Boosted Generative Models

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Abstract

We propose a new approach for using unsupervised boosting to create an ensemble of generative models, where models are trained in sequence to correct earlier mistakes. Our meta-algorithmic framework can leverage any existing base learner that permits likelihood evaluation, including recent latent variable models. Further, our approach allows the ensemble to include discriminative models trained to distinguish real data from model-generated data. We show theoretical conditions under which incorporating a new model in the ensemble will improve the fit and empirically demonstrate the effectiveness of boosting on density estimation and sample generation on synthetic and benchmark real datasets.

1. Introduction

Many of the recent successful applications of machine learning in computer vision, speech recognition, and natural language processing are based on discriminative models. Learning generative models has proven to be much more difficult. A variety of deep generative architectures have recently shown promising results in a range of tasks. These include fully-visible belief networks such as PixelRNN (Oord et al., 2016), latent variable models such as variational autoencoders (Kingma & Welling, 2014), and implicit density models such as generative adversarial networks (Goodfellow et al., 2014). Despite significant progress, existing generative models cannot fit complex distributions with a sufficiently high degree of accuracy, limiting their applicability.

In this paper, we propose a technique for ensembling (imperfect) generative models to improve their overall performance. Our meta-algorithm is inspired by boosting, a technique used in supervised learning to combine weak classifiers (e.g., decision stumps or trees), which individually might not perform well on a given classification task, into a more powerful ensemble. The boosting algorithm will attempt to learn a classifier to correct for the mistakes made, and repeat this procedure recursively. Under some conditions on the weak classifiers’ effectiveness, the boosting meta-algorithm can drive the (training) error to zero (Freund et al., 1999). Boosting can also be thought as a feature learning algorithm, where at each round a new feature is learned by training a classifier on a reweighted version of the original dataset. In practice, algorithms based on boosting perform extremely well in machine learning competitions (Caruana & Niculescu-Mizil, 2006).

We show that a similar procedure can be applied to generative models. Given an initial generative model that provides an imperfect fit to the data distribution, we construct a second model to correct for the error, and repeat recursively. The second model is also a generative one, which is trained on a reweighted version of the original training set. Our meta-algorithm is general and can construct ensembles of any existing generative model that permits (approximate) likelihood evaluation such as fully-visible belief networks and variational autoencoders. Interestingly, our method can also leverage discriminative models, which have been shown to perform extremely well in practice (Krizhevsky et al., 2012; LeCun et al., 2015). Specifically, we train a binary classifier to distinguish true data samples from “fake” ones generated by the current model and provide a principled way to include this discriminator in the ensemble.

A prior attempt at boosting density estimation by Rosset & Segal (2002) proposed a sum-of-experts formulation. We show theoretically the limitations of additive approaches in learning complex distributions, and instead propose to use multiplicative boosting or equivalently a product-of-experts formulation. Building on our core unsupervised boosting formulation, this paper makes the following contributions:

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1. We provide theoretical conditions under which incorporating a new model is guaranteed to improve the ensemble fit, eventually recovering the true distribution.

2. We design and analyze a flexible meta-algorithmic boosting framework for including both generative and discriminative models in the ensemble.

3. We provide an algorithm for boosting normalizing flow models that permits exact and efficient likelihood evaluation and sampling.

4. We empirically demonstrate the superior performance of boosted generative models over baseline models on density estimation and sample generation on mixture of Gaussians, MNIST, and CIFAR-10 datasets.

2. Unsupervised boosting

Supervised boosting provides an algorithmic formalization of the hypothesis that a sequence of weak learners can create a single strong learner (Schapire & Freund, 2012). Here, we propose a framework that extends boosting to unsupervised settings for learning generative models. For ease of presentation, all distributions are w.r.t. any arbitrary $x \in \mathbb{R}^d$, unless otherwise specified. We use upper-case symbols to denote probability distributions and assume they all admit absolutely continuous densities (denoted by the corresponding lower-case notation) on a reference measure $dx$. Our analysis naturally extends to discrete distributions, which we skip for brevity. Please refer to Appendix A for the proofs of all results in the following two sections.

Formally, we consider the following maximum likelihood estimation (MLE) setting. Given some data points $X = \{x_i \in \mathbb{R}^d\}_{i=1}^m$ sampled i.i.d. from an unknown distribution $P$, we provide a model class $Q$ parameterizing the distributions that can be represented by the generative model and minimize the Kullback-Liebler (KL) divergence w.r.t. the true distribution,

$$\min_{Q \in \mathcal{Q}} D_{KL}(P || Q). \quad (1)$$

In practice, we only observe samples from $P$ and hence, maximize the log-likelihood of the observed data $X$. Selecting the model class for maximum likelihood learning is non-trivial; the maximum likelihood estimate w.r.t. a small class can be very far from the true distribution, whereas a large class poses the risk of overfitting in the absence of sufficient data, or even underfitting due to difficulty in optimizing non-convex objectives that frequently arise due to the use of latent variable models, neural networks, etc.

The boosting intuition is to greedily increase model capacity by learning a sequence of weak intermediate models $\{h_t \in \mathcal{H}_t\}_{t=0}^T$ that are able to correct for mistakes made by previous models in the ensemble. Here, $\mathcal{H}_t$ is again some predefined model class (such as $\mathcal{Q}$) for $h_t$. We defer the algorithmic questions pertaining to the learning of such intermediate models to the next section, and first discuss two possible ways in which the individual density estimates at each round can be combined to derive the final estimate $q_T$.

