Introduction to Hypermaterials Informatics

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Data-driven science based on big data is advancing rapidly and transform the world around us. As such, machine learning has received considerable attention as a key driver to the next frontier of materials science, enabling us to reap substantial time and cost savings in the discovery and development of new materials. In this lecture, I will describe a basic concept and some key technologies of machine leaning to achieve this goal. The course covers supervised learning, deep learning, transfer learning, adaptive design of experiments, and so on, which will be illustrated on various practical applications, including quasicrystal research.

Recently, a wide variety of machine learning technologies has been rapidly introduced to materials science. In particular, high-throughput screening (HTS) across extensive libraries of candidate materials, which typically contain millions or even billions of virtually created candidates, is a promising application. HTS relies on the fast computation of a statistical model that describes physical, chemical, electronic, thermodynamic, and mechanical properties and unobserved structural features as a function of the material. Nowadays, many successful case studies of HTS have been reported, including small organic molecules, polymeric materials, inorganic solid-state materials, high-entropy alloys, and bulk metallic glasses. Here, we seek to answer the question: can the HTS based on machine learning technologies predict the compositions of quasicrystals?

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