On Memorization in Probabilistic Deep Generative Models

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Abstract

Recent advances in deep generative models have led to impressive results in a variety of application domains. Motivated by the possibility that deep learning models might memorize part of the input data, there have been increased efforts to understand how memorization arises. In this work, we extend a recently proposed measure of memorization for supervised learning (Feldman, 2019) to the unsupervised density estimation problem and adapt it to be more computationally efficient. Next, we present a study that demonstrates how memorization can occur in probabilistic deep generative models such as variational autoencoders. This reveals that the form of memorization to which these models are susceptible differs fundamentally from mode collapse and overfitting. Furthermore, we show that the proposed memorization score measures a phenomenon that is not captured by commonly-used nearest neighbor tests. Finally, we discuss several strategies that can be used to limit memorization in practice. Our work thus provides a framework for understanding problematic memorization in probabilistic generative models.

1 Introduction

In the last few years there have been incredible successes in generative modeling through the development of deep learning techniques such as variational autoencoders (VAEs) [1, 2], generative adversarial networks (GANs) [3], normalizing flows [4, 5], and diffusion networks [6, 7], among others. The goal of generative modeling is to learn the data distribution of a given data set, which has numerous applications such as creating realistic synthetic data, correcting data corruption, and detecting anomalies. Novel architectures for generative modeling are typically evaluated on how well a complex, high dimensional data distribution can be learned by the model and how realistic the samples from the model are. An important question in the evaluation of generative models is to what extent training observations are memorized by the learning algorithm, as this has implications for data privacy, model stability, and generalization performance. For example, in a medical setting it is highly desirable to know if a synthetic data model could produce near duplicates of the training data.

A common technique to assess memorization in deep generative models is to take samples from the model and compare these to their nearest neighbors in the training set. There are several problems with this approach. First, it has been well established that when using the Euclidean metric this test can be easily fooled by taking an image from the training set and shifting it by a few pixels [8]. For this reason, nearest neighbors in the feature space of a secondary model are sometimes used, as well as cropping and/or downsampling before identifying nearest neighbors (e.g., [9–11]). Second, while there may not be any neighbors in the training set for a small selection of samples from the model, this does not demonstrate that there are no observations that are highly memorized. Indeed, in several
Memorization in generative models is not always surprising. When the training data set contains a number of highly similar observations, such as duplicates, then it would be expected that these receive an increased weight in the model and are more likely to be generated. The fact that commonly-used data sets contain numerous (near) duplicates \cite{12} therefore provides one reason for memorization of training observations. While important, memorization due to duplicates is not the focus of this work. Instead, we are concerned with memorization that arises as an increased probability of generating a sample that closely resembles the training data in regions of the input space where the algorithm has not seen sufficient observations to enable generalization. For example, we may expect that highly memorized observations are either in some way atypical or are essential for properly modeling a particular region of the data manifold.

Figure 1a illustrates this kind of local memorization in probabilistic generative models. We focus on explicit density models as these are more amenable to a direct analysis of the learned probability distribution (as opposed to implicit density models such as GANs). The figure shows that in certain regions of the input space the learned probability density can be entirely supported by a single, potentially outlying, observation. When sampling from the model in these parts of the space it is thus highly likely that a sample similar to an input observation will be generated. The figure also illustrates that in regions of the input space that are densely supported by closely-related observations, sampling will yield observations that resemble the input data. The change in the probability density of an observation that occurs when it is removed from the data forms the basis of the memorization score we propose in Section 3. This form of memorization should be contrasted with what is commonly associated with memorization due to overfitting (illustrated in Figure 1b). Overfitting is a global property of a model that typically occurs when it is trained for too long or with too high a learning rate (i.e., overtraining), so that a gap develops between the training and test performance. Thus, we emphasize that in generative models memorization and generalization can occur simultaneously at distinct regions of the input space, and that memorization is not necessarily caused by overtraining.

To understand memorization further, consider the simple case of fitting a multivariate normal distribution. In this scenario, the presence or absence of a particular observation in the data set will have a small effect on the learned model unless the observation is an outlier. By contrast, a kernel density estimate (KDE) \cite{13, 14} of the probability density may be more sensitive to the presence or absence of a particular observation. To see why this is the case, consider that in sparsely-populated regions of the input space the KDE can be supported by a relatively small number of observations. Although deep generative models typically operate in much higher dimensional spaces than the aforementioned methods, the same problem can arise when generalizing to regions of the space that are weakly supported by the available data. Because these models are optimized globally, the model has to place some probability mass in these regions. As we will demonstrate below, it is not necessarily the case that the model places low probability on such observations, resulting in observations that are both highly memorized and not significantly less likely under the model than other observations.

In this work, we extend a recently proposed measure of memorization for supervised learning \cite{15, 16} to probabilistic generative models and introduce a practical estimator of this memorization score. We subsequently investigate memorization experimentally, where we focus on the variational autoencoder.
In our experiments we demonstrate that highly memorized observations are not necessarily outliers, that memorization can occur early during the training process, and show the connection between nearest neighbor tests for memorization and the proposed memorization score. Finally, we discuss approaches that can limit memorization in practice.