2.1. Additive boosting

Similar to supervised boosting, the intermediate models $\{h_t\}_{t=0}^T$ can be combined by taking an arithmetic average,

$$q_T = \sum_{t=0}^{T} \alpha_t \cdot h_t$$

where $0 \leq \alpha_t \leq 1$ denote the weights assigned to the intermediate models. The weights are re-normalized at every round to sum to 1 which gives us a valid probability density estimate. We can express the density estimate after a given round of boosting recursively as,

$$q_t = (1 - \hat{\alpha}_t) \cdot q_{t-1} + \hat{\alpha}_t \cdot h_t$$

where $\hat{\alpha}_t$ denotes the normalized weight for $h_t$ at round $t$. The base model $h_0$ is learned using MLE. We now derive conditions on the intermediate models that allow us to make “progress” in every round of boosting.
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Theorem 1. Let $\delta_{KL}^t(h_t, \hat{\alpha}_t) = D_{KL}(P\|Q_{t-1}) - D_{KL}(P\|Q_t)$ denote the reduction in KL-divergence at the $t$th round of additive boosting. The following conditions hold:

1. Sufficient: If $\mathbb{E}_P \left[ \log \frac{h_t}{\tilde{q}_{t-1}} \right] \geq 0$, then $\delta_{KL}^t(h_t, \hat{\alpha}_t) \geq 0$ for all $0 \leq \hat{\alpha}_t \leq 1$.

2. Necessary: If there exists $0 < \hat{\alpha}_t \leq 1$ such that $\delta_{KL}^t(h_t, \hat{\alpha}_t) \geq 0$, then $\mathbb{E}_P \left[ \log \frac{h_t}{\tilde{q}_{t-1}} \right] \geq 1$.

The sufficient and necessary conditions require that the expected log-likelihood and likelihood respectively of the current intermediate model, $h_t$, are better-or-equal than those of the combined previous model, $q_{t-1}$ under the true distribution when compared using density ratios. Learning such an intermediate model at every round is algorithmically difficult and furthermore, counterintuitive to the boosting paradigm which combines the strength of weak intermediate learners. Next, we consider an alternative formulation that uses multiplicative boosting to ease the requirements for learning good intermediate models.

2.2. Multiplicative boosting

In multiplicative boosting, we factorize the final density estimate as a geometric average of $T + 1$ intermediate models $\{h_t\}_{t=0}^T$, each assigned an exponentiated weight $\alpha_t$,

$$q_T = \frac{\prod_{t=0}^T h_t^{\alpha_t}}{Z_T}$$

where the partition function $Z_T = \int \prod_{t=0}^T h_t^{\alpha_t} \, dx$. The density estimate can be recursively expressed as,

$$\tilde{q}_t = h_t^{\alpha_t} \cdot \tilde{q}_{t-1}$$  \hspace{1cm} (2)

where $\tilde{q}_t$ is the unnormalized estimate (at round $t$). The base model $h_0$ is learned using MLE. The corresponding conditions on the intermediate models for reducing KL-divergence at every round are stated below.

Theorem 2. Let $\delta_{KL}^t(h_t, \alpha_t) = D_{KL}(P\|Q_{t-1}) - D_{KL}(P\|Q_t)$ denote the reduction in KL-divergence at the $t$th round of multiplicative boosting. The following conditions hold:

1. Sufficient: If $\mathbb{E}_P[\log h_t] \geq \log \mathbb{E}_{Q_{t-1}}[h_t]$, then $\delta_{KL}^t(h_t, \alpha_t) \geq 0$ for all $0 \leq \alpha_t \leq 1$.

2. Necessary: If there exists $0 < \hat{\alpha}_t \leq 1$ such that $\delta_{KL}^t(h_t, \hat{\alpha}_t) \geq 0$, then $\mathbb{E}_P[\log h_t] \geq \mathbb{E}_{Q_{t-1}}[\log h_t]$.

In contrast to additive boosting, the conditions above compare expectations under the true distribution with expectations under the model distribution in the previous round, $Q_{t-1}$. The equality in the conditions holds for $\alpha_t = 0$, which corresponds to the trivial case where the current intermediate model is ignored in Eq. (2). For other valid $\alpha_t$, the non-degenerate version of the sufficient inequality guarantees progress towards the true data distribution. Note that the intermediate models increase the overall capacity of the ensemble at every round.

From the necessary condition, we see that a “good” intermediate model $h_t$ necessarily assigns a better-or-equal log-likelihood under the true distribution as opposed to the model distribution in the previous round, $Q_{t-1}$. This condition suggests two learning objectives for intermediate models which we discuss next.

3. Boosted generative models

In this section, we design and analyze meta-algorithms for multiplicative boosting of generative models. Given a base model $h_0$ which permits (approximate) likelihood evaluation, we provide a mechanism for boosting the base model by adding either a generative or discriminative model to the ensemble. We later generalize this procedure to include arbitrary generative and discriminative model sequences. Finally, we present a graphical model based on normalizing flows that effectively utilizes the boosting meta-algorithms for expressive, yet tractable learning and inference.
3.1. Generative boosting

Supervised boosting algorithms such as AdaBoost [Freund & Schapire 1995] typically involve a reweighting procedure for training weak learners. We can similarly train an ensemble of generative models for unsupervised boosting, where every subsequent model performs \( \text{MLE} \) with respect to a reweighted data distribution \( D_t \),

\[
\max_{h_t} \mathbb{E}_{D_t}[\log h_t] \quad (3)
\]

where \( d_t \propto \left( \frac{p}{q_{t-1}} \right)^{\beta_t} \quad (4) \)

and \( 0 \leq \beta_t \leq 1 \) is the reweighting coefficient (at round \( t \)). These coefficients are in general different from the model weights \( \alpha_t \) that appear in the density estimate in Eq. (2).

**Theorem 3.** If we can maximize the objective in Eq. (3) optimally, then \( \delta_{KL}(h_t, \alpha_t) \geq 0 \) for any \( 0 \leq \beta_t \leq 1 \) with the equality holding for \( \beta_t = 0 \).

While the objective in Eq. (3) can be hard to optimize in practice, note that the target distribution becomes simpler to approximate as we reduce the reweighting coefficient. For the extreme case of \( \beta_t = 0 \), the reweighted data distribution is simply uniform. There is no free lunch however, since reducing the reweighting coefficient would lead to a slower reduction in KL-divergence leading to a computational-statistical trade-off.

