LibKet: Cross-Platform Library for Running Quantum Algorithms on NISQ processors

Variational Quantum Algorithms

IEEE Quantum Week 2022

September 18-23, 2022

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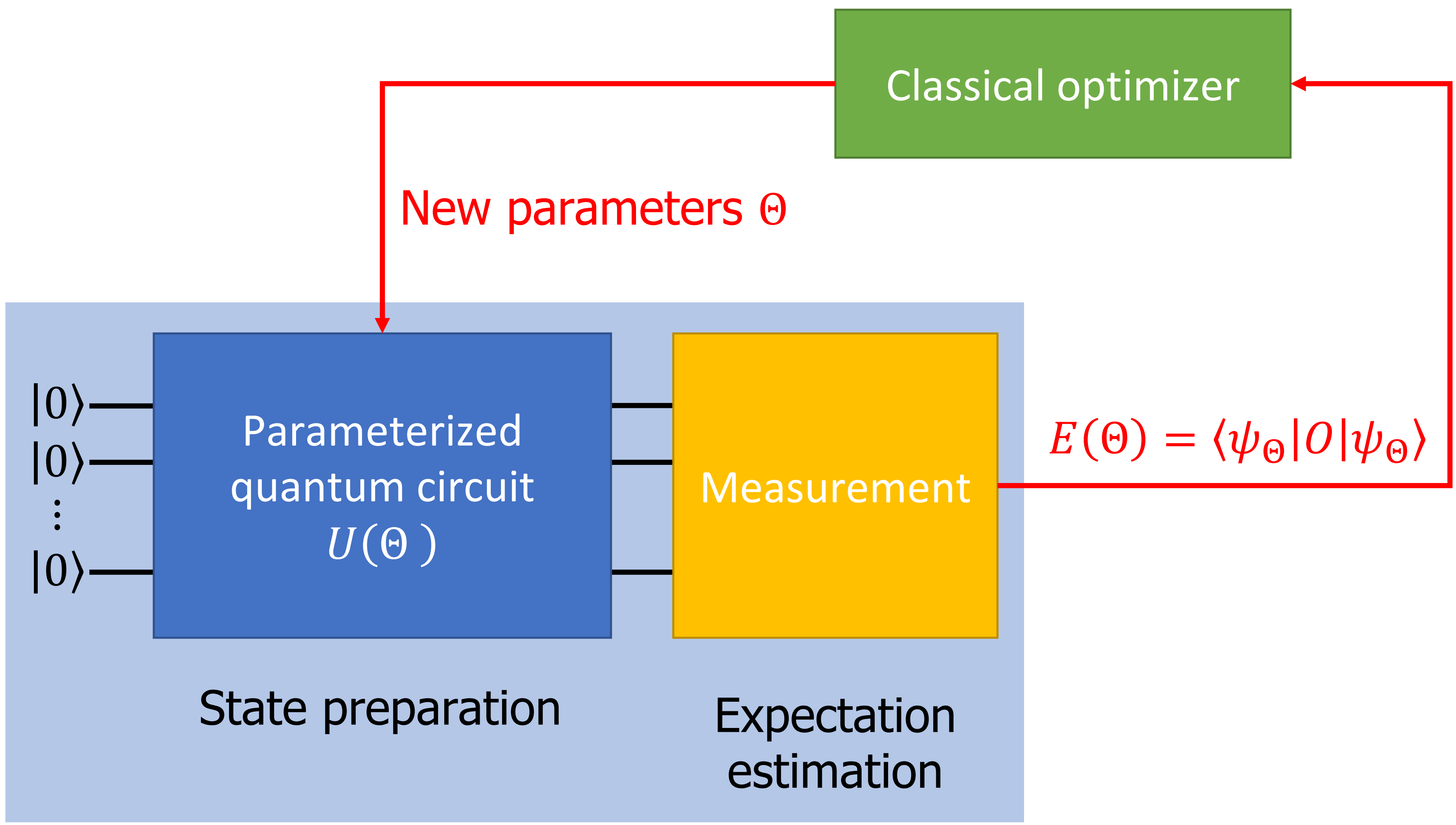
Working principle



