DARTMOUTH COLLEGE
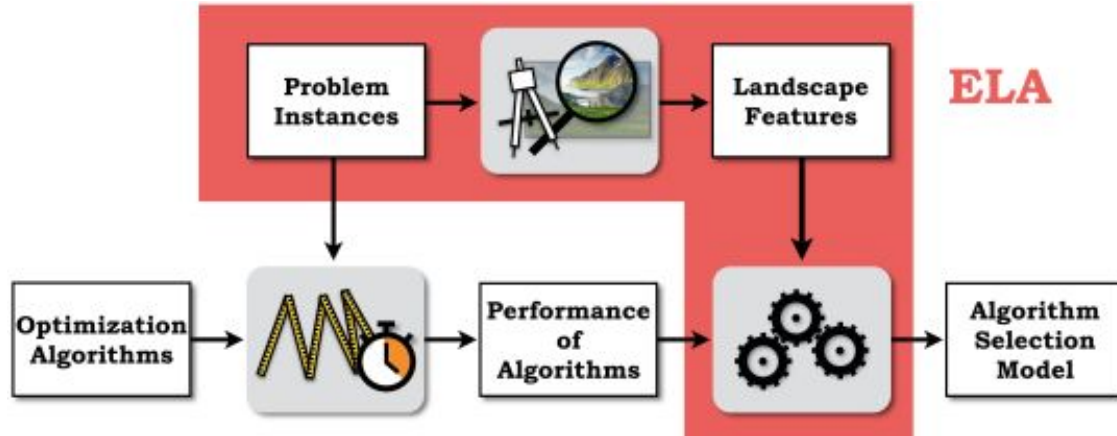PHYSICS AND ASTRONOMY

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Landscape Analysis and Quantum Computing
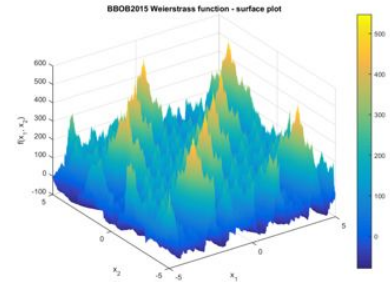
Ben Newhall
James Whitfield
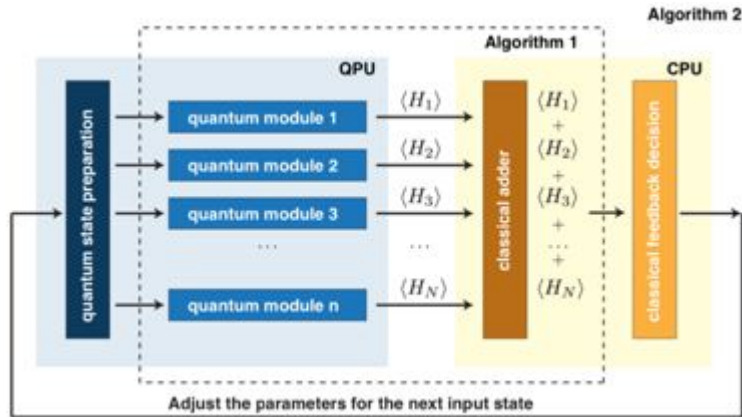Graduate Advisor: Weishi Wang

Exploratory Landscape Analysis (ELA)

- Statistical method
- Determines certain Landscape features
  - "Smoothness"
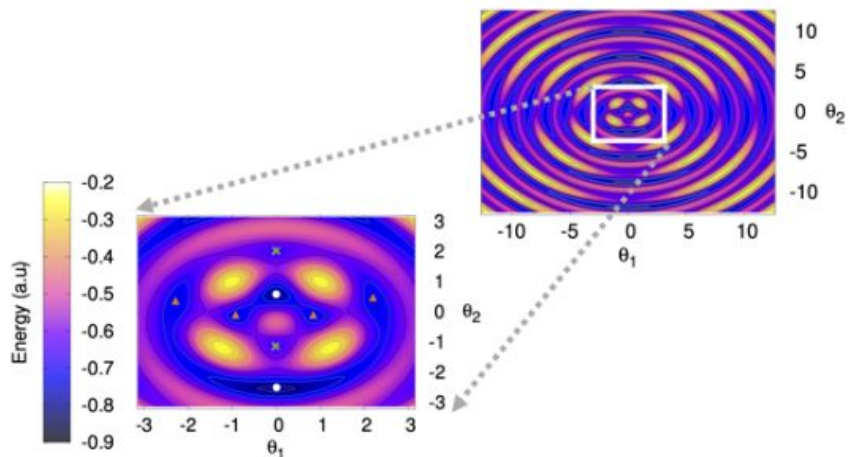- Used to select optimization algorithms

Quantum Optimization

- VQE is a quantum optimization method that uses a classical optimization algorithm

Variational Quantum Eigensolver (VQE)

Motivation

- Application to scientific computing
- Can use VQE to find minimum energies of molecules
  - Image shown is H3 at fixed value of nuclear separation
  - Found using Hartree-Fock
  - From work done by Prof Whitfield at Dartmouth and Sahil Gulania at University of Southern California
- Landscape analysis can be used to select correct optimization algorithm
- Can more generally be used to determine which problems are hard on a quantum computer

