Abstract

This paper proposes a new type of implicit generative model that is able to quickly learn a latent representation without an explicit encoder. This is achieved with an implicit neural network that takes as inputs points in the coordinate space alongside a latent vector initialised with zeros. The gradients of the data fitting loss with respect to this zero vector are jointly optimised to act as latent points that capture the data manifold. The results show similar characteristics to autoencoders, but with fewer parameters and the advantages of implicit representation networks.

1 Introduction

Observable data in nature has some parameters which are known, such as local coordinates, but also some unknown parameters such as how the data is related to other examples. Generative models, which learn a distribution over observables, are central to our understanding of patterns in nature and allow for efficient query of new unseen examples.

In recent years, deep generative models have received significant interest due to their ability to capture a broad set of features when modelling data distributions, offering both direct applications as well as benefits for downstream tasks. A number of methods have been proposed such as Variational Autoencoders (VAEs, Figure 1a), which learn to encode the data to a latent space that follows a normal distribution permitting sampling (Kingma and Welling, 2014). Generative Adversarial Networks (GANs) have two competing networks, one which generates data and another which discriminates from implausible results (Goodfellow et al., 2014). Variational Auto-Decoders (VADs) (Zadeh et al., 2019) do not require an encoder, but to obtain a latent vector for a sample, they require iterative gradient updates. Autoregressive Models (Van Den Oord et al., 2016) decompose the data distribution as the product of conditional distributions and Normalizing Flows (Rezende and Mohamed, 2015) chain together invertible functions; both methods allow exact likelihood inference. Energy-Based Models (EBMs) map data points to energy values proportional to likelihood thereby permitting sampling through the use of Monte Carlo Markov Chains (Du and Mordatch, 2019). In summary, each class of method comes with their own advantages and disadvantages, but they all take considerable time to approximate the data.

Implicit representation learning (Park et al., 2019; Tancik et al., 2020), where a network is trained on data parameterised continuously rather than in discrete grid form, has seen a surge of interest due to the small number of parameters, speed of convergence, and ability to model fine details. In particular, sinusoidal representation networks (SIRENs) (Sitzmann et al., 2020b) achieve impressive results, modelling complex signals with high precision, thanks to their use of periodic activations paired with carefully initialised MLPs. So far, however, these models have currently been limited to modelling single data samples, or use an additional hypernetwork or meta learning (Sitzmann et al., 2020a) to estimate the weights of a simple implicit model which adds significant complexity.
This paper proposes Gradient Origin Networks (GONs), which are a new type of generative model (Figure 1b) where unknown parameters in the latent space are initialised at the origin. This zero vector is concatenated with the known coordinate parameters, which becomes the inputs of an implicit representation network \( F \) with a prior over the gradients (a SIREN whose gradients are normally distributed). This means we can compute gradients of the data fitting loss with respect to these inputs, and jointly optimise for the new latents. At inference, the latent vector can be sampled in a single step without requiring iteration.

2 Method

Consider some dataset \( x \sim p_d \) of a continuous or discrete variable \( x \) that can be represented as a set of coordinates \( x = \{ (c, \Phi_x(c)) \} \) for coordinate \( c \in \mathbb{R}^n \) and corresponding data \( \Phi: \mathbb{R}^n \to \mathbb{R}^m \). As supported by the manifold hypothesis, data samples \( x \) can be represented as low dimensional latent vectors \( z \sim \mathbb{R}^k \); this property is taken advantage of by latent variable generative models such as VAEs. Concatenating a latent variable with coordinates therefore positions data points on a manifold that describes the full dataset, acting as higher dimensional coordinates. An expressive neural network \( F: \mathbb{R}^{n+k} \to \mathbb{R}^m \) can be trained on this space to mimic \( \Phi \) by minimising the Gradient Origin Network loss function:

\[
G_x = \int \mathcal{L}(\Phi_x(c), F(c \oplus -\nabla z_0 \int \mathcal{L}(\Phi_x(c), F(c \oplus z_0))dc)) \, dc,
\]

where both integrations are performed over the space of coordinates, \( c \oplus z \) represents concatenation, \( z_0 = 0 \), and \( \mathcal{L}(a, b) \) is a distance metric between \( a \) and \( b \) that acts as a reconstruction loss (\( L^2 \)-norm is used for the experiments in this paper). From this equation we can see a strong relationship with autoencoder approaches. By negating the gradient of the distance function with respect to the origin, \( z = -\nabla z_0 \int \mathcal{L}(\Phi_x(c), F(c \oplus z_0))dc \), we obtain a latent vector that minimises the reconstruction loss is obtained in a single step, thereby playing a similar role to an explicit encoder. \( F \) in turn can be viewed as a decoder, with the outer loss term determining the overall reconstruction quality. The use of a single network to perform both roles has the advantage of simplifying the overall architecture, avoiding the need to balance networks, and avoiding bottlenecks. In particular, we parameterise \( F \) with a SIREN, finding that it is capable of modelling both high and low frequency components in high dimensional spaces. Additionally, the weight initialisation encourages the posterior to approximately follow a multivariate normal distribution before overfitting occurs thus permitting sampling during this time.