2 Related Work

Here we review work on memorization in deep learning, memorization as it relates to membership inference, the evaluation of generative models, as well as influence functions and stability.

Memorization in deep learning. The observation that deep learning models can learn from patterns of random data has been a catalyst for recent efforts to understand memorization in supervised learning [17–19]. A number of approaches have been proposed to test for memorization in specific applications. In [20] memorization in language models is evaluated using a “canary” string (e.g., if “my social security number is” is in the training data, how often does the model complete the prompt “my social security number is” using $x$ instead of a comparable $y \neq x$ that is not in the training set). Unfortunately, this approach does not translate easily to other contexts, such as images. Moreover, language models often contain explicit memory cells such as LSTMs [21] that can facilitate memorization, which are absent in most generative models.

A memorization score for supervised learning was proposed in [15], which forms the inspiration for our formulation in Section 3. A related “consistency score” for supervised learning was proposed in [22]. We argue, however, that memorization in supervised learning differs fundamentally from that in generative models, as the label prediction task affects the training dynamics, and label noise is known to induce memorization in supervised learning [23, 24]. Building on earlier work by [25, 26], a hypothesis test is proposed in [27] that is based on the premise that memorization has occurred when samples from the trained model are “closer” to the training data than observations from the test set. While this is a useful test for aggregate memorization behavior in (a region of) the input space, our proposed score function allows us to quantify the memorization of a single observation.

Membership inference. A topic closely related to memorization is the problem of membership inference. Here, the goal is to recover whether a particular observation was part of the unknown training data set, either using knowledge of the model, access to the model, or in a black-box setting. Membership inference is particularly important when models are deployed [28], as potentially private data could be exposed. In the supervised learning setting, [29] propose to use an attack model that learns to classify whether a given sample was in the training set. Later work [30, 31] focused on generative models and proposed to train a GAN on samples from the target model. The associated discriminator is subsequently used to classify membership of the unknown training set. A related approach to recovering training images is described in [32], using an optimization algorithm that identifies for every observation the closest sample that can be generated by the network. However this requires solving a highly non-convex problem, which isn’t guaranteed to find the optimal solution.

Evaluating generative models. Memorization is a known issue when evaluating generative models, in particular for GANs [26, 33]. Several approaches are discussed in [8], with a focus on the pitfalls of relying on log-likelihood, sample quality, and nearest neighbors. Using the log-likelihood can be particularly problematic as it has been shown that models can assign higher likelihood to observations outside the input domain [34]. Nowadays, generative models are frequently evaluated by the quality of their samples as evaluated by other models, as is done in the Inception Score (IS) [35] and Fréchet Inception Distance (FID) [36]. Since these metrics have no concept of where the samples originate, the pathological case where a model memorizes the entire training data set will yield a near-perfect score. Motivated by this observation, [37] propose to use neural network divergences to measure sample diversity and quality simultaneously, but this requires training a separate evaluation model and there is no guarantee that local memorization will be detected.

Influence & Stability. The problem of memorization is also related to the concept of influence functions in statistics [38, 39]. Influence functions can be used to measure the effect of upweighting or perturbing an observation and have recently been considered as a diagnostic tool for deep learning [40, 41]. However, it has also been demonstrated that influence function estimates in deep learning models can be fragile [42]. Below, we therefore focus on a relatively simple estimator to gain a
A principled formulation of a memorization score for probabilistic generative models, $X \subseteq \mathcal{X}$ with observations from $\mathcal{X}$. This memorization score measures how much more likely an observation is when it is included in the training set compared to when it is not. For example, if $|I| = 1, \ldots, n$, and we define the leave-one-out (LOO) memorization score as

$$M_{\text{LOO}}(A, D, i) = \log P_A(x_i | D) - \log P_A(x_i | D_{[n]\setminus\{i\}}).$$

(2)

This memorization score measures how much more likely an observation is when it is included in the training set compared to when it is not. For example, if $M_{\text{LOO}}(A, D, i) = 10$, then $P_A(x_i | D) = \exp(10) \cdot P_A(x_i | D_{[n]\setminus\{i\}})$. Moreover, when $M_{\text{LOO}}(A, D, i) = 0$ removing the observation from the training data has no effect at $x_i$, and when $M_{\text{LOO}}(A, D, i) < 0$ the observation is more likely under the model when it is removed from the training data. We will abbreviate the LOO memorization score as $M_{\text{LOO}} := M_{\text{LOO}}(A, D, i)$ when the arguments are clear from context.

**Estimation.** The memorization score in (2) is a leave-one-out estimator that requires fitting the learning algorithm $A$ multiple times for each observation as it is left out of the training data set. As this is computationally infeasible in general, we introduce a practical estimator that simplifies the one proposed in (2). Instead of using a leave-one-out method or random sampling, we use a $K$-fold approach as is done in cross-validation. Let $\mathcal{I}_k$ denote randomly sampled disjoint subsets of the indices $\{1, \ldots, n\}$ of size $n/K$, such that $\bigcup_{k=1}^{K} \mathcal{I}_k = [n]$. We then train the model on each of the training sets $D_{[n]\setminus\mathcal{I}_k}$ and compute the log probability for all observations in the training set and the holdout set $D_{\mathcal{I}_k}$.