The pseudocode for the corresponding boosting meta-algorithm, referred to as GenBGM, is given in Algorithm 1. In practice, we only observe samples from the true data distribution, and hence, approximate \( p \) based on the empirical data distribution which is defined to be uniform over the dataset \( X \). At every subsequent round, GenBGM learns an intermediate model that maximizes the log-likelihood of data sampled from a reweighted data distribution.

3.2. Discriminative boosting

A base generative model can be boosted using a discriminative approach as well. Here, the intermediate model is specified as the density ratio obtained from a binary classifier. Specifically, consider the following binary classification problem: we observe an equal number of samples drawn i.i.d. from the true data distribution (w.l.o.g. assigned the label \( y = +1 \)) and the model distribution in the previous round \( Q_{t-1} \) (assigned the label \( y = -1 \)).

**Definition 1.** Let \( f : \mathbb{R}^+ \to \mathbb{R} \) be any convex, lower semi-continuous function satisfying \( f(1) = 0 \). The \( f \)-divergence between \( P \) and \( Q \) is defined as,

\[
D_f(P||Q) = \int q \cdot f \left( \frac{p}{q} \right) dx.
\]

Notable examples include the Kullback-Liebler (KL) divergence, Hellinger distance and the Jenson-Shannon (JS) divergence among many others. The binary classifier in discriminative boosting at round \( t \) maximizes a variational lower bound
Algorithm 2 DiscBGM($X = \{x_i\}_{i=1}^m, T$ rounds, $f$-div)

Initialize $d_0(x_i) = 1/m$ for all $i = 1, 2, \ldots, m$.
Train generative model $h_0$ to maximize $\mathbb{E}_{D_0} \left[ \log h_0 \right]$.
Set (unnormalized) density estimate $\tilde{q}_0 = h_0$.

for $t = 1, \ldots, T$ do
  - Generate negative samples from $q_{t-1}$.
  - Optimize $r_t$ to maximize RHS in Eq. (5).
  - Set $h_t = [f']^{-1}(r_t)$.
  - Choose $\alpha_t$.
  - Set (unnormalized) density estimate $\tilde{q}_t = h_t^\alpha_t \cdot \tilde{q}_{t-1}$.
end for

Estimate $Z_T = \int \tilde{q}_T \, dx$.
return $q_T = \tilde{q}_T / Z_T$

on any $f$-divergence,
$$D_f (P || Q_{t-1}) \geq \sup_{r_t \in \mathcal{R}_f} \left( \mathbb{E}_P [r_t] - \mathbb{E}_{Q_{t-1}} [f^*(r_t)] \right). \tag{5}$$

where $f^*$ denotes the Fenchel conjugate of $f$ and $r_t : \mathbb{R}^d \rightarrow \text{dom}_f$ is a class of functions parameterizing the classifier. Under mild conditions on $f$ (Nguyen et al., 2010), the lower bound in Eq. (5) is tight if,
$$r_t^* = f' \left( \frac{p}{q_{t-1}} \right). \tag{6}$$

Hence, a solution to Eq. (5) can be used to estimate density ratios. The density ratios naturally fit into the multiplicative boosting framework and provide a justification for the use of objectives of the form Eq. (5) for learning intermediate models as formalized in the proposition below.

**Proposition 1.** For any given $f$-divergence, let $r_t^*$ denote the optimal solution to Eq. (5) in the $t^{th}$ round of boosting. Then, the model density at the end of the boosting round matches the true density if we set $\alpha_t = 1$ and
$$h_t = [f']^{-1}(r_t^*) \tag{7}$$

where $[f']^{-1}$ denotes the inverse of the derivative of $f$.

The pseudocode for the corresponding boosting meta-algorithm, DiscBGM is given in Algorithm 2. At every round, we train a binary classifier to optimize the objective in Eq. (5) corresponding to a chosen $f$-divergence.

As a special case, the negative of the cross-entropy loss commonly used for binary classification is also a lower bound on an $f$-divergence. While Algorithm 2 is applicable for any $f$-divergence, we will refer to the cross-entropy based objective henceforth to streamline the discussion, unless explicitly mentioned otherwise.

**Corollary 1.** Consider the following (negative) cross-entropy objective maximized by a binary classifier,
$$\sup_{c_t \in \mathcal{C}_t} \mathbb{E}_P [\log c_t] + \mathbb{E}_{Q_{t-1}} [\log (1 - c_t)]. \tag{8}$$

If a binary classifier $c_t$ trained to optimize Eq. (8) is Bayes optimal, then the model density at the end of the boosting round matches the true density if we set $\alpha_t = 1$ and
$$h_t = \frac{c_t}{1 - c_t}. \tag{9}$$

In practice, a classifier with limited capacity trained on a finite dataset will not generally be Bayes optimal. The above corollary, however, suggests that a good classifier can provide a “direction of improvement”, in a similar spirit to the gradient boosting algorithm proposed by Freund & Schapire (1995) for supervised learning. Additionally, if the intermediate model distribution $h_t$ obtained using Eq. (9) satisfies the conditions in Theorem 2, it is guaranteed to improve the fit.
The weights $0 \leq \alpha_t \leq 1$ can be interpreted as our confidence in the classifier density estimate, akin to the step size used in gradient descent. While in practice we use heuristic strategies for assigning weights to the intermediate models, the greedy optimum value of these weights at every round is a critical point for $\delta_{KL}$ (defined in Theorem 2). For example, consider the extreme cases below.

- If $c_t$ is uninformative, i.e., $c_t \equiv 0.5$, then $\delta_{KL}(h_t, \alpha_t) = 0$ for all $0 \leq \alpha_t \leq 1$.
- If $c_t$ is Bayes optimal, then $\delta_{KL}$ attains a maxima when $\alpha_t = 1$ (Corollary 1).

### 3.3. Hybrid boosting

Intermediate models need not be exclusively generators or discriminators as presented in Algorithm 1 and Algorithm 2; we can design a boosting ensemble with any combination of generators and discriminators as intermediate models. If an intermediate model is chosen to be a generator, we learn a generative model using MLE after appropriately reweighting the data points. If a discriminator is used to implicitly specify an intermediate model, we set up the corresponding binary classification problem.