Summary

- Landscape analysis is a statistical method for determining the shape of a landscape
- VQE is a quantum optimization algorithm that uses a classical optimizer
- Landscape analysis can be used to:
  - Speed up quantum optimization
  - Determine which problems are difficult on a Quantum Computer

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Appendix
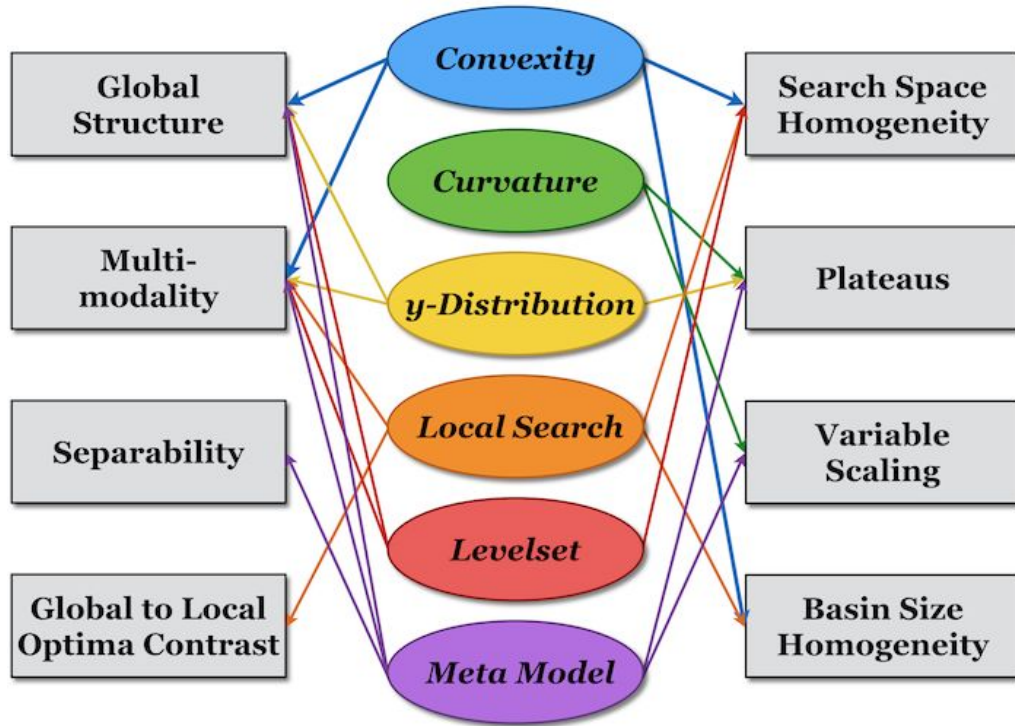
- Flacco: R package for ELA
  - https://github.com/kerschke/flacco
- PFlacco: Python port of flacco
  - https://pypi.org/project/pflacco/
- Mersmann et al. (2011), "Exploratory Landscape Analysis", in Proceedings of the 13th Annual Conference on Genetic and Evolutionary Computation, pp. 829—836. ACM (http://dx.doi.org/10.1145/2001576.2001690).
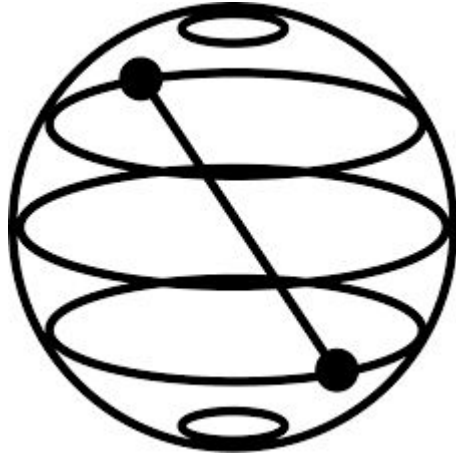
Appendix
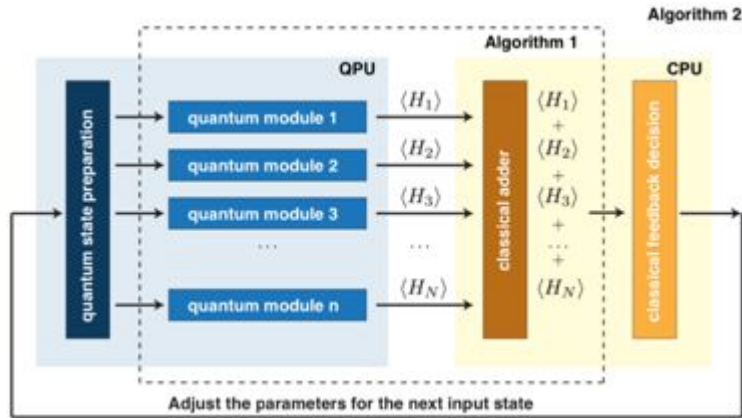
A visual description of VQE. Adapted from "A variational eigenvalue solver on a photonic quantum processor" by Alberto Peruzzo, Jarrod Mcclean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J. Love, … Jeremy L. O'brien. (2014). *Nature Communications*

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Appendix

- Use Qiskit for VQE
- Use python tools to either run locally or remotely on QC
- Tutorial at https://qiskit.org/textbook/ch-applications/vqe-molecules.html

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