Inverse Design with Variational Auto-encoder

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Abstract

Inverse design problems are frequently encountered in many fields of engineering and science. Among the different types of design problems, those involved in layout design are of particularly challenging because of the difficulties encountered in defining a set of independent design variables that characterize the unknown layout. Topological optimization offers an effective method for solving this type of problem. Successful applications of topological optimization can be found in many areas ranging from structure design to design of metamaterials. One major challenge in the current topological optimization techniques is the control of the shape of the optimal layout. Shape control is necessary due to, for example, the need for including a few explicit shapes in the design, manufacturing constraints such as minimum feature size, aesthetic consideration and connection/installation requirements. Despite the continuous efforts on the methodology development, an efficient and general method is yet to come.

In this talk, we will report our recent work on using variational auto-encoder (VAE) [1], a machine learning technique, to conduct inverse design. In recent years, machine-learning techniques have shown remarkable success in various disciplines including image recognition, natural language processing, quantum mechanics, and material design. As one of the most successful machine learning techniques, VAE has emerged as a popular method for unsupervised learning of complicated distributions of datasets and generating new and similar data sets. It has been successfully applied to image processing [2] and various physical problems [3]. We show that VAE can also be applied to solving inverse design problems, and shape control can be easily handled in this approach. In addition, this approach is non-gradient based and can be very efficient. Once trained, the network can quickly produce designs with similar objectives. Examples involving inverse design of surface diffusion and microlithography will be illustrated to demonstrate the performance of the proposed approach.

Keywords: Inverse design, viriational auto-encoder, artificial neural network, surface diffusion, computational microlithography

References

- [1] Kingma, D.P., Welling, M. (2013): Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114.
- [2] Sohn, K., Lee, H., Yan, X. (2015): Learning structured output representation using deep conditional generative models. In: Advances in Neural Information Processing Systems, pp. 3483-3491.
- [3] Rocchetto, A., Grant, E., Strelchuk, S., Carleo, G., Severini, S. (2017): Learning hard quantum distributions with variational autoencoders. arXiv preprint arXiv:1710.00725.