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Constraint reasoning and kernel clustering for pattern decomposition with scaling.


Summary: Motivated by an important and challenging task encountered in material discovery, we consider the problem of finding $K$ basis patterns of numbers that jointly compose $N$ observed patterns while enforcing additional spatial and scaling constraints. We propose a Constraint Programming (CP) model which captures the exact problem structure yet fails to scale in the presence of noisy data about the patterns. We alleviate this issue by employing Machine Learning (ML) techniques, namely kernel methods and clustering, to decompose the problem into smaller ones based on a global data-driven view, and then stitch the partial solutions together using a global CP model. Combining the complementary strengths of CP and ML techniques yields a more accurate and scalable method than the few found in the literature for this complex problem.

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