An Efficient Global Optimization Python Module based on Generalized Simulating Annealing: PyGenSA

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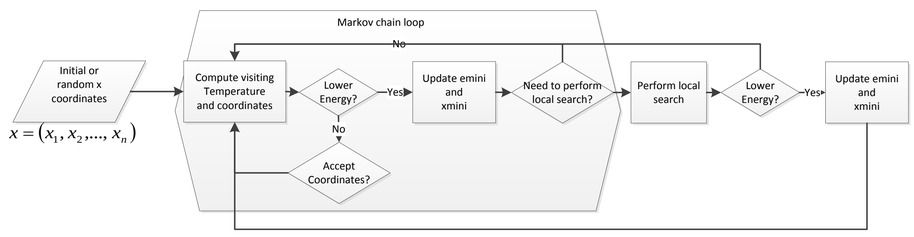
Abstract

Many problems in statistics, finance, biology, pharmacology, physics, mathematics, economics, and chemistry involve the determination of the global minimum of multidimensional functions. Python modules from **SciPy** and **PyPI** for the implementation of different stochastic methods (i.e.: pyEvolve, SciPy optimize) have been developed and successfully used in the Python scientific community. Based on Tsallis statistics, the PyGenSA python module has been developed for generalized simulated annealing to process complicated non-linear objective functions with a large number of local minima. Testing PyGenSA, basinhopping (SciPy) and differential evolution (SciPy) on many standard test functions used in optimization problems shows that PyGenSA is more reliable in general and more efficient in particular for high dimension problems.

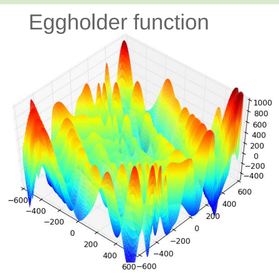
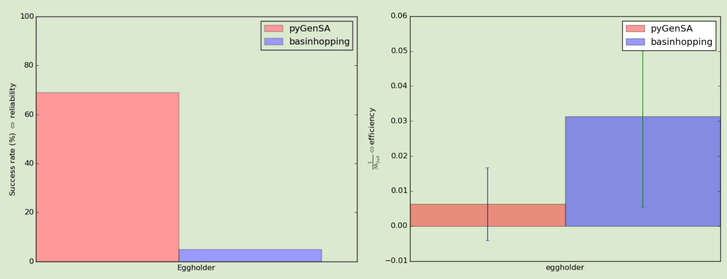
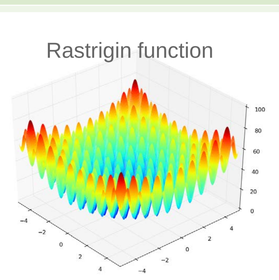
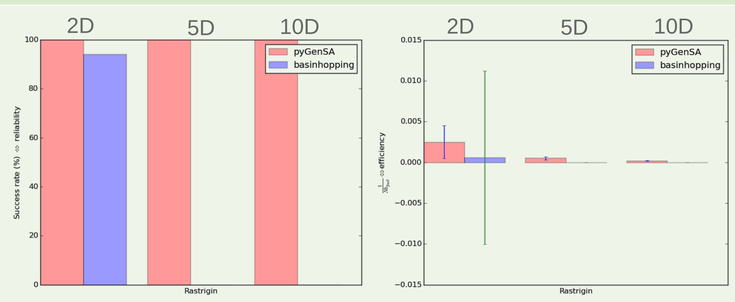
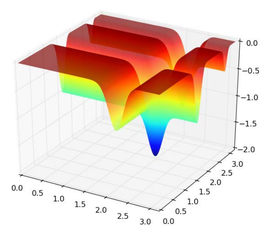
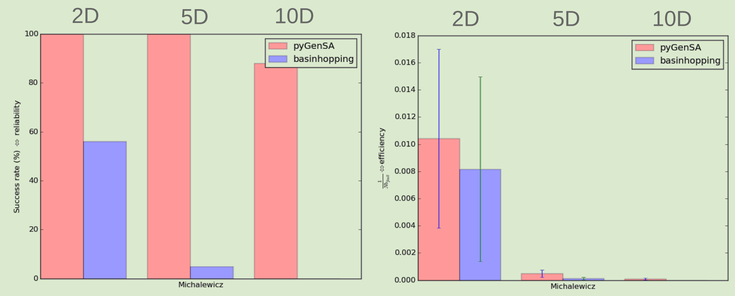
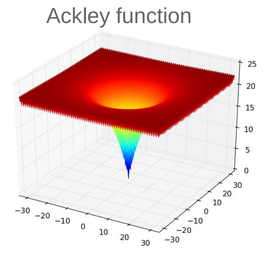
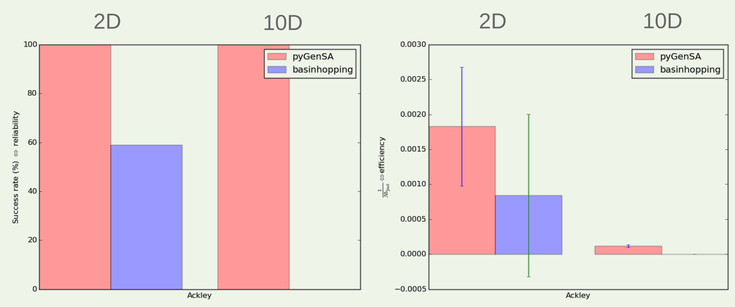
Description of PyGenSA

