frac{\exp(2c_t^*) - 1}{\exp(2c_t^*) + 1} \in (0, 1),
\]

then we again need to ensure \( \nu_{c_t^*} \leq \mu_P c_t^*/(2 + \mu_P c_t^*) \), which again yields to the first PS property.

We are not yet done as we now have to replace \( \mu_P \) by its estimate, \( \hat{\mu}_P \), in (51). Under \( E \), we obtain

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \frac{\hat{\mu}_P - \kappa \gamma P}{8} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right),
\]

and under the (EWLA), we know that \( \hat{\mu}_P \geq \gamma P \), so if we also put the constraint \( \kappa \leq 1/2 \), then \( \kappa \gamma P \leq \gamma P / 2 \leq \hat{\mu}_P / 2 \) and so:

\[
\text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \frac{\hat{\mu}_P}{16} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right),
\]

as claimed. This ends the proof of Step.2 by remarking two additional facts: (i) we have not changed the PS properties, and (ii) we have two constraints over \( \kappa \) (also considering (50)), which can be both satisfied by choosing (since \( \gamma Q \leq 1 \)) \( \kappa \) satisfying

\[
\kappa \leq \frac{1}{4}. \tag{52}
\]

**Theorem 23.** Suppose EWLA\(_{\delta,T}\) holds. Then with probability of at least \( 1 - \delta \),

\[
(\forall t = 1, 2, ..., T) \quad \text{KL}(P, Q_t) \leq \text{KL}(P, Q_{t-1}) - \Delta_t,
\]

where

\[
\Delta_t = \begin{cases} 
\frac{\hat{\mu}_P}{16} \log \left( \frac{1 + \hat{\nu}_{Q_{t-1}}}{1 - \hat{\nu}_{Q_{t-1}}} \right) & \text{in the non-clamped regime,} \\
\frac{\hat{\mu}_P c_t^*}{2} + \nu_{c_t^*} \cdot \left( \frac{1}{4} + \frac{\hat{\delta}_{t-1}}{1 - \nu_{c_t^*}} \right) & \text{otherwise.}
\end{cases}
\]

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\textbf{Proof.} We proceed in exactly the same way as we did for Theorem 17. We first remark that Lemma 21 is still valid in this case, so that we still have
\[ E_{Q_{t-1}} \exp(c_t) \leq \frac{1 - \nu_{Q_{t-1}} \nu_{c_t}}{\sqrt{1 - \nu_{c_t}^2}}. \]
It is not hard to check that we then keep the exact same derivations as for Theorem 17, yielding
\[ KL(P, Q_t) \leq KL(P, Q_{t-1}) - \mu_P c_t^* - \nu_{c_t}^2 \cdot \left( \frac{1}{2} + \frac{\delta_{t-1}}{1 - \nu_{c_t}^2} \right), \]
where we have let \( \nu_{Q_{t-1}} = (1 + \delta_{t-1})\nu_{c_t^*} \). Remark that this time, \( \delta_{t-1} \) is not necessarily positive since we do not have access to \( \nu_{Q_{t-1}} \) — this may happen when \( \nu_{Q_{t-1}} < \nu_{Q_{t-1}}^\star \). What we do, to finish up Step.3, is replace \( \delta_{t-1} \) by the \( \delta_{t-1}^\star \) for which we have \( \nu_{Q_{t-1}}^\star = (1 + \delta_{t-1})\nu_{c_t^*} \), which we are then sure is going to satisfy \( \delta_{t-1}^\star \geq 0 \) under the clamped regime for \( \alpha_t \). Under \( E \), we have
\[ \delta_{t-1} = \frac{\nu_{Q_{t-1}}}{\nu_{c_t}} - 1 \]
\[ \geq \frac{\nu_{Q_{t-1}}^\star}{\nu_{c_t}} - 1 - \kappa \cdot \frac{\gamma_Q}{\nu_{c_t}^2} \]
\[ = \delta_{t-1}^\star - \kappa \cdot \frac{\gamma_Q}{\nu_{c_t}^2} \]
yielding
\[ KL(P, Q_t) \leq KL(P, Q_{t-1}) - \mu_P c_t^* - \nu_{c_t}^2 \cdot \left( \frac{1}{2} \kappa \gamma_Q \left( 1 - \frac{\nu_{c_t}^2}{\nu_{c_t}^2} \right) + \frac{\delta_{t-1}^\star}{1 - \nu_{c_t}^2} \right). \]
Suppose we pick \( \kappa \) such that
\[ \kappa \leq \frac{\nu_{c_t}^2(1 - \nu_{c_t})}{2}, \quad (53) \]
Since \( \nu_{c_t} \in [0, 1] \), we also have
\[ \kappa \leq \frac{\nu_{c_t}^2(1 - \nu_{c_t}^2)}{2}. \]
In this case, we obtain, since \( \gamma_Q \leq 1 \),
\[ KL(P, Q_t) \leq KL(P, Q_{t-1}) - \mu_P c_t^* - \nu_{c_t}^2 \cdot \left( \frac{1}{2} + \frac{\delta_{t-1}^\star}{1 - \nu_{c_t}^2} \right). \]
Finally, we also know under \( E \) that \( \mu_P c_t^* \geq \hat{\mu}_P c_t^* - \kappa \gamma_P c_t^* \). Under the (EWLA), we know that \( \hat{\mu}_P \geq \gamma_P \), so if we again put the constraint \( \kappa \leq 1/2 \) (satisfied from (52)), then \( \kappa \gamma_P c_t^* \leq \gamma_P c_t^*/2 \leq \hat{\mu}_P c_t^*/2 \) and so:
\[ KL(P, Q_t) \leq KL(P, Q_{t-1}) - \frac{\hat{\mu}_P c_t^*}{2} - \nu_{c_t}^2 \cdot \left( \frac{1}{4} + \frac{\delta_{t-1}^\star}{1 - \nu_{c_t}^2} \right), \]
which ends the proof of Step.3 once we remark that (52) and (53) are both satisfied if
\[ \kappa = \min \left\{ \frac{1}{4}, \frac{\nu_{c_t}^2(1 - \nu_{c_t})}{2} \right\} = \frac{\nu_{c_t}^2(1 - \nu_{c_t})}{2} = \kappa^*. \]
E Experimental procedure