### 3.4. Boosting normalized flow models

The boosting meta-algorithms presented above are applicable to a wide range of base generators learned using MLE as well as discriminators maximizing a variational lower bound on a chosen $f$-divergence. At any given round, the model density needs to be specified only up to a normalization constant. Once the boosting rounds are over, the partition function can be estimated using approximate inference based on Monte Carlo techniques such as Annealed Importance Sampling (Neal, 2001) if required. Monte Carlo estimates can have high variance in the absence of good proposals, leading to practical difficulties in density estimation of high-dimensional distributions. Similarly for generating samples from the BGM, we have to resort to Markov chains which can take a long time to mix for simple proposals.

To offset these limitations, consider the normalizing flow model in Figure 1. The model consists of multiple layers of random variables $\{X_t\}_{t=0}^T$, with each layer expressing a distribution $q_t$ over the same space as the data. The connections between the layers $t \rightarrow t + 1$ specify an invertible transformation $g_t = f_t^{-1}$ from one distribution to another formalized using the change-of-variables formula,

$$
q_t(x) = q_{t-1}(f_{t-1}(x)) \left| \frac{\partial f_t(x)}{\partial x} \right|
$$

where $\frac{\partial f_t(x)}{\partial x}$ denotes the Jacobian of $f_t$ at $x$.

Due to the absence of any latent variables, normalizing models also permit exact likelihood evaluation as long as the prior density of the first layer $p_{X_0}$ is tractable and computing the determinant of the Jacobian is inexpensive. Dinh et al. (2014) define affine location-scale transformations parameterized by neural networks that ensure that the Jacobian is an upper triangular matrix and hence, the determinant can be easily computed as the product of diagonal entries. Furthermore, efficient ancestral sampling is possible in flow models since the transformations are invertible as shown by the recursive equations below,

$$
x^{(0)} \sim q_0; \quad x^{(t)} = g_t(x^{(t-1)})
$$

In the boosting setting, the connections between any two layers of a normalizing flow model can be used to specify a weak learner that corrects for the shortcomings of the previous layers. The change-of-variables formula in Eq. (10) matches

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1 For many applications of generative models such as feature learning, we can sidestep computing the partition function.
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Figure 2: Experimental setup for a mixture of Gaussians showing (a) true density and (b) base (misspecified) model.

the multiplicative boosting updates in Eq. (2) with all model weights $\alpha_t$ set to unity and the intermediate model at any round, $h_t$, corresponding to the Jacobian of a parameterized invertible function $f_t$. Importantly, flow models ensure that the resulting density estimate is normalized. We can then apply Algorithm 1 with a simple flow model as a base and greedily train additional layers to optimize the objective in Eq. (3), following an appropriate reweighting step as per Eq. (4).

3.5. Regularization

In practice, we want boosted generative models (BGM) to generalize to data points outside the training set $X$. Regularization in BGMs is imposed primarily in two ways. First, every intermediate model can be independently regularized by early stopping of training based on validation error, incorporating explicit terms in the learning objective, heuristics such as dropout, etc. Moreover, restricting the number of rounds of boosting is another effective mechanism for regularizing BGMs. Fewer rounds of boosting are required if the intermediate models are sufficiently expressive.

4. Empirical evaluation

We evaluated the performance of boosting generative models for the tasks of density estimation and sample generation on real and synthetic datasets.

Figure 3: Multiplicative boosting algorithms such as GenBGM (c-d) and DiscBGM with negative cross-entropy (e-f) and Hellinger distance (g-h) outperform additive boosting (a-b) in correcting for model misspecification.

4.1. Mixture of Gaussians

A common pitfall with training generative models is model misspecification with respect to the true underlying data distribution as illustrated in the following synthetic setting.

Experimental setup. The true data distribution is a equi-weighted mixture of four Gaussians centered symmetrically
Table 1: Average test NLL estimates (with std error) for models over sampled instances of the mixture of Gaussians.

| Model          | NLL (in nats) |
|----------------|--------------|
| Base model     | 4.69 ± 0.01  |
| Add model      | 4.64 ± 0.02  |
| GenBGM         | 4.58 ± 0.10  |
| DiscBGM-NCE    | 4.42 ± 0.01  |
| DiscBGM-HD     | 4.35 ± 0.01  |

around the origin, each having an identity covariance matrix. The contours of the underlying density are shown in Figure 2 (a). We only observe 1,000 training samples drawn i.i.d. from the data distribution (shown as black dots in Figure 3), and the task is to learn this distribution. The test set contains 1,000 samples from the same distribution. For statistical significance, we repeat the process 10 times.

As a base (misspecified) model, we fit a mixture of two Gaussians to the data; the contours for an example instance are shown in Figure 2 (b). We compare multiplicative and additive boosting, each run for \( T = 2 \) additional rounds. For additive boosting (Add model), we use the algorithm proposed by Rosset & Segal (2002) setting \( \hat{\alpha}_0 \) to unity and doing a line search over \( \hat{\alpha}_1, \hat{\alpha}_2 \in [0, 1] \). For the multiplicative boosting algorithms, all model weights, \( \alpha \)'s to unity. The reweighting coefficients, \( \beta \)'s for GenBGM are all set to unity and the intermediate models are mixtures of two Gaussians as well. For DiscBGM, the classifiers are multi-layer perceptrons with two hidden layers (each containing 100 units) maximizing \( f \)-divergences corresponding to the negative cross-entropy (NCE) and Hellinger distance (HD).

The test negative log-likelihood (NLL) estimates are listed in Table 1. Qualitatively, the contour plots for the estimated densities after every boosting round on a sample instance are shown in Figure 3. Multiplicative boosting algorithms outperform additive boosting in correcting for model misspecification. GenBGM initially leans towards maximizing coverage, whereas both versions of DiscBGM are relatively more conservative in assigning high densities to data points away from the modes. Refer to Appendix B.1 for results with additional heuristic model weighting (\( \alpha \)'s) strategies.

