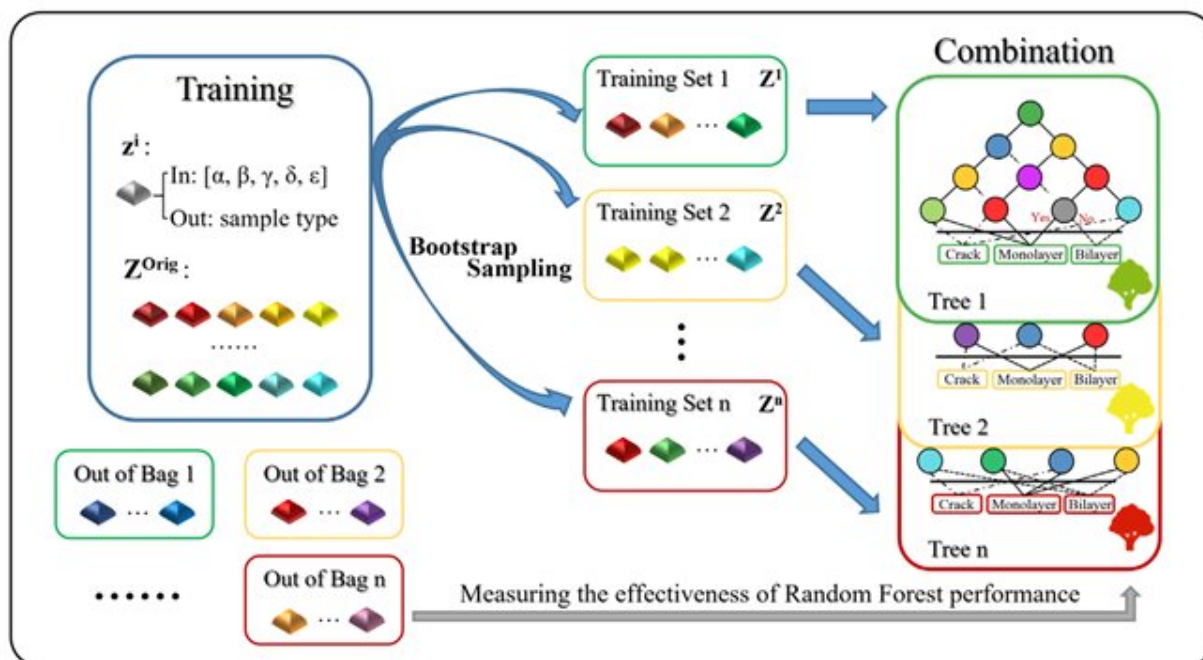


Scientists propose machine learning method for 2-D material spectroscopy

November 19 2020, by Zhang Nannan



Basic architecture of the learning procedure in the random forest method.
Credit: SIOM

Machine learning is an important branch in the field of artificial intelligence. Its basic idea is to build a statistical model based on data and use the model to analyze and predict the data. With the rapid development of big data technology, data-driven machine learning algorithms have begun to flourish in various fields of materials research.

Recently, a research team led by Prof. Wang Jun from the Shanghai Institute of Optics and Fine Mechanics of the Chinese Academy of Sciences (CAS) proposed a recognition method to distinguish the monolayer continuous film and random defect areas of two-dimensional (2-D) semiconductors using the [machine learning](#) method with Raman signals.

Their work revealed the application potential of machine learning algorithms in the field of 2-D material spectroscopy, and was published in *Nanomaterials*.

The Raman spectrum of 2-D materials is very sensitive to molecular bonding and sample structure, and can be used for research and analysis of chemical identification, morphology and phase, internal pressure/stress, and composition. Although Raman spectroscopy provides enough information, how to mine the depth of information and use multiple information to make comprehensive decisions still needs further research.

In this study, the researchers used various feature information including the Raman frequency and intensity of MoS₂. They used the bootstrap sampling process to obtain sub-training sets containing different spatial location information, and established a random forest [model](#) composed of the certain number of decisions through the learning procedure.

When a new sample point enters the model for prediction and judgment, each decision tree in the random forest will make independent judgments, and then give relatively accurate prediction results through majority voting. In addition to judging the monolayer and bilayer samples, the model can also predict cracks and randomly distributed nuclei that are easily introduced during sample growth.

The research program proposed in this work introduces machine

learning algorithms into the study of two-dimensional material spectroscopy, and can be extended to other materials, providing important solutions for material characterization in different fields.

More information: Yu Mao et al. Machine Learning Analysis of Raman Spectra of MoS₂, *Nanomaterials* (2020). [DOI: 10.3390/nano10112223](https://doi.org/10.3390/nano10112223)

Provided by Chinese Academy of Sciences

Citation: Scientists propose machine learning method for 2-D material spectroscopy (2020, November 19) retrieved 21 May 2024 from <https://phys.org/news/2020-11-scientists-machine-method-d-material.html>

<p>This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.</p>
--