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What can global optimisation and coarse-graining reveal about energy landscapes?

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The description of biological systems often requires a large number of degrees of freedom. Exploring their energy landscape is an important but computationally demanding task. We apply a new methodology that identifies global or local minima of interest without sampling or exhaustive searching. Rather, it relies on a relaxation of the interactions of interest to a special sum of squares convex function that can be solved in polynomial time by exploiting computationally efficient semidefinite programming methods. Another advantage of the method is that the level of any approximation is controllable and hence known. We will apply the method to model problems and discuss how it can be used to guide coarse-graining to few but relevant degrees of freedom in protein-protein interactions.

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