Examples of variational algorithms

- Variational Quantum Eigensolver (VQE)
  – *Peruzzo et at. 2014, McClean et al. 2015*
- Quantum Approximate Optimization Algorithm (QAOA)
  – *Farhi et al. 2014*
- Quantum Alternating Operator Ansatz (QAOA)
  – *Hadfield et al. 2019*
- Variational Quantum Linear Solver (VQLS)
  – *Bravo-Prieto et al. 2019, Xu et al. 2019*
- …

Parameterized rotation gates

$$R_x(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -i\ \sin\frac{\theta}{2} \\ -i\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}, \qquad R_y(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}, \qquad R_z(\theta) = \begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix}$$

Valid substitutions of the Hadamard gate

$$H \mapsto R_x(\pi)R_y(\pi/2), \qquad H \mapsto R_y(-\pi/2)R_x(\pi)$$
$$H \mapsto R_y(\pi/2)R_z(\pi), \qquad H \mapsto R_z(\pi)R_y(-\pi/2)$$

Exercise 1
Check the above substitution rules with the QuEST simulator

Exercise 2
Try to find the correct rotation angles by grid search

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https://tinyurl.com/3vw4zdc8

IEEE QUANTUM WEEK IEEE International Conference on Quantum Computing and Engineering – QCE22

Tutorial at IEEE QCE22, September 18-23, 2022

LibKet: A Cross-Platform Library for Running Quantum Algorithms on NISQ Processors

Organizers: Carmen G. Almudever, Matthias Möller

Session 1: Sunday, September 18, 10:00 AM – 11:30 AM MDT (UTC-6)

Time	Content	Lecturer	Slides	Binder
10:00-11:00 am	Hands-on Introduction to Quantum Computing	Carmen	slides	tutorial 01
11:00-11:30 am	Libket - The Basics	Matthias	slides	tutorial 02

Session 2: Sunday, September 18, 12:00 AM – 1:30 PM MDT (UTC-6)

Time	Content	Lecturer	Slides	Binder
1:00-1:45 pm	LibKet - Advanced Features	Matthias	slides	tutorial 03
1:45-2:30 pm	Variational Quantum Algorithms	Carmen/Matthias	slides	tutorial 04

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Reference solution

```
QVar_t<0> var0(0.0); QVar_t<1> var1(0.0);
auto expr = rx(var0, ry(var1, init()));
QDevice<QDeviceType::quest, 1> device; device(expr);

for (int i = 0; i < 11; i++) {
    for (int j = 0; j < 11; j++) {
      var0 = 3.14159265358979323846/10*i;
      var1 = 1.57079632679489661923/10*j;
      device.eval(1);
      std::cout << "i=" << i << " j=" << j << "\n"
                    << device.reg() << std::endl;
    }
}
```