Since there is randomness in the algorithm $A$ and in the chosen folds $\mathcal{I}_k$, we repeat the cross-validation procedure $L$ times and average the results. Writing $\mathcal{I}_{\ell,k}$ for the $k$-th holdout index set in run $\ell$ and at observed data $x$. We estimate $M_{\text{LOO}}(A, D, i)$ by averaging over multiple $K$-fold cross-validation fits (see Section 3). Related to influence functions is the concept of stability in learning theory [45]. In particular, the point-wise hypothesis stability is an upper bound on the expected absolute change in the loss function when an observation is removed from the training set (where the expectation is over all training sets of a given size). We instead focus on the change in the density of a probabilistic model when trained on a specific data set.

**3 Memorization Score**

We present a principled formulation of a memorization score for probabilistic generative models, inspired by the one proposed recently in [15, 16] for supervised learning. Let $A$ denote a randomized learning algorithm, and let $\alpha$ be an instance of the algorithm (i.e., a trained model). Here, $A$ captures a complete description of the algorithm, including the chosen hyperparameters, training epochs, and optimization method. The randomness in $A$ arises from the particular initial conditions, the selection of mini-batches during training, as well as other factors. Denote the training data set by $D = \{x_i\}_{i=1}^{n}$ with observations from $\mathcal{X} \subseteq \mathbb{R}^D$. Let $|n| = \{1, \ldots, n\}$ and write $D_I = \{x_i : x_i \in D, i \in I\}$ for the subset of observations in the training data indexed by the set $I \subseteq [n]$. The posterior probability assigned to an observation $x \in \mathcal{X}$ by a model $A$ when trained on a data set $D$ is written as $p(x | D, A)$.

We are interested in the posterior probability of an observation assigned by the algorithm $A$, not merely by an instantiation of the algorithm. Therefore we introduce the probability $P_A(x | D)$ and its sampling estimate as

$$P_A(x | D) = \int p(x | D, \alpha)p(\alpha) \, d\alpha \approx \frac{1}{T} \sum_{\ell=1}^{T} p(x | D, a_\ell),$$

(1)

for some number of repetitions $T$. We see that $P_A(x | D)$ is the expectation of $p(x | D, \alpha)$ over instances of the randomized algorithm $A$.

To facilitate meaningful interpretation of the memorization score we use the difference in log probabilities, in contrast to [15, 16]. Thus we define the leave-one-out (LOO) memorization score as

$$M_{\text{LOO}}(A, D, i) = \log P_A(x_i | D) - \log P_A(x_i | D_{[n]\setminus\{i\}}).$$

(2)

This memorization score measures how much more likely an observation is when it is included in the training set compared to when it is not. For example, if $M_{\text{LOO}}(A, D, i) = 10$, then $P_A(x_i | D) = \exp(10) \cdot P_A(x_i | D_{[n]\setminus\{i\}})$. Moreover, when $M_{\text{LOO}}(A, D, i) = 0$ removing the observation from the training data has no effect at $x_i$, and when $M_{\text{LOO}}(A, D, i) < 0$ the observation is more likely under the model when it is removed from the training data. We will abbreviate the LOO memorization score as $M_{\text{LOO}} := M_{\text{LOO}}(A, D, i)$ when the arguments are clear from context.
We employ the variational autoencoder (VAE) [1, 2] as the probabilistic generative model in our experiments that advance our understanding of memorization in probabilistic deep generative models, with a focus on the variational autoencoder setting. Additional results are available in Supplement C. Code to reproduce our experiments can be found in an online repository.

4.1 Background

We employ the variational autoencoder (VAE) [1, 2] as the probabilistic generative model in our experiments, although it is important to emphasize that the memorization score introduced above is equally applicable to methods such as normalizing flows, diffusion networks, and other generative models that learn a probability density over the input space. The VAE is a latent-variable model, where we model the joint distribution \( p_\theta(x, z) \) of an observation \( x \in \mathcal{X} \subseteq \mathbb{R}^D \) and a latent variable \( z \in \mathcal{Z} \subseteq \mathbb{R}^d \). The joint distribution can be factorized as \( p_\theta(x, z) = p_\theta(x \mid z)p(z) \), and in the VAE the prior distribution \( p(z) \) is typically assumed to be a standard multivariate Gaussian. The posterior

\[
M_i^{K\text{-fold}} = \log \left[ \frac{1}{L(K - 1)} \sum_{\ell=1}^{L} \sum_{k=1}^{K} \mathbb{1}_{i \notin I_{\ell,k}} p(x_i \mid D_{\ell,k}, a_{\ell,k}) \right] - \log \left[ \frac{1}{L} \sum_{\ell=1}^{L} \sum_{k=1}^{K} \mathbb{1}_{i \in I_{\ell,k}} p(x_i \mid D_{\ell,k}, a_{\ell,k}) \right],
\]

abbreviating the respective training set as \( D_{\ell,k} = D_{[n] \setminus I_{\ell,k}} \), the memorization score becomes

When is memorization significant? A natural question is what values of the memorization score are significant and of potential concern. The memorization scores can be directly compared between different algorithm settings on the same data set, for instance to understand whether changes in hyperparameters or model architectures increase or decrease memorization. Statistical measures such as the mean, median, and skewness of the memorization score or the location of, say, the 95th percentile, can be informative when quantifying memorization of a particular model on a particular data set, but can not necessarily be compared between data sets. In practice, we also find that the distribution of the memorization score can differ between modes in the data set, such as distinct object classes. This can be understood by considering that the variability of observations of distinct classes likely differs, which affects the likelihood of the objects under the model, and in turn the memorization score. We will return to this question in Section 6.

