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Finding saddle points using Gentlest ascent dynamics AMIT SAMANTA, XIANG ZHOU, Applied and Computational Mathematics, Princeton University, WEINAN E, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University — We present dynamical equations for determining transition states and escape paths from basins of attraction of a stable system on a potential energy landscape. It is shown that the stable fixed points of such dynamical systems are the index-1 saddle points. The method relies on determining the smallest eigenvalue of the Hessian matrix. The formalism is easy to extend to systems of higher dimensions and can be used to explore the free energy landscapes of systems whose large time scale separation makes the standard molecular dynamics inefficient. The utility of the algorithm is demonstrated by evaluating the activation parameters for homogeneous and heterogeneous dislocation nucleation.

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