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TEMImageNet, AtomSegNet and TomoFillNet, open-source libraries and models that enable defect localization in 2D and 3D atomic resolution images

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Deep learning schemes have already impacted areas such as cognitive game theory (e.g., computer chess and the game of Go), pattern (e.g., facial or fingerprint) recognition, event forecasting, and bioinformatics. They are beginning to make major inroads within physics, chemistry and materials sciences and hold considerable promise for accelerating the discovery of new theories and materials. In this talk, I will introduce deep convolutional neural networks and how they can be applied to the computer vision problems in transmission electron microscopy and tomographic imaging for atomic defect localization in nanomaterials. [1-4]

Electron tomography, as an important 3D imaging method, offers a powerful method to probe 3D structure of materials from the nano- to the atomic-scale. However, as a grant challenge, information loss and artifacts induced by missing-wedge greatly hindered us from obtaining 3D structure of nano-objects with high fidelity. Mathematically speaking the tomography inverse problem is ill defined because the solution is non-unique. Traditional methods, such as weighted back projection (WBP) and simultaneous algebraic reconstruction technique (SART), lack the ability to recover the unacquired project information as a result of the limited tilt range; consequently, the tomograms reconstructed using these methods are distorted and contaminated with the elongation, streaking, and ghost tail artifacts. Total variance minimization (TVM) which combines iterative reconstruction and regularization has been developed to recover the lost information and reduce artifacts induced by missing-wedge. However, one of the caveats of TVM is that it is not parameter free and computationally expensive. These aside, the real problem of TVM or any generalized TVM approach is that they are bound to one regularization that promotes one prior constraint on the solution which may or may not be suitable for the object of interest. In this paper, we apply machine learning, particularly deep learning to tackle this problem. Fig. 1 shows that the unacquired projection information can be effectively recovered by joining two inpainting generative adversarial network (GAN) models in the sinogram and tomogram domains separately [2,4]. We first design a sinogram filling model based on the use of Residual-in-Residual Dense Blocks in a Generative Adversarial Network (GAN). Then, an U-net structured Generative Adversarial Network to reduce the residual artifacts. The joint deep-learning model achieves remarkable tomography reconstruction quality for missing-wedge sinograms with a missing angle as large as 45 degrees. The improved performance of this model stems from the fact that the problem was decoupled into two separate domains. In each domain, a unique solution, based on trained 'priors', can be learned efficiently. In addition, compared with regularization-based method, this deep-learning method is an end-to-end method without any hyperparameters. Its performance is independent of prior knowledge or the human operator's experience in setting hyperparameters. [5]

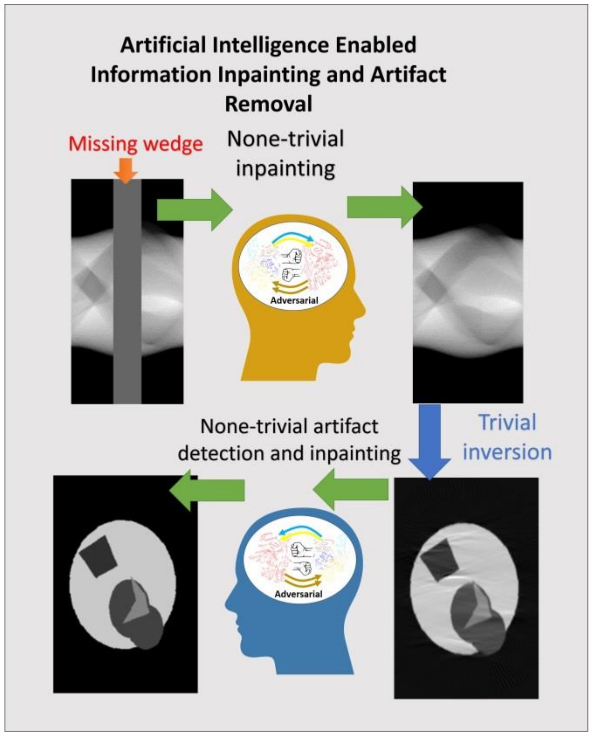

Figure 1. A newly proposed deep-learning approach that utilize two generative adversarial models to jointly fill the missing-wedge information and remove artifacts for electron tomography reconstructions.

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