4 Experiments

We next describe several experiments that advance our understanding of memorization in probabilistic deep generative models, with a focus on the variational autoencoder setting. Additional results are available in Supplement C. Code to reproduce our experiments can be found in an online repository.

Algorithm 1 Computing the Cross-Validated Memorization Score

Input: Algorithm \( A \), data set \( D \), repetitions \( L \), folds \( K \)

Output: \( M_i^{K\text{-fold}} \), \( \forall i \)

1: for \( \ell = 1, \ldots, L \) do
2: \( G_\ell \leftarrow \text{Random partition of } [n] \text{ into } K \text{ disjoint subsets} \)
3: for \( I_{\ell,k} \in G_\ell \text{ with } k = 1, \ldots, K \) do
4: \( a_{\ell,k} \leftarrow \text{Train } A \text{ on } D_{[n] \setminus I_{\ell,k}} \)
5: \( \pi_{\ell,k,i} \leftarrow \text{Compute } \log p(x_i \mid D_{[n] \setminus I_{\ell,k}}, a_{\ell,k}), \forall i \in [n] \)
6: end for
7: end for
8: \( U_i \leftarrow \text{LOGMEANEXP}(\{\pi_{\ell,k,i} : \ell \in [L], k \in [K], i \notin I_{\ell,k}\}), \forall i \)
9: \( V_i \leftarrow \text{LOGMEANEXP}(\{\pi_{\ell,k,i} : \ell \in [L], k \in [K], i \in I_{\ell,k}\}), \forall i \)
10: \( M_i^{K\text{-fold}} \leftarrow U_i - V_i, \forall i \)

\footnote{See: https://github.com/alan-turing-institute/memorization.}
We first explore memorization qualitatively. Figure 2 shows examples of observations with low, median, and high memorization scores in the CIFAR-10 data set, when learning the distribution with a convolutional VAE. Memorization scores range from about −180 in the top left of figure (a) to about 900 in the bottom right of figure (c), with a median of 97.

The distribution \( p_\theta(z \mid x) \) is generally intractable, so it is approximated using an inference model, or encoder, \( q_\phi(z \mid x) \). Analogously, the model \( p_\theta(x \mid z) \) is often referred to as the decoder. The VAE is trained by maximizing the lower bound on the evidence (ELBO), see (5), since

\[
\log p_\theta(x) \geq \mathbb{E}_{q_\phi(z \mid x)} \left[ \log p_\theta(x, z) - \log q_\phi(z \mid x) \right] = -D_{KL} (q_\phi(z \mid x) \| p(z)) + \mathbb{E}_{q_\phi(z \mid x)} \left[ \log p_\theta(x \mid z) \right],
\]

with \( D_{KL}(\cdot \| \cdot) \) the Kullback-Leibler (KL) divergence [46]. By choosing a simple distribution for the encoder \( q_\phi(z \mid x) \), such as a multivariate Gaussian, the KL divergence has a closed-form expression, resulting in an efficient training algorithm.

We use importance sampling on the decoder [47] to approximate \( \log p_\theta(x_i) \) for the computation of the memorization score, and focus on the MNIST [48], CIFAR-10 [49], and CelebA [50] data sets. We use a fully connected encoder and decoder for MNIST and employ convolutional architectures for CIFAR-10 and CelebA. For the optimization we use Adam [51] and we implement all models in PyTorch [52]. The memorization score is estimated using \( L = 10 \) repetitions and \( K = 10 \) folds. Additional details of the experimental setup and model architectures can be found in Supplement B.

4.2 Results

We first explore memorization qualitatively. Figure 2 shows examples of observations with low, median, and high memorization scores in the VAE model trained on CIFAR-10. While some of the highly-memorized observations may stand out as odd to a human observer, others appear not unlike those that receive a low memorization score. This shows that the kind of observations that are highly memorized in a particular model may be counterintuitive, and are not necessarily visually anomalous.

If highly memorized observations are always given a low probability when they are included in the training data, then it would be straightforward to dismiss them as outliers that the model recognizes as such. However, we find that this is not universally the case for highly memorized observations, and a sizable proportion of them are likely only when they are included in the training data. If we consider observations with the 5% highest memorization scores to be “highly memorized”, then we can check how many of these observations are considered likely by the model when they are included in the training data. Figure 3a shows the number of highly memorized and “regular” observations for bins of the log probability under the VAE model for CelebA, as well as example observations from both groups for different bins. Moreover, Figure 3b shows the proportion of highly memorized observations in each of the bins of the log probability under the model. While the latter figure shows that observations with low probability are more likely to be memorized, the former shows that a considerable proportion of highly memorized observations are as likely as regular observations when they are included in the training set. Indeed, more than half the highly memorized observations fall within the central 90% of log probability values (i.e., with \( \log P_D(x \mid D) \in [-14500, -12000] \)).

