Advances in Auto-Fitting of Mixture Models

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The development of high-accuracy mixture models has historically been a slow-and-steady approach governed by intuition and deterministic optimization. This framework has proven successful as a means of developing mixture models for a wide range of the technically most important systems, like those of natural gas mixtures described by the GERG model. There are quite a few systems for which enough data is available to fit more accurate mixture models, and in some cases, there is enough data available to fit entire departure functions, which allow for much more accurate representations of the thermodynamic properties of the mixture, particularly for densities. The use of evolutionary optimization for global optimization is not a new idea -- nature has been doing it for eons. In this case, we use nature-inspired evolutionary optimization to find the "best" mixture model. These mixture models are typically structured as empirical departure terms with many adjustable parameters - as many as 30 or 40. Just as for pure fluids, the fitted departure function will have a strong effect on the shape of the thermodynamic surface, and therefore on properties like the shape of the phase envelope. In this work, we have leveraged a number of open-source libraries developed by the authors for parallel processing and optimization. Global optimization with evolutionary methods is very well-suited algorithm to parallel-processing, and we have been able to achieve quasi-linear speedup as we add more computational cores. Currently we are working on a new mixture model for ammonia + water, perhaps the industrially most important mixture. This optimization approach is showing great promise, and is able to reliably find reasonable candidate models. The solutions are then fed into a deterministic optimization routine that applies additional constraints on the model to control its shape and thermodynamic behavior. In the long term, the goal is to develop a method that is entirely hands-off: the user enters the data and starts the optimizer and walks away; the output is the fitted model. We are still some distance from this dream, but it is within sight.