MSMExplorer: Data Visualizations for Biomolecular Dynamics

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Summary

MSMExplorer is a Python package for visualizing data generated from biomolecular dynamics. While molecular visualizations have been a large focus of the molecular dynamics (MD) community (Humphrey, Dalke, and Schulten 1996, Schrödinger, LLC (2015)), data visualizations for the analyses of MD trajectories have been less developed. *MSMExplorer* seeks to fill this niche by providing publication-quality statistical plots with an easy-to-use Python API that works seamlessly with commonly used Python libraries, such as `numpy` and `scikit-learn` (Walt, Colbert, and Varoquaux 2011, Pedregosa et al. (2011)). Additionally, plots are generated using already established plotting libraries, like `seaborn`, to provide a consistent aesthetic (Waskom et al. 2016, Hunter (2007), Hagberg, Schult, and Swart (2008), Foreman-Mackey (2016)).

Plotting functionality in *MSMExplorer* is centered around the statistical tools available in `msmbuilder` (M. P. Harrigan et al. 2017). Because of this focus, in addition to standard time-series plots, users can choose to plot more involved measures, such as Gibbs free energy and implied timescales estimated from Markov models.

MSMExplorer is actively developed and maintained by researchers at Stanford University. Source code for *MSMExplorer* is hosted on GitHub and is continuously archived to Zenodo (C. Hernández, Harrigan, and Pande 2016). Full documentation, including a practical example gallery, can be found at http://msmbuilder.org/msmexplorer.

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