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Quantifying cluster expansions in multicomponent systems: Precise expansions from noisy databases ALEJANDRO DIAZ-ORTIZ, HELMUT DOSCH, Max Planck Institute for Metals Research, RALF DRAUTZ, Department of Materials, University of Oxford — We have performed a systematic analysis of the ubiquitous numerical errors contained in the databases used in cluster expansions of multicomponent alloys. Our results underscore the importance of numerical noise on the effective cluster interactions and on the selection mechanisms. The relevance of the size of and the information contained in the input database is highlighted. It is shown that cross-validators approaches by themselves can produce unphysical expansions characterized by non-negligible, long-ranged coefficients. A selection criterion that combines both forecasting ability and the physical limiting behavior for the expansion is proposed. Expansions performed under this criterion exhibit the remarkable property of noise filtering. We illustrate our findings on bcc-based Fe-Co alloys.

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