The memorization score can be a useful diagnostic tool to evaluate the effect of different hyperparameter settings and model architectures. For example, in Figure 4c we illustrate the distribution of the memorization score for a VAE trained on MNIST with two different learning rates, and we show the train and test set losses during training in Figure 4a. With a learning rate of \( \eta = 10^{-3} \) (blue curves), a clear generalization gap can be seen in the loss curves, indicating the start of overtraining (note the test loss has not yet started to increase). This generalization gap disappears when training with the smaller learning rate of \( \eta = 10^{-4} \) (yellow curves). The absence of a generalization gap is
(a) Counts

(b) Proportions

Figure 3: In (a) we show a histogram of the number of highly memorized (yellow) and regular (blue) observations for bins of the log probability under a VAE model trained on the CelebA data set (where \( n = 162,770 \)). The numbers above the bars correspond to the number of highly memorized observations in each bin. Randomly selected training observations from several bins are shown as well, with dashed lines illustrating the bin where the images in a particular column can be found. Images with a yellow frame are highly memorized whereas those with a blue frame have low memorization scores. Figure (b) shows the proportion of highly memorized and regular observations for each bin.

4.3 Memorization during training

To continue on the relation between memorization and overtraining, we look at how the memorization score evolves during training. In Figure 4b we show the 0.95 and 0.999 quantiles of the memorization score for the VAE trained on MNIST using two different learning rates. The quantiles are chosen such that they show the memorization score for the highly memorized observations. For both learning rates we see that the memorization score quantiles increase during training, as can be expected. However we also see that for the larger learning rate of \( \eta = 10^{-3} \) the memorization score quantiles already take on large values before the generalization gap in Figure 4a appears. This is additional evidence that determining memorization by the generalization gap is insufficient, and implies that early stopping would not fully alleviate memorization. Moreover, we see that the rate of increase for the peak memorization quantiles slows down with more training, which suggests that the memorization score stabilizes and does not keep increasing with the training epochs. This is reminiscent of [20], who demonstrated that their metric for memorization in language models peaks when the test loss starts to increase. The difference is that here memorization appears to stabilize even before this happens.

4.4 Nearest Neighbors

As discussed in the introduction, nearest neighbor illustrations are commonly used to argue that no memorization is present in the model. Moreover, hypothesis tests and evaluation metrics have been proposed that measure memorization using distances between observations and model samples [26, 27]. Because of the prevalence of nearest neighbor tests for memorization, we next demonstrate the relationship between our proposed memorization score and a nearest neighbor metric.

As an example of a nearest neighbor test, we look at the relative distance of observations from the training set to generated samples and observations from the validation set. Let \( S \subseteq \mathcal{X} \) be a

\[ \log P_A(x_i | D_{\{i\}} \setminus \{1\}) \approx -178 \] when the observation is excluded from the training data, and \[ \log P_A(x_i | D) \approx -97 \] when it is included, and the latter value is approximately equal to the average log probability of the other observations with the same digit.

\[ \text{count} \]

Regular

High mem.

\[ \log P_A(x | D) \]

Proportion

Regular

High mem.

\[ \text{proportion} \]
We describe two strategies that can be used to mitigate memorization in probabilistic generative models. First, the memorization score can be directly related to the concept of Differential Privacy (DP) \cite{54,55}. Note that the memorization score in (2) can be rewritten as

\[ \eta = 10^{-3}, \text{train} \]

\[ \eta = 10^{-3}, \text{test} \]

\[ \eta = 10^{-4}, \text{train} \]

\[ \eta = 10^{-4}, \text{test} \]

Since this must hold for all subsets \( D \) of \( \mathcal{X} \), it must also hold for the case where \( W = \{ x_i \} \). Moreover, when \( x_i \) is removed from \( D \) it can be expected that the largest change in density occurs at \( x_i \). It then follows that the memorization score can be bounded by employing \( \varepsilon \)-DP estimation techniques when

\[ \rho_i = \frac{\min_{x \in V} d(x_i, x)}{\min_{x \in S} d(x_i, x)} \] \hspace{1cm} (6)

If \( \rho_i > 1 \), then the nearest neighbor of \( x_i \) in the sample set is closer than the nearest neighbor in the validation set, and vice versa. Thus \( \rho_i > 1 \) suggests memorization is occurring, but as it depends on sampling it is expected to be very noise at an individual data point. Investigating if the average ratio for a set of observations differs significantly from 1 is an example of using hypothesis testing approaches to measure memorization.

\[ P_A(x_i | D) = \exp(M_i^{K \text{-fold}}) P_A(x_i | D_{[n]} \setminus \{i\}) \] \hspace{1cm} (7)

and recall that a randomized algorithm \( A \) is \( \varepsilon \)-differentially private if for all data sets \( D_1, D_2 \) that differ in only one element the following inequality holds

\[ P_A(W | D_1) \leq \exp(\varepsilon) P_A(W | D_2), \quad \forall W \subseteq \mathcal{X}. \] \hspace{1cm} (8)

We therefore argue that while nearest neighbor examples and hypothesis tests can be informative and may detect global memorization, to understand memorization at an instance level the proposed memorization score is to be preferred.

