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Information-Based Examination of Variable Hierarchy in Radiation Detection KIM FERRIS, BOBBIE-JO WEBB-ROBERTSON, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC — Of considerable importance in the development of a general program of information-based materials design is the manner in which materials data are stored, retrieved and analyzed. In the area of radiation detection materials, the variable spaces tend to be large and property measurements (and computations) of candidate materials are not abundant. Moreover, measurements and calculations of the same nominal quantity (e.g. bandgap) are typically based on differing and incompletely defined environments, and may not be directly comparable. The identification of parameter degeneracies, reduced spaces and transferability within the information hierarchy have become critical issues for the development of effective structure mappings for making inferences on these systems. As the initial framework for a materials-informatics approach to radiation detection materials, we have explored the use of both supervised (Support Vector Machines(SVM); Linear Discriminant(LDA)) and unsupervised (Principal Component (PCA)) learning methods for the development of structural signature models. Application of these methods yields complementary results, both of which are necessary to reduce parameter space and variable degeneracy. Using a crystal structure classification test, nonlinear SVM significantly increases predictive performance, suggesting trade-offs between smaller descriptor spaces and simpler linear models.

Kim Ferris
Pacific Northwest National Laboratory

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