All models were trained using the ADAM optimiser with the default settings from Flux.jl [Innes, 2018]: \( \eta = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \varepsilon = 1e-08 \). In all experiments we divide the data into training (75\%) and test (25\%) sets, which we use to early stop on certain experiments. The reset of the experimental conditions are presented in Table 13. Each experiment was run 20 times.
| Experiment | $P$ | $Q_0$ | $\alpha_t$ | Sample size ($P,Q$) | Epochs | Batch size | Early stop$^a$ | Network topolgy of $c_t$ |
|------------|-----|-------|-------------|----------------------|--------|-----------|---------------|------------------|
| §4.1.1, §4.1.2 | 8 mode Gaussian ring mixture $\sigma = 1$ | Isotropic Gaussian $\sigma = 1$ | 1/2 | (1000,1000) | 3000 | 50 | Not used | $\mathcal{X}$ ReLU dense $\rightarrow$ $\mathbb{R}$ 5 ReLU dense $\rightarrow$ $\mathbb{R}$ |
| §4.1.3 | 8 mode Gaussian ring mixture $\sigma = 1$ | Isotropic Gaussian $\sigma = 1$ | 1/2 | (1000,1000) | 3000 | 50 | Not used | varies |
| §4.1.4 | randomly arranged 8 mode Gaussian mixture | Isotropic Gaussian $\sigma = 1$ | 1/2 | (1000,1000) | 2000 | 250 | 20% | $\mathcal{X}$ ReLU dense $\rightarrow$ $\mathbb{R}$ 10 ReLU dense $\rightarrow$ $\mathbb{R}$ 10 ReLU dense $\rightarrow$ $\mathbb{R}$ |
| §4.1.5 | randomly arranged 8 mode Gaussian mixture | Empirically fit Gaussian | Selected to minimise NLL | (1000,1000) | 3000 | 50 | Not used | $\mathcal{X}$ ReLU dense $\rightarrow$ $\mathbb{R}$ 10 ReLU dense $\rightarrow$ $\mathbb{R}$ 10 ReLU dense $\rightarrow$ $\mathbb{R}$ |
| §4.1.6 | Adagan generated randomly arranged 8 mode Gaussian mixture | Empirically fit Gaussian | Selected to minimise NLL | (5000,5000)$^b$ | 1000 | 250 | 3% | $\mathcal{X}$ ReLU dense $\rightarrow$ $\mathbb{R}$ 10 ReLU dense $\rightarrow$ $\mathbb{R}$ 10 ReLU dense $\rightarrow$ $\mathbb{R}$ |

$^a$This parameter terminates training when the test error falls this amount below the training error. Useful to stabilise training that might otherwise fail due to exploding test error.

$^b$Adagan trains on a set of (64000,64000) samples, we take a subset of these to use for training $Q_t$.

Table 13: Experimental procedure