5 Mitigation Strategies

We describe two strategies that can be used to mitigate memorization in probabilistic generative models. First, the memorization score can be directly related to the concept of Differential Privacy (DP) \cite{54,55}. Note that the memorization score in (2) can be rewritten as

\[ P_A(x_i | D) = \exp(M_i^{K \text{-fold}}) P_A(x_i | D_{[n]} \setminus \{i\}) \] \hspace{1cm} (7)

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Since this must hold for all subsets \( W \) of \( \mathcal{X} \), it must also hold for the case where \( W = \{ x_i \} \). Moreover, when \( x_i \) is removed from \( D \) it can be expected that the largest change in density occurs at \( x_i \). It then follows that the memorization score can be bounded by employing \( \varepsilon \)-DP estimation techniques when
training the generative model, as this will guarantee that $M_{i}^{\text{LOO}} \leq \varepsilon, \forall i$. The converse is however not true: observing a maximum memorization score of $M_{i}^{\text{LOO}} = \varepsilon$ for a particular model does not imply that the model is also $\varepsilon$-DP. This connection of the memorization score to differential privacy offers additional support for the proposed formulation of the memorization score.

An alternative approach to limit memorization is to explicitly incorporate an outlier component in the model that would allow it to ignore atypical observations when learning the probability density. This technique has been previously used to handle outliers in factorial switching models [56] and to perform outlier detection in VAEs for tabular data [57]. The intuition is that by including a model component with broad support but low probability (such as a Gaussian with high variance), the log probability for atypical observations will be small whether they are included in the training data or not, resulting in a low memorization score. Other approaches such as using robust divergence measures instead of the KL-divergence in VAEs [58] may also be able to alleviate memorization.

6 Discussion

We have introduced a principled formulation of a memorization score for probabilistic generative models. The memorization score directly measures the impact of removing an observation on the model, and thereby allows us to quantify the degree to which the model has memorized it. We explored how the memorization score evolves during training and how it relates to typical nearest neighbor tests, and we have shown that highly memorized observations are not necessarily unlikely under the model. The proposed memorization score can be used to determine regions of the input space that require additional data collection, to understand the degree of memorization that an algorithm exhibits, or to identify training observations that must be pruned to avoid memorization by the model.

A question that requires further study is what constitutes a “high” memorization score on a particular data set. One of the main difficulties with this is that density estimates returned by a model, and thus probability differences, are not necessarily comparable between data sets [34]. We expect that future work will focus on this important question, and suggest that inspiration may be taken from work on choosing $\varepsilon$ in differential privacy [59, 60]. Furthermore, exploring the relationship between memorization and the double descent phenomenon [61, 62] could be worthy of investigation. Improving the efficiency of the estimator is also considered an important topic for future research.

If we want diversity in the samples created by generative models, then the model will have to learn to generalize to regions of the data manifold that are not well represented in the input data. Whether this is achieved by extrapolating from other regions of the space or fails due to memorization is an important question. Our work thus contributes to the ongoing effort to understand the balance between memorization and generalization in deep generative neural networks.
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A Memorized observations in recently proposed generative models

While experimenting with the proposed memorization score on CIFAR-10 [49], we noticed that the images of automobiles shown in Figure 6 are present in the training set multiple times (with slight variation). We subsequently spotted these images in the illustrations of generated samples in [7] (Figure 13, example (a) can be seen twice) and [63] (Figure 11 and Figure 13, truck class). These works are recently proposed probabilistic generative models that achieve impressive performance on sample quality metrics such as the inception score (IS) [35] and the Fréchet inception distance (FID) [36], and also achieve high log likelihoods. However, the fact that we were able to serendipitously spot images from the training set in the generated samples might suggest that some unintended memorization occurs in these models. We do not know if there are other images in the presented samples that are present in the training data.

Of course, spotting near duplicates of training observations is only possible because these models yield realistic samples. As we argue in the main text and as has been shown by previous works [32, 37], quality metrics such as IS and FID do not detect memorization.

We emphasize that this evidence is presented mainly to support the notion that (unintended) memorization can occur in probabilistic deep generative models, and to provide additional motivation for understanding and quantifying when and how memorization arises, which is the focus of our work.

B Experimental Details

This section describes additional details of the data sets, model architectures, and experimental setup.

B.1 Datasets

We use the MNIST [48], CIFAR-10 [49], and CelebA [50] data sets, which are widely used and are freely available for research purposes (although to the best of our knowledge explicit licenses are not available). For MNIST we binarize the images dynamically during training by considering each grayscale pixel value as the parameter of an independent Bernoulli variable, as is common [11, 64]. Images in all data sets are resized to $32 \times 32$ pixels for efficiency and ease of implementation. CIFAR-10 contains color images from 10 different categories and does not require further preprocessing. CelebA contains potentially identifiable images of faces of celebrities sourced from publicly available images on the Internet. We used the predefined cropping function of [11] to center the face region. For CIFAR-10 and CelebA we used random horizontal flips during training as data augmentation. All data sets have predefined train and test sets, and CelebA additionally has a validation set. We mainly used the training sets in the experiments, with the exception of the experiments for Figure 4a, which uses the MNIST test set, and the experiments in Section 4.4, which use the CelebA validation set.