There are a number of interesting generalisations that make this approach applicable to other tasks. One possibility is modality conversion, where in addition to \( c \) and \( z \), \( F \) also takes the content of the source signal and outputs the target signal. In Equation 1 we use the same \( \mathcal{L} \) and \( \Phi \) in both the inner term and outer term however it is possible to use different functions; through this, training a GON concurrently as a generative model and classifier is possible. It is also possible through some minor modifications to train a Gradient Origin Network solely as a classifier:

\[
C_x = \mathcal{L}_{CE}(y, f \left( -\nabla z_0 \int \mathcal{L}(\Phi_x(c), F(c \oplus z_0))dc \right)),
\]

where \( y \) are the target labels, \( f \) is a single linear layer followed by softmax, and \( \mathcal{L}_{CE} \) is the categorical cross entropy loss function.
3 Results & Discussion

In this section, we show that Gradient Origin Networks are not only competent autoencoders but also generative models in their own right. We evaluate on a variety of image datasets using simple models of approximately 4 hidden layers of 256 units trained with Adam (Kingma and Ba, 2017).

The representation ability of GONs is shown in Figure 2 where we overfit to large image datasets using a relatively small number of parameters. In particular, Figure 2a shows MNIST can be well-represented with just 4,385 parameters (a SIREN with 3 hidden layers each with 32 hidden units, and 32 latent dimensions). The structure of the GON latent space is shown by sampling latent codes from pairs of images, and then spherically interpolating between them to synthesise new samples (Figure 3). These samples are shown to capture variations in shape (the shoes in Figure 3b), size, and rotation (Figure 3d). To obtain new samples, we train GONs with early stopping, ensuring that a multivariate distribution follows the true prior. Samples (see Figure 4) are high quality, diverse, and mostly non-blurry. GONs are also found to converge quickly; we plot reconstructions at multiple time points during the first minute of training (Figure 5). After only 3 seconds of training on a single GPU, a substantial amount of signal information from MNIST is modelled. Figure 6 shows a GON trained as a classifier where the latent space is squeezed into 2D for visualisation (Equation 2) and Figure 7 shows that the gradients after 800 steps of training are approximately normally distributed.

(a) 4,385 parameters (b) 297k parameters (c) 270k parameters (d) 270k parameters (e) 396k parameters

Figure 2: Overfitting small GONs with few parameters demonstrates their representation ability.

(a) MNIST (b) FashionMNIST (c) Small NORB (d) COIL20 (e) CIFAR-10

Figure 3: Spherical linear interpolations between points in the latent space for trained GONs using different datasets (approximately 2-10 minutes training per dataset on a single GPU).

(a) 4,385 parameters (b) 70k parameters (c) 270k parameters (d) 270k parameters (e) 270k parameters

Figure 4: Random samples drawn from the multivariate distributed latent space for different networks, which are trained with early stopping to ensure quality samples.
Despite similarities with autoencoder approaches, the absence of an explicit encoding network offers several advantages. This simplicity ensures that latent codes must be utilised, unlike VAEs with powerful decoders (Chen et al., 2017). Similar to GONs, Normalizing Flow methods are also capable of encoding and decoding with a single set of weights. They, however, achieve this using invertible functions thereby allowing the network to run in reverse. This requires considerable architectural restrictions that affect performance and make them much less parameter efficient. GONs on the other hand use gradients as encodings which allow arbitrary functions to be used.

Due to the integration terms in Equation 1 computation time scales with data dimension. This makes training slower for very high dimensional data, although we have not yet investigated Monte Carlo integration. While learning rates are quite resilient, some tuning is required. Despite these disadvantages, GONs are stable, capable of generating quality samples with an exceptionally small number of parameters, and converge to diverse results in a matter of seconds. Nevertheless, there are avenues to explore so as to improve the quality of samples and scale to more complex datasets. In particular, it would be beneficial to focus on how to better sample these models, perform formal analysis of the gradients, and assess whether the distance function could be improved as with adversarial strategies.

**Availability**

The source code is available under the MIT license on GitHub at https://github.com/cwkx/GON. This implementation uses PyTorch and all reported experiments use a Nvidia RTX 2080 Ti GPU.

**Conclusion**

In conclusion, we have proposed a new type of implicit generative model that captures the dataset without requiring an explicit encoder. By initialising a latent vector of our unknown parameters with zeros, we have shown that it is possible to compute the gradients of the data fitting loss with respect to this origin, and then jointly fit the data while learning this new point of reference in the latent space. The results show this approach is able to represent datasets using a small number of parameters, with the advantage of implicit representation networks being able to model many different types of discrete signals.
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