An optimal quantum sampling regression algorithm for variational eigensolving in the low qubit number regime

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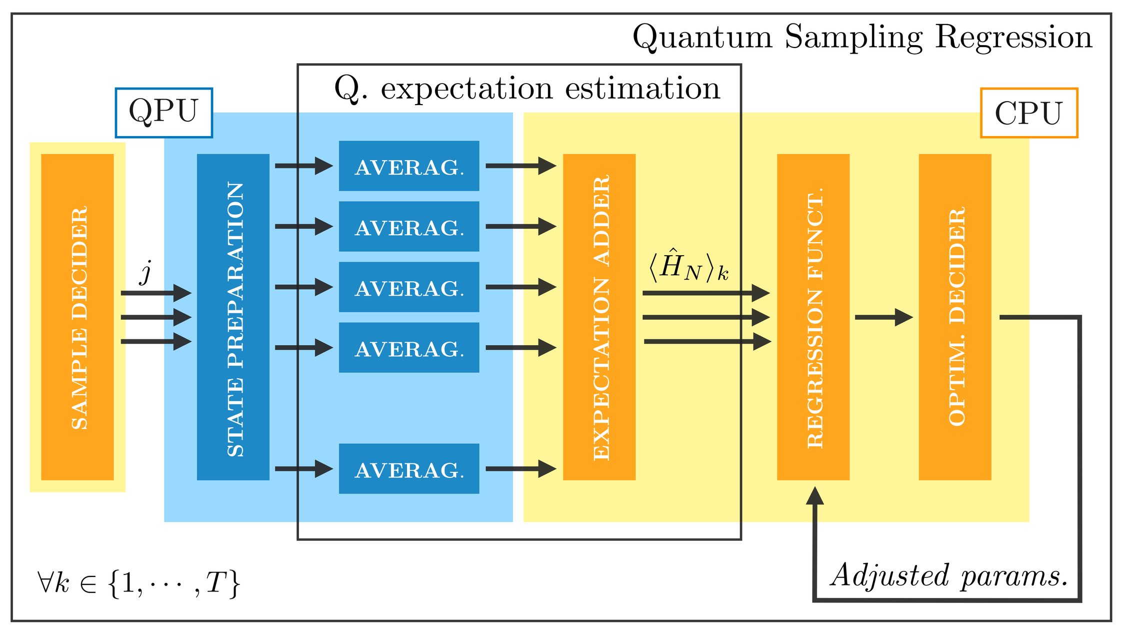


Figure: Diagrammatic representation of the Quantum Sampling Regression algorithm (QSR).

Introduction

Variational quantum eigensolver (VQE):

1. Prepare a quantum state in the quantum processor according to some parameters.
2. Evaluate the expectation value of the computable addends in the target operator.
3. Combine the previous expectation values by adding them up classically according to their respective weights.
4. Use a classical optimization decider to generate a new set of parameters.
5. Return to step one or stop if convergence has been reached.

$$\hat{H}_N = \sum_{j=1}^{\mathcal{O}(N^q)} w_j \hat{H}_N^j \quad \Rightarrow \quad \left\langle \hat{H}_N \right\rangle = \sum_{j=1}^{\mathcal{O}(N^q)} w_j \left\langle \hat{H}_N^j \right\rangle$$