B.2 Model Architectures

Let $L$ denote the size of the latent space and recall that $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^D$. For all experiments we used a Gaussian encoder with a learned diagonal covariance matrix, $q_\phi(z \mid x) = \mathcal{N}(z; \mu_\phi(x), \text{diag}(\sigma^2_\phi(x)))$ and a standard multivariate Gaussian prior on the latent variables, $p(z) = \mathcal{N}(z; 0, \mathbf{I}_L)$. As mentioned above we used a dynamically binarized version of the MNIST data set, and therefore used a Bernoulli likelihood for the decoder of the VAE. Both the encoder and decoder used fully connected layers with the ReLU activation on the intermediate layers [65] and a sigmoid activation on the output of the decoder that represents the parameter of the Bernoulli distribution. For MNIST we used $L = 16$. Full details of the model architecture are given in Table 1.

For CIFAR-10 and CelebA we used a Gaussian likelihood for the decoder, employed uniform dequantization on the pixel values [66], and trained the models in logit space following [67]. For both data sets
we used Adam [51] to optimize the parameters of the model with learning rate $\eta = 10^{-3}$ for the main experiments and $\eta = 10^{-4}$ for the experiments on MNIST in Section 4.2. We used a batch size of 64 and left the remaining parameters for Adam at their default values in PyTorch [52]. For both MNIST and CIFAR-10 we trained for 100 epochs, and used 50 epochs for CelebA. These settings were chosen by taking into consideration the available computational resources and aimed to avoid overtraining. The parameter settings were determined through some preliminary experimentation. Electricity needed for the experiments came from carbon-free sources. Experiments were conducted on a desktop machine running Arch Linux, using an NVIDIA GeForce GTX 1660 SUPER GPU, 32GB of RAM, and an AMD Ryzen 5 3600 processor. Total wall-clock time was about 200 hours for the main results, excluding preliminary experimentation.}

As mentioned in the main text, importance sampling was used to approximate $p(x)$, such that

$$p(x) \approx \frac{1}{N} \sum_{i=1}^{N} \frac{p_\theta(x | z_i) p(z_i)}{q_\phi(z_i | x)}, \quad z_i \sim q_\phi(z_i | x).$$

(9)

This was computed in log space for numerical accuracy. For MNIST we used $N = 256$ and for CIFAR-10 and CelebA we used $N = 128$ samples.

Table 1: Model architectures used for the experiments. We used fully connected (FC) layers with the RELU activation for MNIST, with the SIGMOID activation on the decoder. For CIFAR-10 and CelebA we used convolutional layers for the encoder (CONV2D with kernel size 4, stride 2, and padding 1), followed by batch normalization (BN), and the Leaky RELU activation (LReLU, using slope 0.2). For these data sets the decoder consists of transposed convolution layers (CONVT2D, with kernel size 4, stride 2, and padding 1 except for the layer marked with an asterisk (*), which uses kernel size 2, stride 1, and padding 0 to get the correct output size), followed by batch norm and the RELU activation. We use the abbreviations ENCBlock($C_1, C_2$) = CONV2D($C_1, C_2$) $\rightarrow$ BN $\rightarrow$ LReLU and DECBlock($C_1, C_2$) = CONVT2D($C_1, C_2$) $\rightarrow$ BN $\rightarrow$ RELU.

| Data set   | Encoder network                                                                 | Decoder network                                                                 | Likelihood ($p_\theta(x | z)$) |
|------------|---------------------------------------------------------------------------------|---------------------------------------------------------------------------------|-------------------------------|
| MNIST      | FC(1024, 512) $\rightarrow$ RELU $\rightarrow$ FC(512, 256) $\rightarrow$ RELU | FC(L, 256) $\rightarrow$ RELU $\rightarrow$ FC(512, 1024) $\rightarrow$ SIGMOID | $\mathcal{B}(x_i; \pi_i(z))$ |
| CIFAR-10   | CONV2D($C, F$) $\rightarrow$ LReLU $\rightarrow$ ENCBlock($F, 2F$) $\rightarrow$ DECBlock$^*$($L, 8F$) | $\rightarrow$ DECBlock(8F, 4F) $\rightarrow$ DECBlock(4F, 2F) $\rightarrow$ DECBlock(2F, F) $\rightarrow$ CONVT2D($F, 2C$) | $\mathcal{N}(x; \mu_\theta(z), \text{diag} (\sigma_\theta(z)))$ |
| CelebA     | Same as for CIFAR-10, except final layer uses CONVT2D($F, C$)                   | Same as for CIFAR-10, except final layer uses CONVT2D($F, C$)                   | $\mathcal{N}(x; \mu_\theta(z), \gamma_\theta I_D)$ |

we used an architecture similar to DCGAN [68], consisting of four convolutional layers in the encoder, each followed by batch normalization [69] and leaky RELU activation [70], and five transposed convolution layers in the decoder followed by batch normalization and RELU, see Table 1. For CIFAR-10 the Gaussian likelihood on the decoder was parameterized as $p_\theta(x | z) = \mathcal{N}(x; \mu_\theta(z), \text{diag} (\sigma_\theta(z)))$ and for CelebA we used the simpler formulation $p_\theta(x | z) = \mathcal{N}(x; \mu_\theta(z), \gamma_\theta I_D)$ with a learned parameter $\gamma_\theta$, as the more general decoder was unnecessary. For CIFAR-10 and CelebA the number of input channels is $C = 3$ and we used $L = 64$ and $L = 32$, respectively. For the convolutional networks the feature map multiplier was set to $F = 32$ (see Table 1).