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The eigenvalue problem

Given the Hamiltonian

$$H = c_0 X \otimes I + c_1 I \otimes X, \qquad c_0, c_1 \in \mathbb{R}$$

find the *smallest* eigenvalue of H, that is

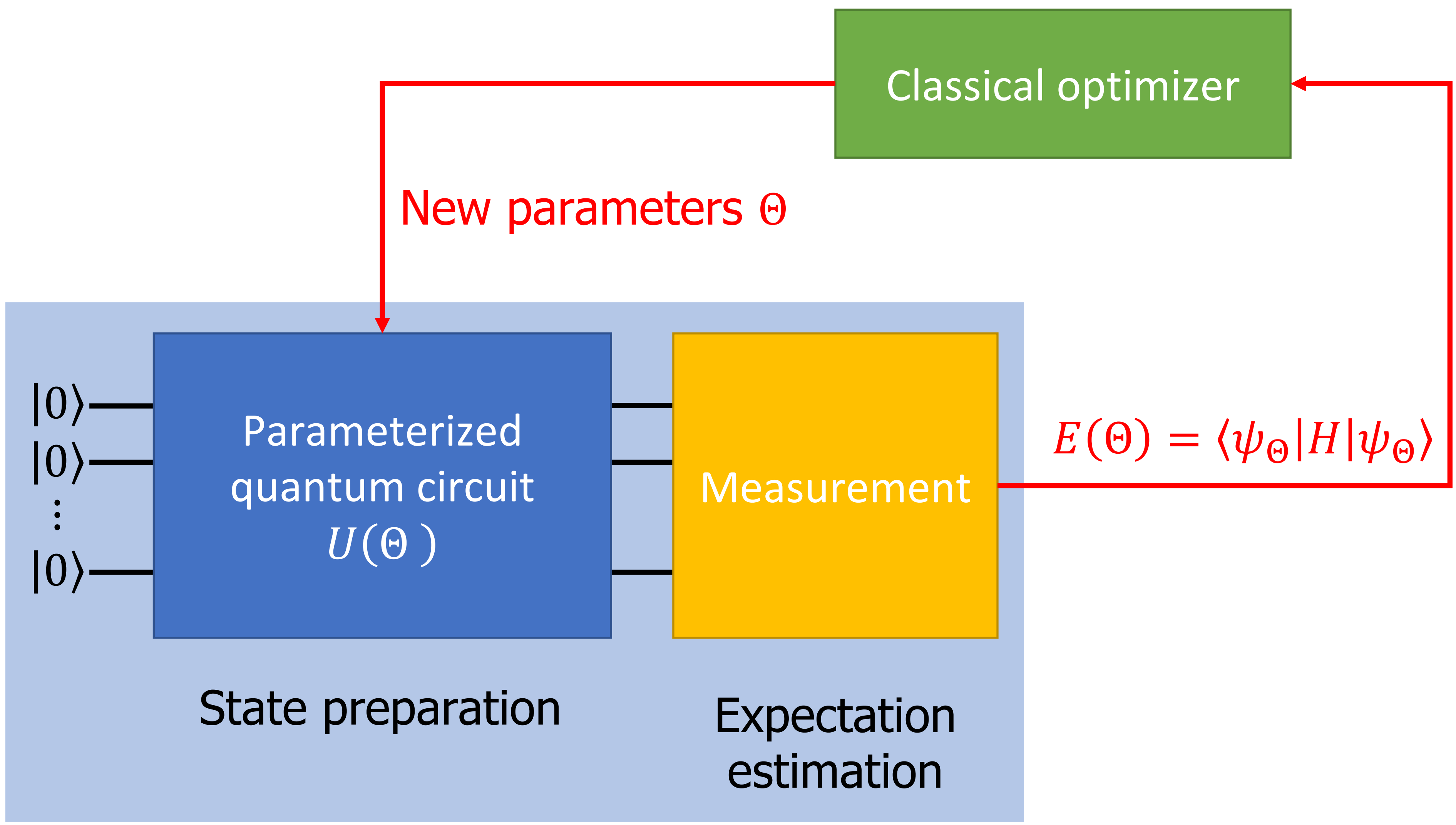
$$H\psi_{\min} = \lambda_{\min}\psi_{\min}$$

Example

$$H = 0.5 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + 0.6 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0.6 & 0.5 & 0 \\ 0.6 & 0 & 0 & 0.5 \\ 0.5 & 0 & 0 & 0.6 \\ 0 & 0.5 & 0.6 & 0 \end{bmatrix} \Rightarrow \lambda_i \in \{-1.1, -0.1, 0.1, 1.1\}$$

Variational Quantum Eigensolver



VQE – state preparation

All possible 1-qubit states can be created from $|0\rangle$ with the **U3 ansatz**

$$U_3(\theta,\varphi,\lambda)|0\rangle = \begin{bmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\varphi}\sin(\theta/2) & e^{i(\varphi+\lambda)}\cos(\theta/2) \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