4.2. MNIST

The binarized MNIST dataset contains 50,000 train, 10,000 validation, and 10,000 test images of handwritten digits, each of dimensions \( 28 \times 28 \) (LeCun et al., 2010).

**Experimental setup.** Consider a baseline variational autoencoder (VAE) (Kingma & Welling, 2014) trained for sufficiently long. Ancestral samples obtained by the baseline VAE model are shown in Figure 4 (a). We use the evidence lower bound (ELBO) as a proxy for approximately evaluating the marginal log-likelihood during learning.

The conventional approach to improving the performance of a latent variable model is to increase its representational capacity by adding hidden layers (Baseline VAE + depth) or increasing the number of hidden units in the existing layers (Baseline VAE + width). These lead to a marginal improvement in sample quality as seen in Figure 4 (b) and 4 (c). Table 4.1 lists the architecture for the baseline models. Appendix B.2 provides more details regarding the model structure, learning procedure and hyperparameter settings.

In contrast, we make steady improvements in sample quality using boosting. We start with a VAE roughly half the size of Baseline VAE and generate samples after boosting it using GenBGM, DiscBGM, and GenDiscBGM (Figures 4 (d), 4 (e), and 4 (f) respectively). The discriminator used is a convolutional neural network (CNN) (LeCun & Bengio, 1995) trained to maximize the negative cross-entropy. The model weights, \( \alpha \)'s and reweighting coefficient, \( \beta \)'s are set to unity. The boosted sequences generate sharper samples than all the baselines in spite of having similar model capacity. The samples are generated using independent Monte Carlo Markov Chain (MCMC) sampling. See Appendix B.2 for details on the MCMC procedure.

Since boosting is particularly attractive for improving weak learners, it does not require the models in the ensemble to be trained until convergence. Tables 4.1 and 4.2 in Figure 4 compare the wall-clock time taken during training of baseline models and BGM sequences. In an attempt to equalize for training time, we train the VAEs used in the BGM sequences for only 70 epochs, such that the training time of the most expensive BGM sequence (GenDiscBGM) matches that of the
Figure 4: The boosted generative models (d-f) demonstrate how boosting may be used to ensemble weak learners into stronger models generating sharper samples, compared to naively increasing model capacity (a-c). Note that we show actual samples and not mean pixels. The VAEs used in the boosting sequences have a 784-100-50 layered architecture.

weakest baseline (Baseline VAE). The convergence curves are shown in Appendix B.2 for reference. Hence, the boosting framework does not contribute towards any significant overhead during training.

4.3. CIFAR-10

The dataset contains 50,000 train and 10,000 test images, each of dimensions 32×32×3 [Krizhevsky & Hinton, 2009].

**Experimental setup.** We perform density estimation and sampling using a boosted normalized flow model. The base model is a multi-scale architecture similar to the one proposed by [Dinh et al., 2016], marginally downsized due to constraints on available computational resources. Every “scale” of the architecture consists of multiple layers. The scale compositions and elaborate learning procedure are derived from prior work and deferred to Appendix B.3.

The prior density, $q_0$, is an isotropic unit norm Gaussian. The base model implicitly specifies an intermediate learner $h_1$. A second intermediate learner $h_2$ is obtained by adding another scale to the model. Learning the parameters for the final architecture ($h_1$ and $h_2$) can be done in two ways. The “Joint” baseline jointly learns the parameters based on MLE. Alternatively, we learn the model greedily (i.e., $h_1$ followed by $h_2$) using the boosting procedure described in Section 3.4. The reweighting coefficient $\beta_1$ is set to zero (i.e., all points have same weights) since the prior density is not expected to be very informative. For subsequent learning of $h_2$, we do a line search for different values of $\beta_2$.

The test NLLs are listed in Table 2. Following common practice, the results are expressed in bits and normalized by the total number of dimensions ($32 \times 32 \times 3$). We observe that boosted models are significantly better than the jointly trained baseline (up to 90 bits over the full space). Joint training of very deep networks through backpropagation is difficult due to many reasons, including vanishing or exploding gradient signals [Glorot & Bengio, 2010]. Hence, boosting indirectly provides a better optimization mechanism in this particular setting. Samples generated from the best performing boosted model are shown in Figure 5. Given the high variation across the images in CIFAR-10, it is hard to make a definite comparison with samples generated from the joint model. For completeness, we show samples from the latter in Appendix B.3.

5. Discussion and related work

Boosting has offered interesting theoretical insights into the fundamental limits of supervised learning and led to the development of algorithms that work well in practice [Schapire, 1990; Freund et al., 1999; Friedman, 2002; Caruana & Niculescu-Mizil, 2006]. Our work provides a foundational framework for unsupervised boosting. Many key components of our framework exhibit connections with prior work in generative modeling.
Table 2: Test NLL (in bits/dim) for the CIFAR-10 dataset.

| Model | NLL  |
|-------|------|
| Joint | 3.58 |
| \(\beta_2 = 0\) | 3.56 |
| \(\beta_2 = 0.25\) | **3.55** |
| \(\beta_2 = 0.50\) | **3.55** |
| \(\beta_2 = 1.0\) | 3.57 |

**Sum- vs. product-of-experts.** Rosset & Segal (2002) proposed an algorithm for density estimation using Bayesian networks similar to gradient boosting. Theorem 1 highlights the key limitation of additive formulations for learning complex multi-modal distributions as requiring a more powerful learner at every round. These models are normalized and easy to sample, but are generally outperformed by multiplicative formulations in correcting for model misspecification as we demonstrated empirically. Recent preprints use additive boosting in the context of variational inference (Miller et al., 2016; Guo et al., 2016) and generative adversarial networks (Tolstikhin et al., 2017).