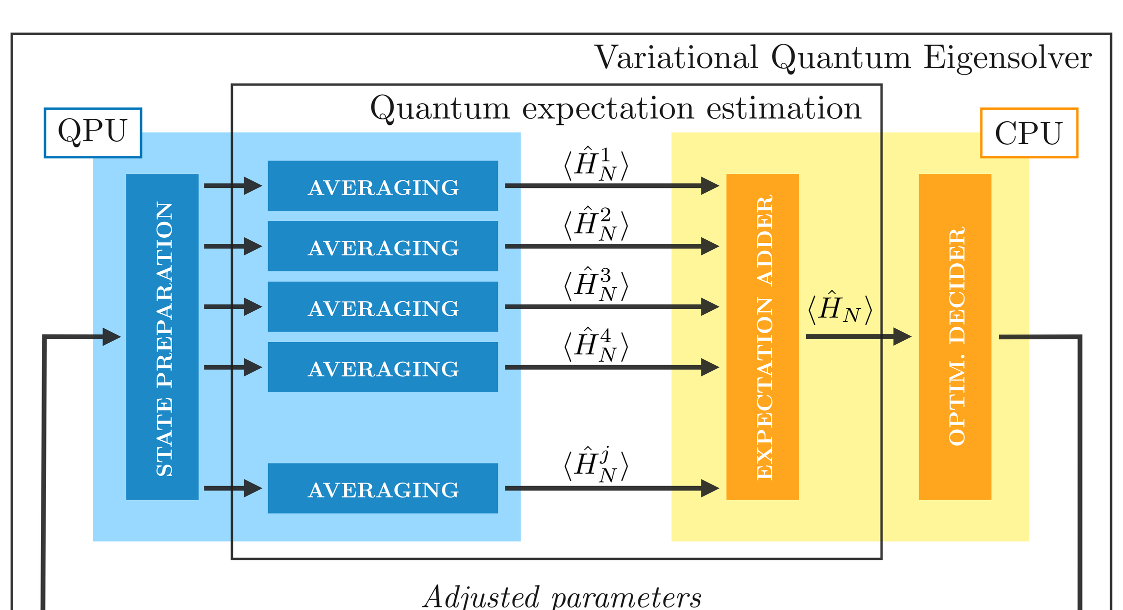


Figure: Diagrammatic representation of the Variational Quantum Eigensolver algorithm (VQE).

Algorithm outline

Quantum sampling regression (QSR):

1. Determine the bandwidth associated to each parameter in the parametrization ansatz.
2. Sample the objective function using a quantum processor in the same way as for VQE.
3. Compute the Fourier coefficients from the measured samples.
4. In a classical machine, solve for the global minimum of the resulting regression function.

$$h(\theta) \triangleq \left\langle \hat{H}_N \right\rangle (\theta) \equiv a_0 + \sum_{k=1}^{S} \left[a_k \cos(k\theta) + b_k \sin(k\theta) \right]$$

$$T = \prod_{j=1}^{n} (2S_j + 1) \leq (2S_{\max} + 1)^n \equiv 2^{sn}$$

Theoretical bedrock

- **Quantum circuit topology** implies a frequency-bounded periodic domain.
- Fourier analysis: **Nyquist-Shannon sampling theorem** as proof of optimality.

Performance comparison

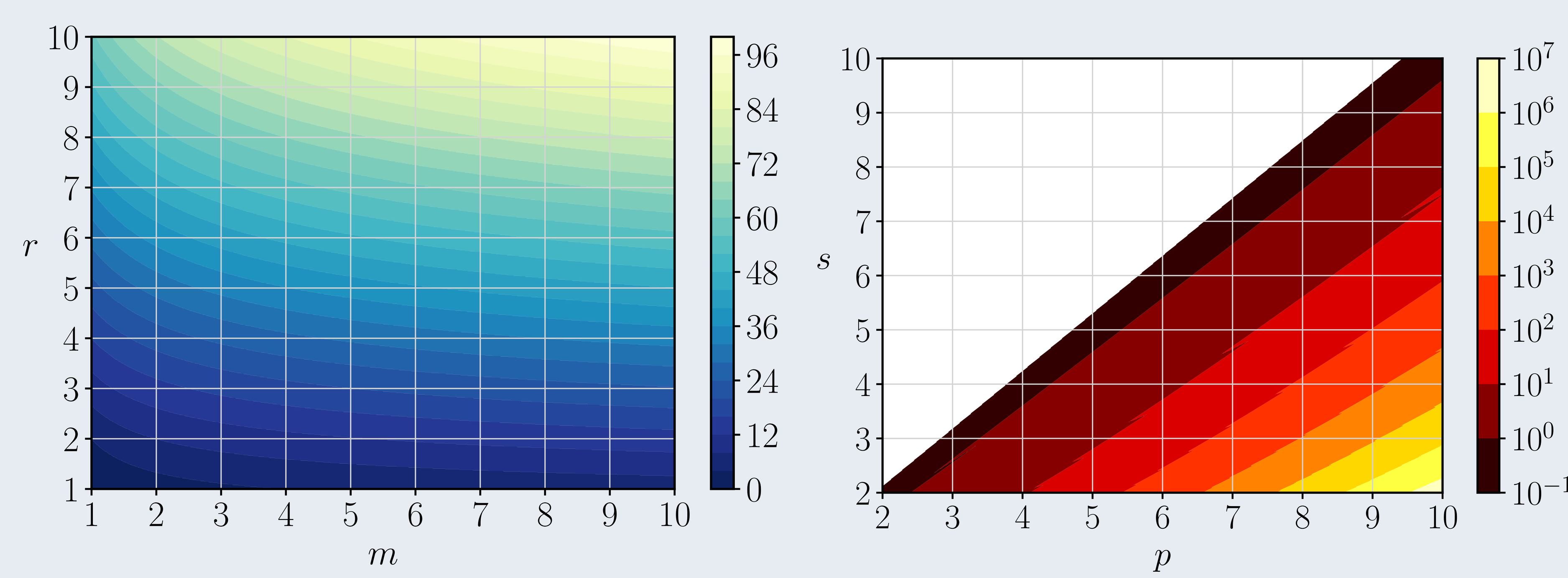


Figure: (Left) VQE threshold a. (Right) QSR average efficieny gains E in the low qubit number regime.

