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An information geometric approach to least squares minimization

MARK TRANSTRUM, BENJAMIN MACHTA, JAMES SETHNA, LASSP, Cornell University — Parameter estimation by nonlinear least squares minimization is a ubiquitous problem that has an elegant geometric interpretation: all possible parameter values induce a manifold embedded within the space of data. The minimization problem is then to find the point on the manifold closest to the origin. The standard algorithm for minimizing sums of squares, the Levenberg-Marquardt algorithm, also has geometric meaning. When the standard algorithm fails to efficiently find accurate fits to the data, geometric considerations suggest improvements. Problems involving large numbers of parameters, such as often arise in biological contexts, are notoriously difficult. We suggest an algorithm based on geodesic motion that may offer improvements over the standard algorithm for a certain class of problems.

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