Inverse Problems in Designing New Materials

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Abstract: Our present work deals with the modeling and simulation of an inverse problem in Material Science application with tolerances. The development of new materials with certain properties has become one of the most challenging tasks for engineers nowadays. For example, high performance metals are required for the continuous development of cars, airplanes and other complex structures. A high-throughput screening method has been recently introduced in which many small alloy samples are synthesized and exposed to different thermal and mechanical treatments. Properties of materials are predicted by a black box model based on some descriptors which are obtained from these samples. This model is approximated locally by machine learning techniques such as Neural Networks and Support Vector Regression. Our task is to find values for the descriptors such that the predicted properties satisfy certain performance profile which might include some tolerances. It turns out that this is an ill-posed inverse problem. For solving it, Tikhonov regularization methods are used and tolerances are incorporated into the discrepancy term. Numerical results are compared with using machine learning techniques to solve the inverse problem directly. Finally, we discuss possible ways of how to determine not only exact values but also tolerances for the descriptors.

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