

Using graph traversal techniques to explore energy landscapes

Applying the max-product algorithm to find the minimum energy pathway and avoid local minima.

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Abstract

We explore the issue of local minima when finding minimum energy pathways in energy landscapes. We then apply the max-product algorithm to efficiently explore the landscape and hence find a better route. We then evaluate the performance of this approach in different scenarios and with respect to different parameters.

Introduction

Minimum energy pathways are important because...