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Synthetic Nanomechanical Data and Kernel-Averaged Mechanical Mismatch for Robust Phase Clustering

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We present an unsupervised machine learning framework to enhance phase identification in nanoindentation mapping of multiphase materials, combining physics-informed features with synthetic data generation. Central to this approach is the Kernel-Averaged Mechanical Mismatch (KAMM), a spatial descriptor that quantifies local gradients in elastic modulus (E) and hardness (H). KAMM is incorporated into multiple clustering algorithms—including k-means, Gaussian Mixture Models, DBSCAN, and agglomerative clustering—to evaluate its effect on clustering robustness and accuracy. To systematically benchmark performance, we generate synthetic indentation datasets with controlled gradients in mechanical properties, emulating multiphase composites and interfacial zones. These datasets enable parametric studies of clustering behavior under varying phase contrast, noise, and sampling density. Results show that incorporating KAMM consistently enhances intra-cluster compactness and inter-cluster separability, particularly in low-contrast or graded materials, enabling a more quantitative benchmarking of unsupervised learning approaches for nanomechanical data analysis. Finally, we demonstrate a lightweight, interactive application that integrates these clustering workflows —allowing users to visualize indentation maps, compare algorithms, and assess the impact of KAMM in real time for advanced phase-mapping analysis.

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