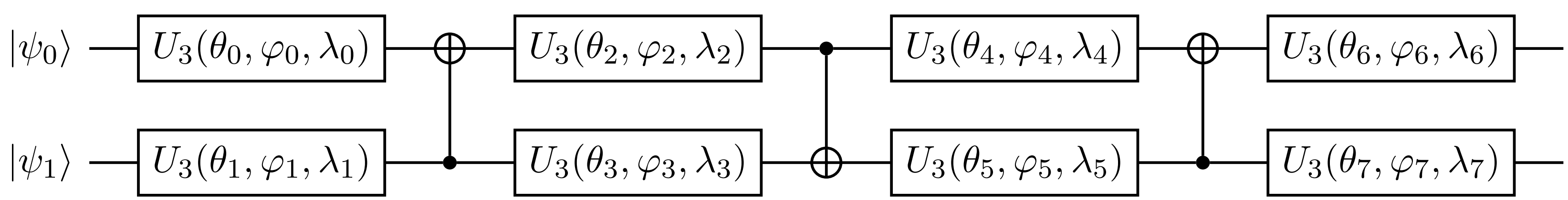
$$= \cos(\theta/2)\,|0\rangle + e^{i\varphi}\sin(\theta/2)$$

The U3 ansatz can be represented as **parameterized quantum circuit**

$$U_3(\theta,\varphi,\lambda) = R_z(\varphi)R_x(-\pi/2)R_z(\theta)R_x(\pi/2)R_z(\lambda)$$

VQE – state preparation

Shende et al. 2003 has extended the U3 ansatz to two qubits



So we need to find the optimal value of 24 parameters.

VQE – expectation estimation

$$\langle\psi_\Theta|H|\psi_\Theta\rangle = \langle\psi_\Theta|c_0 X \otimes I + c_1 I \otimes X|\psi_\Theta\rangle$$

Due to the properties of the inner product this can be decomposed into

$$\langle\psi_\Theta|H|\psi_\Theta\rangle = c_0\langle\psi_\Theta|X \otimes I|\psi_\Theta\rangle + c_1\langle\psi_\Theta|I \otimes X|\psi_\Theta\rangle$$

