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Crystallization Learning with Delaunay Triangulation

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High-dimensionality is known to be the bottleneck for both nonparametric regression and Delaunay triangulation. To efficiently exploit the geometric information for nonparametric regression without conducting the Delaunay triangulation for the entire feature space, we develop the crystallization search for the neighbour Delaunay simplices of the target point similar to crystal growth. We estimate the conditional expectation function by fitting a local linear model to the data points of the constructed Delaunay simplices. Because the shapes and volumes of Delaunay simplices are adaptive to the density of feature data points, our method selects neighbour data points more uniformly in all directions in comparison with Euclidean distance based methods and thus it is more robust to the local geometric structure of the data. We further develop the stochastic approach to hyperparameter selection and the hierarchical crystallization learning under multimodal feature data densities, where an approximate global Delaunay triangulation is obtained by first triangulating the local centres and then constructing local Delaunay triangulations in parallel.

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