



THE UNIVERSITY OF
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STATISTICS COLLOQUIUM

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Multimarginal Optimal Transport, Density Functional
Theory, and Convex Relaxation

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Eckhart 133, 5734 S. University Avenue

ABSTRACT

Density functional theory has been a popular tool in solid state physics and quantum chemistry for electronic structure calculation. However, current functionals used in density functional theory face difficulties when dealing with strongly correlated systems. In this talk, we examine the regime where the electrons are strictly correlated. This gives rise to a multimarginal optimal transport problem, a direct extension of the optimal transport problem that has applications in economics and operations research as well. In particular we introduce methods from convex optimization to provide a lower bound to the cost of the multimarginal transport problem with a practical running time. We further propose projection schemes based on tensor decomposition to obtain upper bounds to the energy. Numerical experiments demonstrate a gap of order 10^{-3} to 10^{-2} between the upper and lower bounds.

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