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Self-assemby of shapes via generalized centroidal Voronoi tessellations

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Self-assembly of shapes from spheres to non-smooth and possibly non-convex shapes, are pervasive throughout the sciences. These arrangements arise in biology for animal flocking and herding, in condensed matter physics with molecular and nano self assembly, and in control theory for coordinated motion problems. While idealizing these often non-convex objects as points or spheres aids in analysis, the effects of shape curvature and convexity are often dramatic, especially for short-range interactions. In this talk, we develop a general purpose model for arranging rigid shapes in Euclidean domains and on flat tori. The shapes are arranged optimally with respect to minimization of a geometric Voronoi-based cost function which generalizes the notion of a centroidal Voronoi tessellation from point sources to general rigid shapes. The functional can naturally be phrased in terms of Wasserstein distances.

We present an efficient and fast algorithm for the minimization of this nonlocal, albeit finite-dimensional variational problem. The algorithm applies in any space dimension and can be used to generate self-assemblies of any collection of non convex, piecewise smooth shapes. We will also provide an approximate result for the minimizers of this cost function which supports the intuition that self-assembled shapes should be centered in and aligned with their Voronoi regions.

This is joint work with Lisa Larsson (Credit-Suisse) and J.C. Nave (McGill).

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