Title	指向性生成ネットワーク:あらかじめ用意されたデータセットを用いない構造化オブジェクトの生成方法に関する研究
Author(s)	伊藤, 康明
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Description	Supervisor: NGUYEN, Minh Le, 先端科学技術研究科, 博士

Abstract

This research proposes a new method of machine learning for structured artifacts. The technique is called Directional Generative Networks (DGN). This study demonstrates that this method has the potential to be industrially applicable. Here, structured artifacts mainly mean industrial products that are physically tangible. Examples are the structure of a building, the molecular structure of a medicine, etc.

Although various industrially applicable machine learning methods have been proposed, their application to the design or search process of physical products such as the above is limited. The reasons for the limited application are:

1. Product data and business processes are not easily disclosed as trade secrets, and even if they are disclosed, the amount of data is often insufficient,
2. It is challenging to avoid over-fitting due to a lack of data and
3. The difficulty of avoiding biases originating from the data due to the small amount of data.

The performance of machine learning depends on the quantity and quality of the data set. It is presumed that companies dealing with products with physical entities must use machine learning sparingly for the above reasons.

In this study, the structure of physically tangible products is focused on. DGN, the proposal method, is examined to compensate for the lack of data by combining a function that evaluates based on the structure with a machine learning model. Methods or functions to evaluate a product based on its structure are often publicly available. One of the neural network models that make up the DGN is an approximation function of the evaluation function. It is well-known that a neural network with multi-layers can be an approximate function for any function. The scheme of DGN, combining the approximate function as an estimator with a generator, is similar to Generative Adversarial Networks(GAN) generator and discriminator. However, the way ground truth is given differs between GAN and DGN. The return value of the evaluation function is used as the ground truth when training the estimator in DGN. When training the generator, the weights of the estimator, the approximate function model, are fixed. The favorable value the designer wants as the evaluation function output is given as a constant target value. This gives the direction of the training to the generative model. In DGN, the generator and the estimator are trained alternately, like the generator and discriminator are trained alternately in GAN. If the estimator is trained enough, the outputs of the estimator are almost the same as the outputs of the evaluation functions. If the generator is trained enough, the outputs of the generator represent desired products that obtain the desired values of evaluation functions' results. Due to the methods above, you do not have to prepare datasets for the training.

Evolutionary Algorithms(EA) use not training data but feedback from the environment. EA using the evaluation functions as the environment can get suitable results. However, if the complexity of the product parts combination is increased, it will become challenging to get the desired results. On the

other hand, due to training DGN with a gradient of exploration field, DGN may get more suitable results than EA in complex problems.
In this research, DGN was applied to the structural design of buildings and the molecular discovery of drugs. The appropriate representation of data and model structure are examined for each task and confirmed its usefulness for both tasks. If the generator and the estimator are well-trained, the generator can generate various products with the desired structure with a sound output(s) of the evaluation function.
Structural design of buildings and molecular search for pharmaceuticals are completely different industrial fields. It was confirmed that the DGN method can be used in these technologically distant industrial fields. Therefore, it may be applied in various industrial fields, even if a sufficient data set cannot be prepared for the intended training.

Keywords: Generative Model, Unsupervised Learning, Evolutionary Algorithms, Generative Adversarial Networks