

Geometric Optimization for Material Sciences

Geometric optimization is the computational technique of choice for a wide variety of problems in material sciences. This talk dwells on predicting functional properties of biological materials at both molecular and tissue scales. Combinatorial and geometric optimization occurs naturally for solutions to rigid and flexible molecular and macromolecular, shape complementarity matching problems, such as predicting multi-component assemblies. For this class of problems the optimization functional is in general is a non-convex multi-dimensional correlation integral while the search space is the product of transformations groups with dimension growth exponential in the number of movable components. For some cases i shall show how to reduce the approximation solution to semi-definite programming. Geometric optimization also occurs frequently in analyzing spectroscopy data of biological tissue, in an attempt to diagnose malignancy. I shall show how we use a kernel regression optimization functional for de-noising FTIR spectroscopy data. We then utilize the Riesz representation theorem of appropriately chosen reproducing kernel Hilbert spaces, related to this optimization functional to find a representative solution for the minimizer.

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