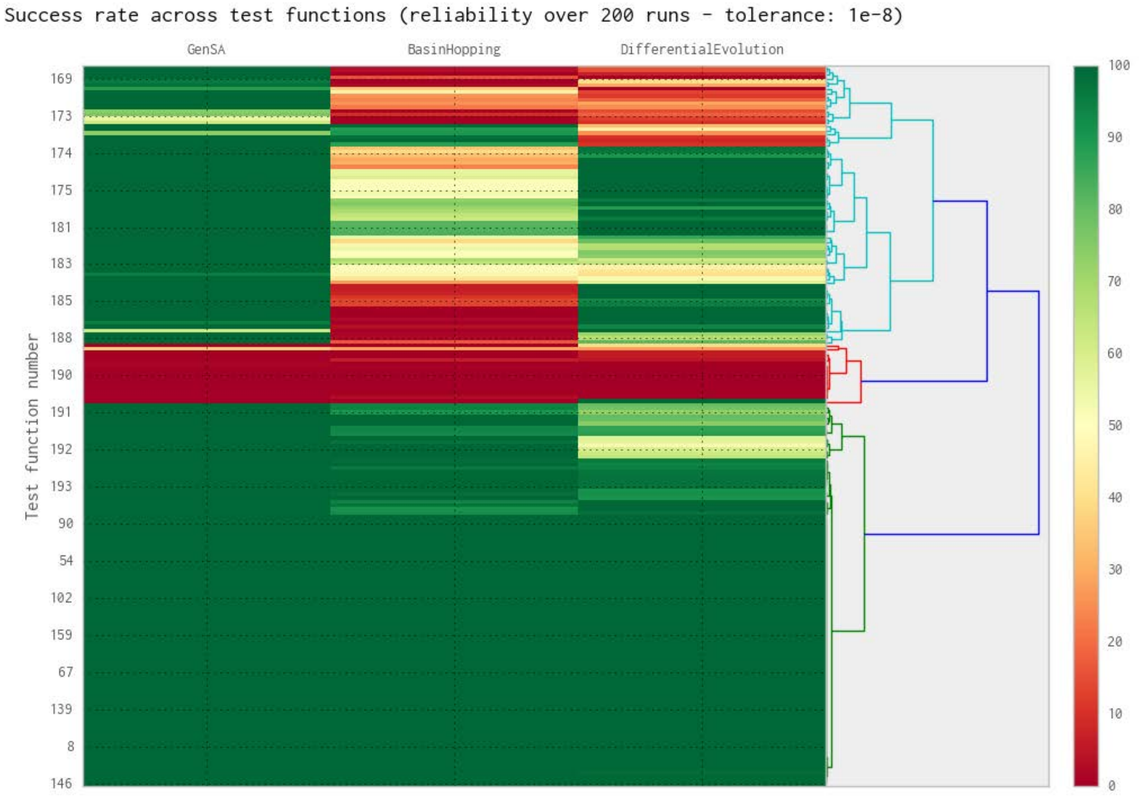
Generalized Simulated Annealing (GSA) is an implementation of the generalization of CSA (Classical Simulated Annealing) and FSA (Fast Simulated Annealing) combined using Tsallis statistics. The algorithm switches between the CSA and FSA techniques depending on the “visiting temperature” along the different jump distances in the search domain. **PyGenSA**’s approach is a “hybrid” algorithm combining GSA and local minimum search that is performed strategically. It is a pure Python implementation using Numpy and the SciPy bindings for local minimum search. The simplified flow chart of the algorithm is illustrated below:



Comparison with basinhopping and differential evolution

SciPy already provides powerful global optimization tools called basinhopping and differential evolution, which we selected for performing comparisons against PyGenSA. To ensure a fair comparison, a tolerance of 1.e-8 is used in both cases and the number of iterations is set to a large value to allow both approaches to reach the global minimum. “Reliability” in the table below corresponds to the percentage of successful runs (the correct minimum was found) and “efficiency” is the inverse average number of objective function calls to reach the solution. The results presented have been obtained by running 100 searches using 196 testing functions with different initial conditions.

Plot of the testing function	Benchmarking results “Reliability” | “Efficiency”
Eggholder function 	
Rastrigin function 	
Michalewicz function 	
Ackley function 	



The above heatmap shows successful rate% of PyGenSA, basinhopping and differential evolution for the 196 testing functions. The color scaling from red to green represents successful rate% from 0 to 100. Clearly PyGenSA has more green region (high successful rate%) than basinhopping and differential evolution.

The mean of successful rate% over all the benchmark functions are 92%, 85%, and 86% for PyGenSA, basinhopping and differential evolution respectively. As the number of function calls changes drastically, the median rather than the mean of number of function calls is given here: 244.3 for PyGenSA, 1625.9 for basinhopping, and 1709.4 for differential evolution.

GenSA R package at pmiscience.com:
https://www.pmiscience.com/library/generalized-simulated-annealing-global-optimization-gensa-package

Further comparisons have been performed using the R/C++ implementation of the algorithm and have been published in the literature:
http://www.jstatsoft.org/v60/i06/paper

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