The product-of-experts formulation, which is also the one we adopt in the current work, was initially proposed for feature learning in energy based models such as Boltzmann machines. For example, the hidden units in a restricted Boltzmann machine can be interpreted as weak learners performing MLE. If the number of weak learners is fixed, they can be efficiently updated in parallel but there is a risk of learning redundant features (Hinton, 1999; 2002). Weak learners can also be added incrementally based on the learner’s ability to distinguish observed data and model-generated data (Welling et al., 2002).

Tu (2007) generalized the latter to boost arbitrary probabilistic models; their algorithm is a special case of DiscBGM with all \(\alpha\)'s set to 1 and the discriminator maximizing the negative cross-entropy. Hence, DiscBGM additionally accounts for imperfections in learning classifiers and can be adapted to maximize any \(f\)-divergence.

**Unsupervised-as-supervised learning.** The use of density ratios learned by a binary classifier for estimation was first proposed by Friedman et al. (2001) and has been subsequently applied elsewhere, notably for parameter estimation using noise-contrastive estimation (Gutmann & Hyvärinen, 2010) and sample generation in generative adversarial networks (GAN) (Goodfellow et al., 2014).

GANs consist of a pair of generative-discriminative networks. The discriminator maximizes the negative cross-entropy as in Eq. (8) and the generator minimizes the same objective. GANs generate extremely good samples, but are unstable to train in practice, and the training objective is not guaranteed to converge (Goodfellow, 2014). Borrowing terminology from Mohamed & Lakshminarayanan (2016), GANs can be seen as *implicit* probabilistic models that are directly optimizing for generating visually appealing samples as opposed to *prescribed* probabilistic models such as BGMs that provide an explicit characterization of the log-likelihood and are typically stable to train. While the original GAN formulation

![Figure 5: Samples generated by the boosted normalizing flow model (\(\beta_2 = 0.5\)) for the CIFAR-10 dataset.](image-url)
was proposed for a cross-entropy based objective. [Nowozin et al. (2016)] extend it to arbitrary \( f \)-divergences. Their work is based on the same variational divergence minimization framework we use for learning binary classifiers in boosted generative models [Nguyen et al. (2010)].

6. Conclusion

We presented a general-purpose framework for boosting generative models by explicit factorization of the model likelihood as a product of simpler intermediate model densities. These intermediate models are learned greedily using discriminative or generative approaches, gradually increasing the overall model’s capacity. We further designed an algorithm for boosting normalizing flow models which can perform exact and efficient likelihood evaluation and sampling. We demonstrated the effectiveness of boosted generative models by designing several ensemble models which improve upon baseline generative models for the tasks of density estimation and sample generation without incurring any significant computational overhead.

In the future, we will explore the design of models such as normalized flow models that permit efficient learning and inference within our boosting framework. We would like to further examine algorithmic questions concerning weighting strategies for intermediate models and the effect of the choice of \( f \)-divergence on learning. Finally, it would be interesting to design algorithms based on boosted generative models for semi-supervised learning.

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Appendices

A. Proofs of theoretical results

A.1. Theorem

The reduction in KL-divergence can be simplified as,

\[ \delta_{KL}^t(h_t, \hat{\alpha}_t) = \mathbb{E}_P \left[ \log \frac{p}{q_{t-1}} \right] - \mathbb{E}_P \left[ \log \frac{q_t}{q_{t-1}} \right] \]

\[ = \mathbb{E}_P \left[ \log \frac{q_t}{q_{t-1}} \right] \]

\[ = \mathbb{E}_P \left[ \log \left( 1 - \hat{\alpha}_t + \hat{\alpha}_t \frac{h_t}{q_{t-1}} \right) \right]. \]

We first derive the sufficient condition by lower bounding \( \delta_{KL}^t(h_t, \hat{\alpha}_t) \).

\[ \delta_{KL}^t(h_t, \hat{\alpha}_t) = \mathbb{E}_P \left[ \log \left( 1 - \hat{\alpha}_t + \hat{\alpha}_t \frac{h_t}{q_{t-1}} \right) \right] \]

\[ \geq \mathbb{E}_P \left[ (1 - \hat{\alpha}_t) \log 1 + \hat{\alpha}_t \log \frac{h_t}{q_{t-1}} \right] \quad \text{(Arithmetic Mean \( \geq \) Geometric Mean)} \]

\[ = \hat{\alpha}_t \mathbb{E}_P \left[ \log \frac{h_t}{q_{t-1}} \right] \quad \text{(Linearity of expectation)} \]

If the lower bound is non-negative, then so is \( \delta_{KL}^t(h_t, \hat{\alpha}_t) \). Hence,

\[ \mathbb{E}_P \left[ \log \frac{h_t}{q_{t-1}} \right] \geq 0 \]

which is the stated sufficient condition.

For the necessary condition to hold, we know that

\[ 0 \leq \delta_{KL}^t(h_t, \hat{\alpha}_t) \]

\[ = \mathbb{E}_P \left[ \log \left( 1 - \hat{\alpha}_t + \hat{\alpha}_t \frac{h_t}{q_{t-1}} \right) \right] \]

\[ \leq \log \mathbb{E}_P \left[ (1 - \hat{\alpha}_t) + \hat{\alpha}_t \frac{h_t}{q_{t-1}} \right] \quad \text{(Jensen’s inequality)} \]

\[ = \log \left( 1 - \hat{\alpha}_t + \hat{\alpha}_t \mathbb{E}_P \left[ \frac{h_t}{q_{t-1}} \right] \right) \quad \text{(Linearity of expectation)} \]

Taking exponential on both sides,

\[ (1 - \hat{\alpha}_t) + \hat{\alpha}_t \mathbb{E}_P \left[ \frac{h_t}{q_{t-1}} \right] \geq 1 \]

\[ \mathbb{E}_P \left[ \frac{h_t}{q_{t-1}} \right] \geq 1 \]

which is the stated necessary condition.
A.2. Theorem[2]