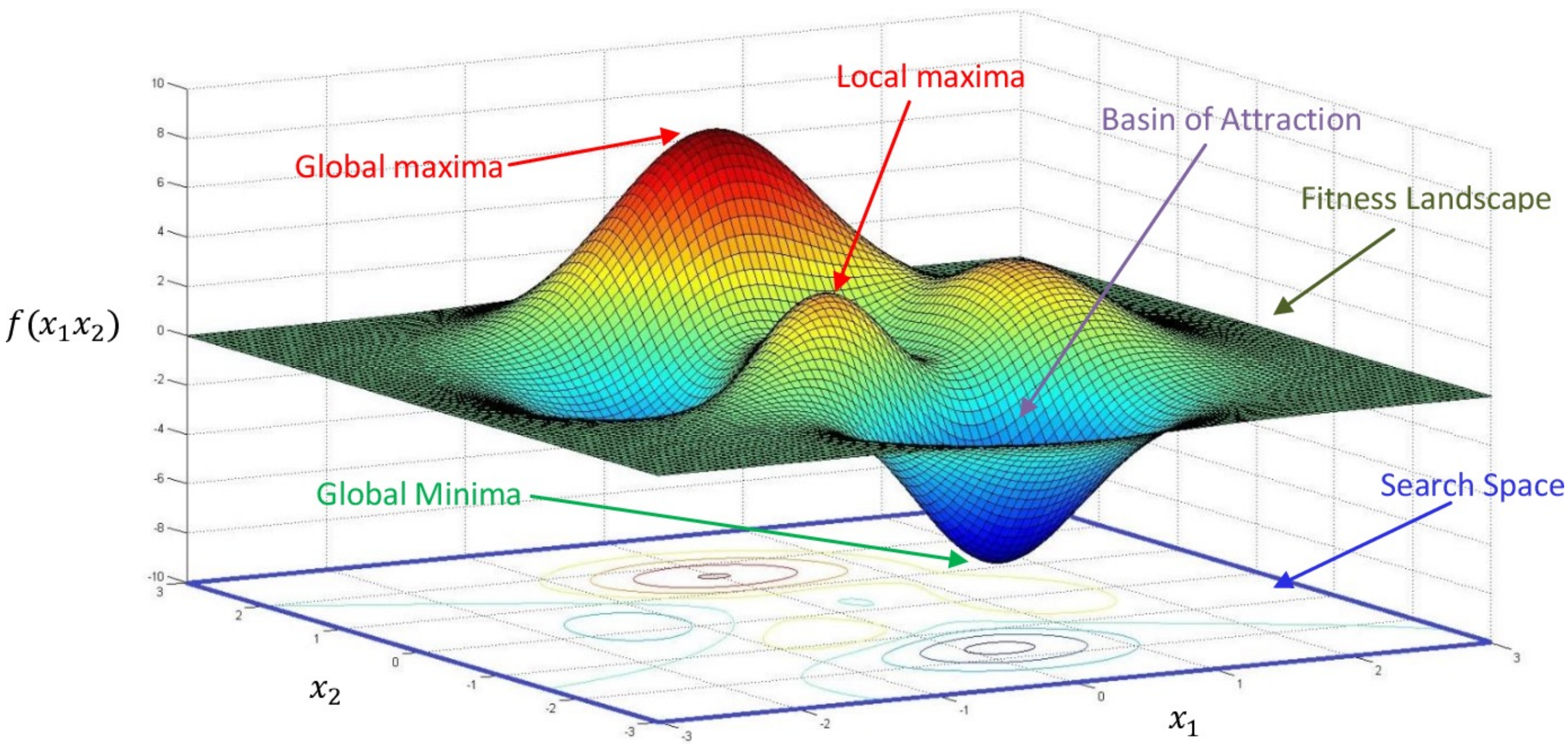
Measurement of q_0 in the X basis

Measurement of q_1 in the X basis

Can be mimicked by

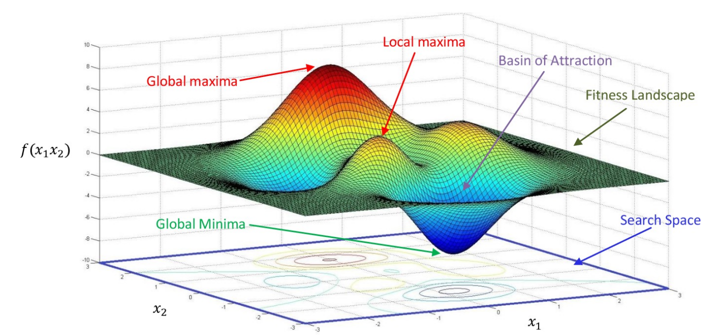
$$\mathrm{meas}_{\mathrm{z}}(H|\psi_\Theta\rangle)$$

