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Automated grouping of spatially distributed detectors in neutron time-of-flight experiments based on multivariate similarity

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Nowadays, in neutron time of flight measurements, there are experimental setups in which many detectors record data during a single experiment. It is usually desirable to be able to sum several spectra in order to increase counting statistics, and therefore decrease uncertainties, for further analysis. A problem arises in time-of-flight experiments when the available spectra are acquired with a set of spatially distributed detectors, each forming a different source-sample-detector angle and at different sample-detector distances. Since these spectra record the neutron's time of flight after scattering, and the neutron scattering depends on the Q vector, then these spectra are not arbitrarily summable. In this work, we propose an automated methodology for wisely adding spectra based on their multivariate similarity by means of machine learning techniques, such as k nearest neighbors combined with T-distributed Stochastic Neighbor Embedding (t-SNE). We exemplify it in the effective temperature determination of hydrogen in ethane and triphenylmethane samples by means of Deep Inelastic Neutron Scattering, measured at the VESUVIO spectrometer (ISIS facility, UK). The proposed methodology can be applied in other time-of-flight experiments, in which detectors located at different angles record complete spectra, and with this method their degree of compatibility can be determined.

Primary author: ROBLEDO, Jose (JCNS-2 Forschungszentrum Jülich)

Co-authors: Dr CANTARGI, Florencia (CNEA); DAWIDOWSKI, Javier (Bariloche Atomic Centre)

Presenter: ROBLEDO, Jose (JCNS-2 Forschungszentrum Jülich)

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