The prediction of liquidus temperatures of oxide glasses by nonlinear "neutral" regression

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Neural networks techniques are gaining wide acceptance in a large variety of engineering disciplines, such as nonlinear process modeling, process control, pattern recognition, and others. They are useful whenever prior domain knowledge is non-existent or inaccurate. They can serve either as black-box or semi-physical models. Formulation is a natural candidate for successful applications of these techniques, especially for complex materials. We illustrate these concepts with the prediction of liquidus temperatures of glass-forming oxide blends.

Numerous properties of glasses and glass-forming liquids of oxide mixtures vary in a relatively simple and regular way with the concentration of the oxides. The liquidus temperature is an exception: the surface to be estimated is fairly complex, so that usual regression methods involve a large number of free parameters. It can be proved that a neural network will provide more accurate predictions than conventional nonlinear regression methods. We demonstrate this property on some examples of oxide mixtures involving up to five components. In the latter case, we show that neural networks provide a sizeable improvement over polynomial methods.