The role of convolutional neural networks in scanning probe microscopy: a review

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1 Introduction

Scanning Probe Microscopy (SPM) is a powerful tool for extracting nanoscale information, yet interpreting its images can be a challenge. Unlike electron microscopes, SPM requires complex and time-consuming processes to generate high-resolution images, involving large amounts of data. SPM produces multimodal data, including topography and electronic properties, making it difficult to distinguish relevant features without advanced image processing techniques and expert judgment. Analyzing these images requires deep knowledge of SPM principles and the ability to identify key features. To address this, the article explores the use of Convolutional Neural Networks (CNNs), a type of deep learning algorithm, to automate and accelerate the analysis [1].

2 Review

2.1 Machine learning (ML)

Machine learning (ML) is a branch of artificial intelligence that allows computers to learn from data without being explicitly programmed. It is typically categorized into three main types of learning: supervised, unsupervised and reinforcement learning. Conventional machine learning methods typically involve converting image data into one-dimensional vectors or extracting features manually, which may result in a loss of information.

2.2 Deep learning (DL)

Deep learning (DL), a subset of machine learning, includes various types for specific tasks. In image classification, a model consists of an input layer, hidden layers, and an output layer. The input layer processes the image, which is passed through hidden layers to extract features. More hidden layers allow the model to learn more complex, non-linear patterns. The output layer provides the final classification result.

2.3 Convolutional neural network (CNN)

Category labels are supplied with images. Together these create the dataset that will be used to train the model and evaluate it.

- **Convolutional layer:** A convolutional layer consists of filters, each filter is an array that contains parameters. Each filter is convoluted with each image resulting in mapping of the extracted features (called feature maps) the number of feature maps is the number of filters applied to the image. In CNNs, the parameters of the filters are not known *a priori* and the CNN model learns the best parameters during the training process to extract the features that best differentiate between images from different categories.

- **Activation layer:** The activation layer is applied to the feature maps to activate the maps. This is a non linear operation that produce non linear decision boundaries.
- **Pooling layer:** Is used for down sampling the extracted features in the feature maps and is usually applied after the activation layer. It compresses the feature maps while keeping the most important information of the features.
- **Operation block:** A combination of convolutional layer + activation layer + pooling layer forms an operation block, usually this block is applied several times. Each block corresponds to a hidden layer. The number of filters can be increased or remain the same in each successive block, and the feature maps are down sampled leading to dimension reduction while keeping the most important information.
- **Flatten layer:** The flatten layer enables the use of linear algebraic operations in further mathematic processing. This is followed by a dense layer, that is, a "fully connected layer" that connects the flattened output to subsequent neurons.
- **Output layer**: The output layer is the last layer that contains neurons. The number of neurons is the number of image categories in the image classification task.
- **Output activation function:** A number between 0-1 is assigned for each image corresponding to the probability that it belongs to a specific category.
- **Loss function:** The loss function computes the error between the network's predictions and the true labels, guiding the optimization process during training.

3 Application of CNN with SPM

CNNs are now widely used in SPM to improve image analysis. They help by automatically finding important features in images, even when the pictures are noisy or of low quality. SPM images often take a long time to create, and CNNs can speed up the process by enhancing low-resolution images. These networks also help remove unwanted background and other errors from the images. They can detect small differences in sample features, such as changes in cell structure, more reliably than manual methods. However, they usually need a large amount of training data, which can be hard to get for SPM applications. They also require careful tuning and can overfit if the data is not varied enough. The use of CNNs in SPM makes it easier to analyze complex samples accounting for all variables. CNN was used to distinguish healthy blood samples from diseased samples infected with malaria based on 122 and 109 images [1]. The images were created with High-Speed Atomic Force Microscopy (HS-AFM). The CNN achieved an accuracy of 99.0% and 96.6%, respectively. Additionally, the CNN was used for class activation to mark relevant areas for each sample type.

4 Conclusion

In conclusion, the integration of CNNs with SPM has proven to be a valuable advancement for image analysis. These networks significantly reduce the time needed to capture and process high-resolution images. By automatically identifying important features and removing noise, CNNs enhance the overall quality and consistency of SPM data. Although they require a substantial amount of training data and careful tuning to avoid overfitting. The review of machine learning and deep learning concepts, along with a detailed breakdown of CNN components, demonstrates the solid and technical foundation upon which these techniques are built. CNNs not only streamline the extraction of sample details but also support the analysis of complex multimodal data. Future research should focus on minimizing the data requirements and enhancing model robustness. Overall, CNNs are transforming SPM into a more efficient and reliable tool for studying materials and biological samples.

References

[1] Ido Azuri, Irit Rosenhek-Goldian, Neta Regev-Rudzki, Georg Fantner, and Sidney R. Cohen. The Role of Convolutional Neural Networks in Scanning Probe Microscopy: A Review. *Beilstein Journal of Nanotechnology*, 12:878–901, 2021.