B.3 Training details

We used Adam [51] to optimize the parameters of the model with learning rate $\eta = 10^{-3}$ for the main experiments and $\eta = 10^{-4}$ for the experiments on MNIST in Section 4.2. We used a batch size of 64 and left the remaining parameters for Adam at their default values in PyTorch [52]. For both MNIST and CIFAR-10 we trained for 100 epochs, and used 50 epochs for CelebA. These settings were chosen by taking into consideration the available computational resources and aimed to avoid overtraining. The parameter settings were determined through some preliminary experimentation and were not extensively optimized. Experiments were conducted on a desktop machine running Arch Linux, using an NVIDIA GeForce GTX 1660 SUPER GPU, 32GB of RAM, and an AMD Ryzen 5 3600 processor. Total wall-clock time was about 200 hours for the main results, excluding preliminary experimentation. Electricity needed for the experiments came from carbon-free sources.
C Additional Results

Below we show additional results that confirm the findings presented in the main text for different data sets.

C.1 Qualitative Illustrations

In Figures 7, 8, and 9 we illustrate observations with low, median, and high memorization scores for a VAE trained on MNIST using $\eta = 10^{-3}$, MNIST using $\eta = 10^{-4}$, and CelebA, respectively. As can be seen from the figures and as discussed in the main text in Section 4.2, while some of the highly memorized observations have visual anomalies, others are not unlike those that receive low memorization scores. For instance, for the VAE trained on MNIST with learning rate $\eta = 10^{-4}$, we see that images from both the low and high memorization groups have active pixels that are not part of the digit (compare, for instance, the images of 9s on the middle of the bottom rows of Figure 8a and Figure 8c).

![Figure 7: Observations with low, median, and high memorization scores in the MNIST data set, for a VAE trained using learning rate $\eta = 10^{-3}$. Memorization scores range from about -18 in the top left of figure (a) to about 200 in the bottom right of figure (c), with a median of 4.4.](image)

![Figure 8: Observations with low, median, and high memorization scores in the MNIST data set, for a VAE trained using learning rate $\eta = 10^{-4}$. Memorization scores range from about -13 in the top left of figure (a) to about 80 in the bottom right of figure (c), with a median of 3.5.](image)

![Figure 9: Observations with low, median, and high memorization scores in the CelebA data set when the density is learned using a convolutional VAE. Memorization scores range from about -450 in the top left of figure (a) to about 6500 in the bottom right of figure (c), with a median of about 60.](image)
C.2 Outliers vs. Memorization

Figures 10 and 11 replicate the experiments shown in Figure 3 in the main text for the VAE trained on the MNIST data set using two different learning rates. We again see that relatively high memorization is not exclusive to observations that receive a low probability under the model. Note that for this particular data set the density estimated by the VAE is slightly multimodal, with the peak in density for higher values of $\log P_A(x | D)$ corresponding to observations for digit 1.

Figure 10: In (a) we show a histogram of the number of highly memorized (yellow) and regular (blue) observations for bins of the log probability under a VAE model trained on the MNIST data set using learning rate $\eta = 10^{-3}$. The numbers above the bars correspond to the number of highly memorized observations in each bin (for MNIST, $n = 60,000$). Randomly selected training observations from several bins are shown, with dashed lines illustrating the bin where the images in a particular column can be found. Images with a yellow frame are highly memorized whereas those with a blue frame have low memorization scores. Figure (b) shows the proportion of highly memorized and regular observations for each bin.

Figure 11: Similar to Figure 10, but for the VAE trained on MNIST with learning rate $\eta = 10^{-4}$.
C.3 Nearest Neighbors

The nearest neighbor experiments demonstrated in Section 4.4 are repeated below in Figures 12 and 13 for the VAEs trained on the MNIST data set using learning rates of $10^{-3}$ and $10^{-4}$. For these models and data set we again do not see a clear relation between the nearest neighbor distance ratio $\rho_i$ and the proposed memorization score $M_{\text{K-fold}}^i$, as discussed in the main text.

Figure 12: Illustration of the nearest neighbor distance ratio in (6) compared to the memorization score for a VAE trained on MNIST using a learning rate of $\eta = 10^{-3}$. We present the average of $\rho_i$ for bins of the memorization score of width 2, and show error bars representing the confidence interval of the standard error of the mean of distance ratio measurements in each bin. The horizontal axis in figure (a) trims off one observation at $M_{\text{K-fold}}^i \approx 210$ for clarity. Figure (b) shows the distribution of the distance ratio for observations with a high memorization score (top 5%) and the regular ones.

Figure 13: Similar to Figure 12 but for the VAE trained on MNIST using a learning rate of $\eta = 10^{-4}$. The horizontal axis in figure (a) trims off one observation at $M_{\text{K-fold}}^i \approx 80$ for clarity.