**Proof.** We first derive the sufficient condition,

\[
\delta_{KL}^t(h_t, \alpha_t) = \int p \log q_t \, dx - \int p \log q_{t-1} \, dx
\]

\[
= \int p \log \frac{h_t^\alpha \cdot q_{t-1}}{Z_t} \, dx - \int p \log q_{t-1} \quad \text{(using Eq. (2))}
\]

\[
= \alpha_t \cdot \mathbb{E}_p[\log h_t] - \mathbb{E}_{Q_{t-1}}[h_t^\alpha]
\]

\[
\geq \alpha_t \cdot \mathbb{E}_p[\log h_t] - \mathbb{E}_{Q_{t-1}}[h_t]^{\alpha_t}
\]

(Jensen’s inequality)

\[
\geq 0 \quad \text{(by assumption)}.
\]

Note that if \( \alpha_t = 1 \), the sufficient condition is also necessary. For the necessary condition,

\[
0 \leq \delta_{KL}^t(h_t, \alpha_t) = \alpha_t \cdot \mathbb{E}_p[\log h_t] - \mathbb{E}_{Q_{t-1}}[h_t^\alpha]
\]

\[
\leq \alpha_t \cdot \mathbb{E}_p[\log h_t] - \mathbb{E}_{Q_{t-1}}[\log h_t]^{\alpha_t}
\]

(Jensen’s inequality)

\[
= \alpha_t \cdot \mathbb{E}_p[\log h_t] - \mathbb{E}_{Q_{t-1}}[\log h_t]
\]

(Linearity of expectation)

\[
\leq \mathbb{E}_p[\log h_t] - \mathbb{E}_{Q_{t-1}}[\log h_t] \quad \text{(since } \alpha_t > 0).\]

\[
\]

A.3. Theorem[3]

**Proof.** By assumption, we can optimize Eq. (3) to get,

\[
h_t \propto \left( \frac{p}{q_{t-1}} \right)^{\beta_t}.
\]

Substituting for \( h_t \) in the multiplicative boosting formulation in Eq. (2),

\[
q_t \propto \frac{q_{t-1} \cdot h_t}{Z_{q_t}}
\]

\[
\propto \frac{q_{t-1}}{Z_{q_t}} \left( \frac{p}{q_{t-1}} \right)^{\beta_t}
\]

\[
= \frac{p^{\beta_t} \cdot q_{t-1}^{1-\beta_t}}{Z_{q_t}}
\]

where the partition function \( Z_{q_t} = \int p^{\beta_t} \cdot q_{t-1}^{1-\beta_t} \).

In order to prove the inequality, we first obtain a lower bound on the log-partition function, \( Z_{q_t} \). For any given point, we have,

\[
p^{\beta_t} \cdot q_{t-1}^{1-\beta_t} \leq \beta_t p + (1 - \beta_t)q_{t-1}
\]

using the Arithmetic Mean \( \geq \) Geometric Mean inequality given that densities are non-negative. Integrating over all points in the domain,

\[
\log Z_q \leq \log \left[ \beta Z_p + (1 - \beta)Z_{q_{t-1}} \right] = 0
\]

(12)

where we have used the fact that \( p \) and \( q_{t-1} \) are normalized densities.
Now, consider the following quantity \[^5\]

\[
D_{KL}(P || Q_t) = E_P \left[ \log \frac{p}{q_t} \right]
\]

\[
= E_P \left[ \log \frac{p}{p^{q_{t-1}} q_t^{-1}} \right]
\]

\[
= (1 - \beta_t) E_P \left[ \log \frac{p}{q_{t-1}} \right] + \log Z_{q_t}
\]

\[
\leq (1 - \beta_t) E_P \left[ \log \frac{p}{q_{t-1}} \right]
\]

\[
\leq E_P \left[ \log \frac{p}{q_{t-1}} \right] \quad (\text{since } \beta_t \geq 0)
\]

\[
= D_{KL}(P || Q_{t-1})
\]

where the second last inequality is due to Eq. (12). This finishes the proof.

**A.4. Proposition** \[^1\]

**Proof.** By the \(f\)-optimality assumption,

\[
r_t = f' \left( \frac{p}{q_{t-1}} \right).
\]

Hence, \(h_t = \frac{p}{q_{t-1}}\). From Eq. (2),

\[
q_t = q_{t-1} \cdot h_t^{\alpha_t} = p
\]

finishing the proof. \(\square\)

**A.5. Corollary** \[^1\]

**Proof.** Let \(u_t\) denote the joint distribution over \((x, y)\) at round \(t\). We will prove a slightly more general result where we have \(m\) positive training examples sampled from \(p\) and the \(k\) negative training examples sampled from \(q_{t-1}\). Hence,

\[
p = u(x | y = +1) \quad \quad \quad u(y = +1) = \frac{m}{m + k}
\]

\[
q_{t-1} = u(x | y = -1) \quad \quad \quad u(y = -1) = \frac{k}{m + k}.
\]

The Bayes optimal density \(c_t\) can be expressed as,

\[
c_t = u(y = +1 | x)
\]

\[
= u(x | y = +1)u(y = +1)/u(x).
\]

Similarly,

\[
1 - c_t = u(x | y = -1)u(y = -1)/u(x).
\]

From Eqs. (13-16), we have,

\[
h_t = \gamma \cdot \frac{c_t}{1 - c_t} = \frac{p}{q_{t-1}}.
\]
where \( \gamma = \frac{k}{m} \). Finally from Eq. (2),
\[
q_t = q_{t-1} \cdot h_t^{\alpha_t} = p
\]
finishing the proof.

Define an adversarial Bayes optimal classifier \( c'_t \) that assigns the density \( c'_t = 1 - c_t \). We prove another corollary for adversarial classifiers below.

**Corollary 2.** For an adversarial Bayes optimal classifier, \( \delta_{KL}^t \) attains a maxima of zero when \( \alpha_t = 0 \).

