A score-based operator Newton construction of transport maps

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Transportation of probability measures underlies many core tasks in statistics and machine learning, from variational inference to generative modeling. A typical goal is to represent a target probability measure of interest as the pushforward of a tractable source measure through a learned map. We present a new construction of such a transport map, given the ability to evaluate the score of the target distribution. Specifically, we characterize the map as a zero of an infinite-dimensional score-residual operator and derive a Newton-type method for iteratively constructing a zero. We prove convergence of these iterations by invoking classical elliptic regularity theory for partial differential equations (PDE) and show that this construction enjoys rapid convergence, under smoothness assumptions on the target score. A key element of our approach is a generalization of the elementary Newton method to infinite-dimensional operators, other forms of which have appeared in nonlinear PDE and in dynamical systems. Our Newton construction, while developed in a functional setting, also suggests new iterative algorithms for approximating transport maps.

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