VQE – classical optimizer



VQE – classical optimizer

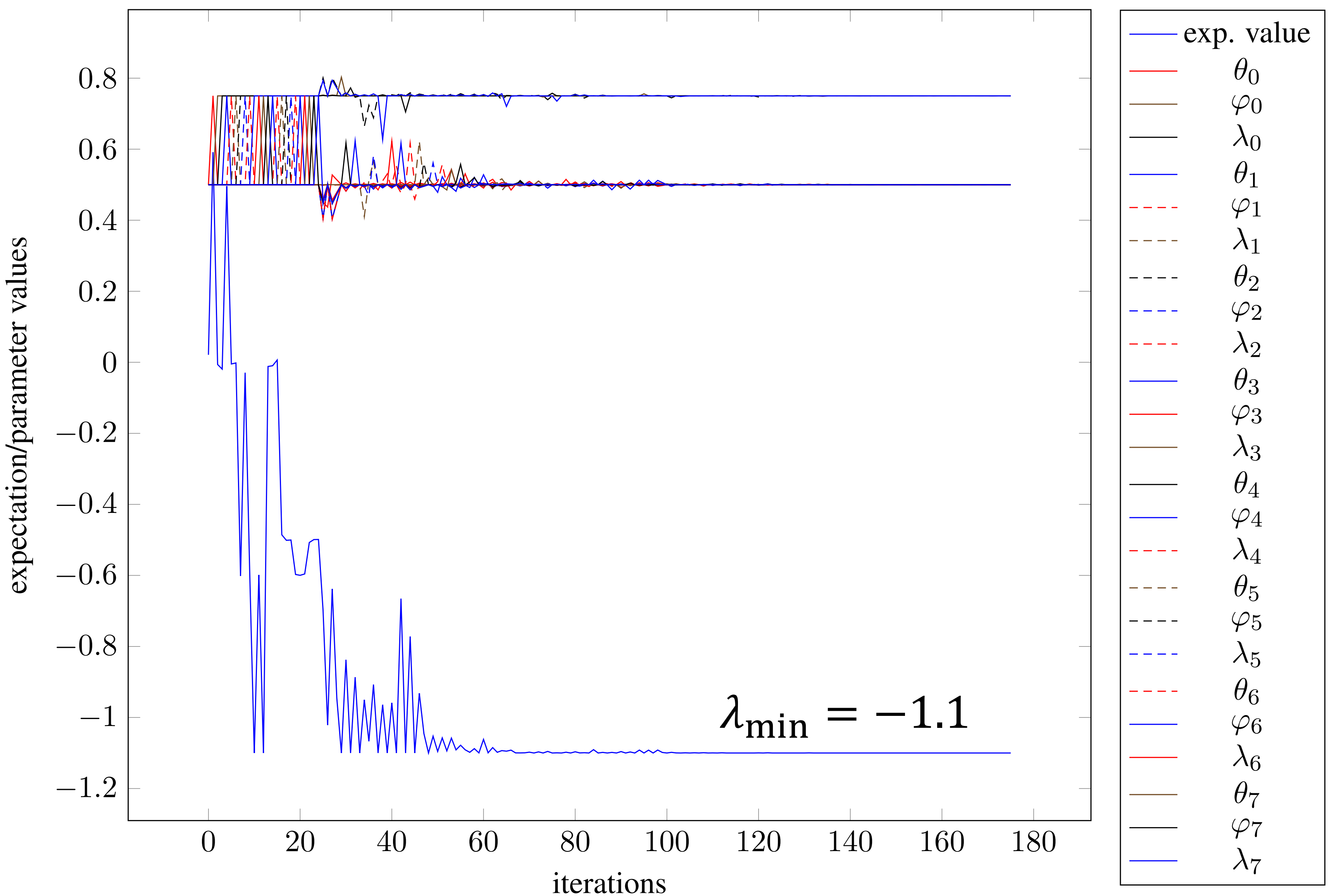
- Global optimizer
  - Genetic algorithm
  - Particle swarm optimization
  - …



- Local optimizer
  - Gradient-free
    - Nelder-Mead Simplex
    - COBYLA
    - …
  - Gradient-based
    - Stochastic gradient descent
    - BFGS / L-BFGS
    - Newton-type
    - …

LibKet integrates the NLopt package https://nlopt.readthedocs.io

Parameters and expectation value



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At the end of the tutorial

- Hands-on introduction into quantum computing
- LibKet – The basics and some of the advanced features
- Variational quantum algorithms – VQE as an example

Scan me

Feedback, bug reports, and feature requests are welcome.

Thank you very much!