Low qubit number regime

Algorithmic complexity model:

$$\frac{\text{VQE}}{\text{QSR}} = \left(mn2^{-n/r} \right)^p$$

Threshold and average efficiency gains:

$$a \triangleq \left[-\frac{r}{\ln 2} W_{-1} \left(-\frac{\ln 2}{mr} \right) \right]$$

$$E \approx \frac{1}{as \ln 2} \left(\frac{m}{s \ln 2} \right)^p \Gamma(p+1, s\ln 2, as\ln 2)$$

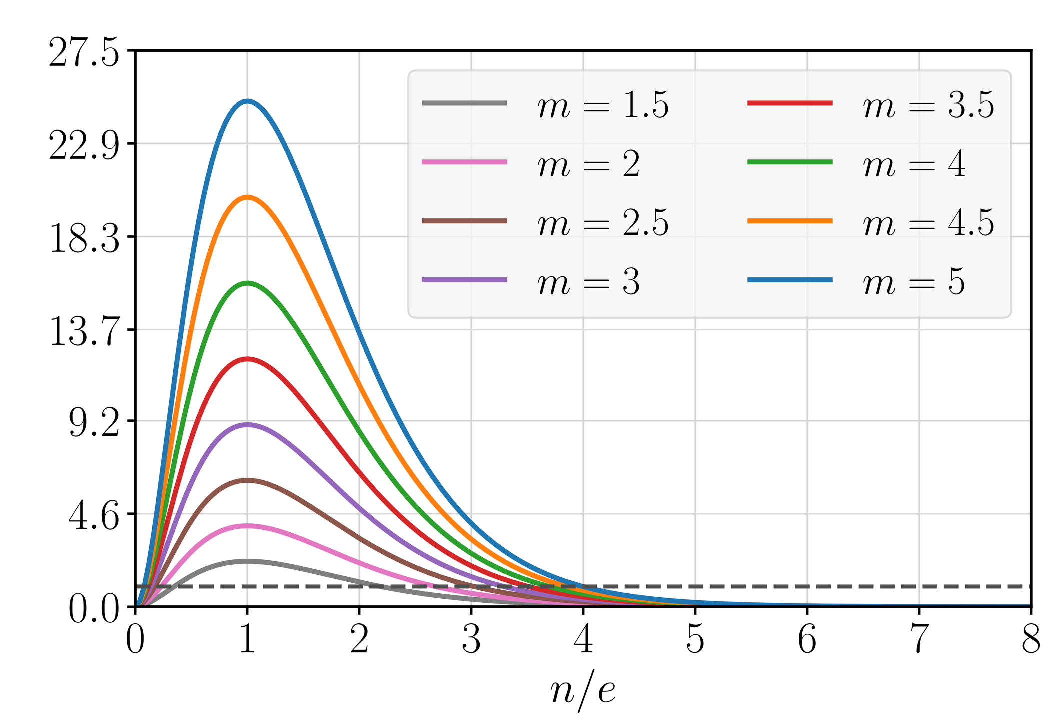
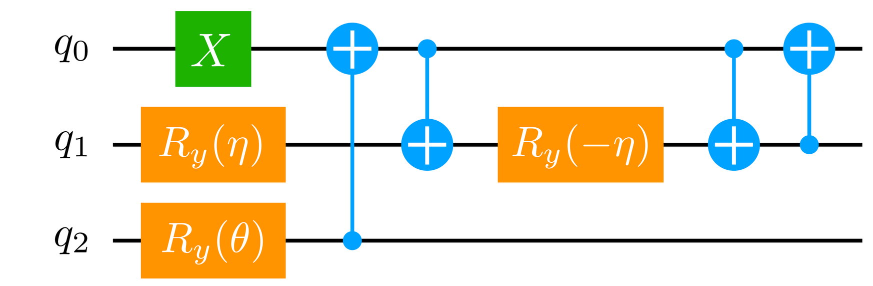


Figure: Comparison between the amount of quantum resources required by VQE and QSR with respect to the number of parameters in the ansatz.



Applications

- **Oversampling** to attain higher precision.
- **Undersampling** to boost performance and get rid of small-wavelength oscillations leading to burdensome local minima.
- VQE low-resolution start-up **supplement**.
- **Proxy** between simulators and real devices.
- Improve convergence by removing stochastic behavior, while retaining important features.
- Avoid the exponential matrix formulation in classical computation.

Benchmarking

Table: Comparison between results for the deuteron binding energy as reproduced using the VQE and QSR algorithms.

n	Algorithm	Samples	Queries	Error
1	VQE	24	24	3.5%
1	QSR	3	1	1.0%
2	VQE	183	183	0.3%
2	QSR	25	1	0.2%

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General Information

- **Contact**: priveroramirez@anl.gov
- **ePrint**: arXiv:2012.02338