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Cold, warm, warmer, hot! Impact of distance metrics on autonomous experimentation

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Artificial intelligence (AI), when interfaced with laboratory automation, can accelerate materials optimization and scientific discovery. For example, it may be used to efficiently map a phase-diagram with intelligent sampling along phase boundaries, or in 'retrosynthesis'problems where a material with a target structure is desired but its synthetic route is unknown. These AI-driven laboratories are especially promising in polymer physics, where design parameters (e.g. chemical composition, MW, topology, processing) are vast and where properties and function are intimately tied to design features. However, for AI to operate efficiently in these spaces, they must be 'encoded'with domain expertise specific to the problems being tackled. In this talk, we focus on the problem of defining appropriate 'distance'metrics to describe differences between functions sampled within a design space. Such functions may be spectroscopic (e.g. UV-Vis absorption, fluorescence, impedance) or scattering profiles (SAXS, SANS) of materials, among others. Traditional 'distance'metrics, such as Euclidean and parametric definitions, often fail when important features of the measured functions are subtle and/or when sampling takes place far from the target. We have thus developed a new shape-based similarity metric using Riemannian geometry (Phase-Amplitude Distance) that has been successfully implemented in both retrosynthesis and phase mapping problems. This talk will first discuss the definition of the Phase-Amplitude Distance metric. We then demonstrate its implementation in an autonomous batch retrosynthesis problem using spectroscopic signatures in a model system of metal nanostructures. Finally, we implement the new distance metric in phase-mapping problems involving block-copolymers, polymer blends, and inorganic materials to showcase the broad applicability of the method. Mathematically, these phase maps need to be continuous over the design space and correlations are usually defined by shape-based similarity between profiles. We pose both constraints as a geometric feature of the phase map where continuity is obtained by diffusing the shape-based similarity of SAS profiles via a local geometry defined by the linear operators on the design space.

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