**Proof.** For an adversarial Bayes optimal classifier,
\[
c'_t = u(x \mid y = -1)u(y = -1)/u(x)
\]
(17)
\[
1 - c'_t = u(x \mid y = +1)u(y = +1)/u(x).
\]
(18)

From Eqs. (13, 14, 17, 18),
\[
h_t = \gamma \cdot \frac{c'_t}{1 - c'_t} = \frac{q_{t-1}}{p}.
\]

Substituting the above intermediate model in Eq. (11),
\[
\delta_{KL}^t(h_t, \alpha_t) = \alpha_t \cdot \mathbb{E}_P \left[ \log \frac{q_{t-1}}{p} \right] - \mathbb{E}_{Q_{t-1}} \left[ \frac{q_{t-1}}{p} \right]^{\alpha_t}
\]
\[
\leq \alpha_t \cdot \mathbb{E}_P \left[ \log \frac{q_{t-1}}{p} \right] - \mathbb{E}_{Q_{t-1}} \left[ \alpha_t \cdot \log \frac{q_{t-1}}{p} \right] \quad \text{(Jensen’s inequality)}
\]
\[
= \alpha_t \cdot \left[ \mathbb{E}_P \left[ \log \frac{q_{t-1}}{p} \right] - \mathbb{E}_{Q_{t-1}} \left[ \log \frac{q_{t-1}}{p} \right] \right] \quad \text{(Linearity of expectation)}
\]
\[
= -\alpha_t \left[ KL(P \mid \mid Q_{t-1}) + KL(Q_{t-1} \mid \mid P) \right]
\]
\[
\leq 0 \quad \text{(} KL \text{ is non-negative).}
\]

By inspection, the equality holds when \( \alpha_t = 0 \) finishing the proof.

**B. Implementation details and additional experimental results**

**B.1. Mixture of Gaussians**

Table 3: Heuristic strategies for setting intermediate model weights.

| Weighting strategy | Per-round weights, \( \alpha_t \) |
|--------------------|----------------------------------|
| Unity              | 1                                |
| Uniform            | 1/(T + 1)                        |
| Decay              | 1/2^t                            |

Our algorithmic framework requires as hyperparameters the number of rounds of boosting (i.e., \( T \)), as well as a set of weights associated with each model in the ensemble (i.e., \( \alpha_t \)’s). For any practical setting, these hyperparameters are specific to the dataset and task under consideration and should be set based on cross-validation. Here, we propose some heuristic weighting strategies for assigning the model weights in Table 3 and study their effect on density estimation for the aforementioned setting of fitting a boosted generative model to a mixture of Gaussians. The partition function is estimated using importance sampling with a Gaussian fitted to the training data as the proposal.
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Figure 6: Train (dashed curves) and test (bold curves) NLL (in nats) of various heuristic strategies on density estimation for a mixture of Gaussians. $T$ is the number of rounds of boosting. The base model is shown as a black cross at $T = 0$.

Figure 7: The baselines are run up till convergence as measured by validation NLL. The training of the VAEs used in the BGMs is terminated early to ensure fairness in total computation time.

In Figure 6 we observe that the performance of the algorithms can however be sensitive to the weighting strategies. In particular, DiscBGM can produce worse estimates as $T$ increases for the “uniform” (red) strategy. GenBGM also slightly degrades in performance with increasing $T$ for the “unity” (green) strategy. For all other strategies, the algorithms are fairly robust to the number of rounds of boosting. Notably, the “decay” (cyan) strategy achieves stable performance for both the algorithms. Intuitively, this heuristic follows the rationale of reducing the step size in gradient based stochastic optimization algorithms, and we expect this strategy to work better even in other settings. However, this strategy could potentially result in slower convergence as opposed to the unity strategy.

B.2. MNIST

VAE architecture and learning procedure details. Only the last layer in every VAE is stochastic, rest are deterministic. The inference network specifying the posterior contains the same architecture for the hidden layer as the generative network. The prior over the latent variables is standard Gaussian, the hidden layer activations are ReLU, and learning is done using Adam (Kingma & Ba, 2015) with a learning rate of $10^{-3}$ and mini-batches of size 100. The convergence curves for the baseline VAEs and the smaller VAE used in the boosted generative model is shown in Figure 7.

CNN architecture and learning procedure details. The CNN contains two convolutional layers and a single fully connected layer with 1024 units. Convolution layers have kernel size $5 \times 5$, and 32 and 64 output channels, respectively. We apply ReLUs and $2 \times 2$ max pooling after each convolution. The net is randomly initialized prior to training, and learning is done for 2 epochs using Adam (Kingma & Ba, 2015) with a learning rate of $10^{-3}$ and mini-batches of size 100.

Sampling procedure for BGM sequences. Samples from the BGM sequences are drawn from a Markov chain run using the Metropolis-Hastings algorithm with a discrete, uniformly random proposal and the BGM distribution as the stationary distribution for the chain. Every sample in Figure 4(d-f) is drawn from an independent Markov chain with a burn-in period
Boosted Generative Models

Figure 8: Samples generated by the jointly trained baseline model for the CIFAR-10 dataset.

of 100,000 samples and a different start seed state.

B.3. CIFAR-10

Model architecture. The overall architecture contains three scales. Every scale is composed of three different kinds of layers: coupling layers (C), squeezing layers (S), and factoring layers (F). Please refer to Dinh et al. (2016) for a complete description of these layers. In increasing order starting from the scale containing the layer expressing the prior density, the scale compositions are as follows,

1. Scale 1: F-C-C-C-C
2. Scale 2: F-C-C-S-C-C-C
3. Scale 3: F-C-C-S-C-C

Our implementation details follow the one by Dinh et al. (2016) closely. The batch size was set to 12 and the images were scaled to lie between [-1, 1] before feeding them into the network. Following common practice when modeling densities, we add real-valued noise to the pixel values to dequantize the data (Uria et al. 2013). We use the ADAM optimizer (Kingma & Ba 2015) with a learning rate of 0.001. For the boosted models, the learning rate was reset for training the additional scale (Scale 3). We used weight normalization (Salimans & Kingma 2016) and batch normalization (Ioffe & Szegedy 2015) to improve the training signal across layers.

Samples. The samples generated by the jointly trained baseline model are shown in Figure 8.