The Energy Landscape Library
- a Platform for Generic Algorithms

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Introduction

The study of energy landscapes of biopolymers and their models is an important field in bioinformatics [1, 2]. For instance, the investigation of kinetics or folding simulations are done using methods that are based on sampling or exhaustive enumeration [3, 4]. Most of such algorithms are independent of the underlying landscape model. Therefore, frameworks for generic algorithms to investigate the landscape properties are needed.

Here, we present the Energy Landscape Library (ELL) that allows such a model-independent formulation of generic algorithms dealing with discrete states. The ELL is a completely object-oriented C++ library that is highly modular, easy to extend, and freely available online. It can be used for a fast and easy implementation of new generic algorithms (possibly based on the provided basic method pool) or as a framework to test their properties for different landscape models, which can be formulated straightforward.

Features of the ELL

The fundamental features of the ELL are:
- Strictly object oriented C++ library following STL coding
- Highly modular by strict partition of algorithms and models
- Development of both layers independent
- Complete API documentation of all classes etc.
- Freely available

Current energy landscape models
- RNA structures for a given sequence
- Lattice protein structures for various contact energies and lattices
- Compressed state representations to reduce memory usage for storing high numbers of states

Available algorithm pool
- Random, gradient, adaptive, ... walks
- Barrier tree generation [5]
- Density of states estimation [3]
- ... Directed walks
- ... More and new energy landscape models from different fields of research

Future Work

The ELL is currently under development and we are focusing our work on:
- More and new energy landscape models from different fields of research
- Implementation of further basic and extended algorithms
- Improving the current ELL in terms of runtime and memory consumption
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Conclusion

The ELL is a C++ programming platform for the study of energy landscapes with generic methods. The partition of the algorithms and the underlying landscape model, interfaced by a state abstraction, allows an independent development of both layers. The ELL supports the user with a pool of common methods and some landscape models (e.g. RNA) to provide a fast and efficient basis for further investigations. It is highly modular, object-oriented and easy to extend. The ELL is available for free under
http://www.bioinf.uni-freiburg.de/sw/ell/

References


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