Universalizing Analog Quantum Simulators

Andrew Shaw1, * 

1University of Maryland, College Park, MD 20742, USA

(Dated: April 1, 2022)

Unitary Sampling Expectation-Value Reconstruction (USER) is used to determine expectation values that are not directly accessible on an analog quantum simulator.

I. UNITARY SAMPLING EXPECTATION-VALUE RECONSTRUCTION

Unitary Sampling Expectation-Value Reconstruction (USER), allows the indirect determination of expectation values.

A. Unitary Operators

For a Hilbert space $\mathcal{H}$, the Haar measure is comprised of all operators that satisfy unitarity [1]:

$$\hat{U} \in \mathcal{H} \otimes \mathcal{H}^*, \quad \hat{U} \hat{U}^\dagger = \mathbb{1} \quad (I.1)$$

A unitary operator can be expressed as follows:

$$\hat{U} = \sum_\alpha e^{i\phi_\alpha} |\alpha\rangle \langle \alpha|, \quad (I.3)$$

$$\phi_\alpha \in [-\pi, \pi] \quad (I.4)$$

The phase separation is the following:

$$\mathcal{P} = |\phi_\alpha - \phi_\beta|_{\text{max}} \quad (I.5)$$

B. Expectation Values

A quantum state and an observable can be expressed as follows:

$$|\psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle \quad (I.6)$$

$$\hat{O} = \sum_{\alpha,\beta} O_{\alpha,\beta} |\alpha\rangle \langle \beta| \quad (I.7)$$

The expectation value of the observable after a similarity transformation is the following:

$$\langle \psi | \hat{U}^\dagger \hat{O} \hat{U} | \psi \rangle = \sum_{\alpha,\beta} e^{i\phi_\alpha} c_\alpha^* c_\beta O_{\alpha,\beta} e^{i(\phi_\beta - \phi_\alpha)} \quad (I.8)$$

$$= \sum_{\alpha,\beta} D_{\alpha,\beta} e^{iK_{\alpha,\beta}} \quad (I.9)$$

C. Reconstruction

A multiplicative subset of the Haar measure is obtained by exponentiating a unitary operator (Figure 1):

$$\langle \psi | \hat{U}^\dagger \hat{O} \hat{U} | \psi \rangle = \sum_{\alpha,\beta} e^{i\phi_\alpha} c_\alpha^* c_\beta O_{\alpha,\beta} e^{i(\phi_\beta - \phi_\alpha)} \quad (I.8)$$

$$= \sum_{\alpha,\beta} D_{\alpha,\beta} e^{iK_{\alpha,\beta}} \quad (I.9)$$

FIG. 1. A unitary operator (golden) is exponentiated to generate a multiplicative subset (blue). A discretization unitary (red) is used to reconstruct inaccessible expectation values.
The discrete multiplicative expectation values must be sampled faster than the aliasing rate \([2]\):

\[
\eta_{\text{alias}} = \frac{\pi}{|\mathcal{K}_{\alpha,\beta}|_{\text{max}}} \tag{I.14}
\]

The sampling procedure is accomplished by iteration with a discretization unitary:

\[
\hat{U}_d = (\hat{U})^\eta_d \tag{I.15}
\]

\[
\eta_d \mathcal{P} < \pi \tag{I.16}
\]

D. Universal Subset

A reconstructive Haar subset can be used to determine the expectation values of the complete Haar measure with USER:

\[
\mathcal{U}_{\text{recon.}} \in \mathcal{U}_{\text{Haar}}. \tag{II.17}
\]

An example reconstructive Haar subset is the following:

1. The subset contains at least one non-trivial unitary operator from each unique multiplicative subset.
2. \( \mathcal{P} < \pi \) for all such non-trivial unitary operators.
3. All integer powers of the non-trivial unitary operators are present in the subset.

II. EXPANDING ANALOG QUANTUM SIMULATORS

A. Simulating Unitary Operators

1. Analog Quantum Simulators

An analog quantum simulator (AQS) can perform time evolution for a Hamiltonian family \([3]\):

\[
\hat{H}_{\gamma}(t) = \sum_\alpha \mathcal{E}_{\gamma,\alpha}(t) \langle \alpha_{\gamma}(t) | \langle \alpha_{\gamma}(t) | \tag{II.1}
\]

Time evolution simulates the AQS unitary operators:

\[
\hat{U}_{\gamma}(t) = \mathcal{T} \left\{ e^{-i \int_0^t dt' \hat{H}_{\gamma}(t')} \right\} \tag{II.2}
\]

2. Magnus Expansion

The AQS unitary operators can be expressed in terms of the time-independent Hermitian operators:

\[
\hat{U}_{\gamma}(t) = e^{i \hat{M}_{\gamma}^{(t)}} \tag{II.3}
\]

\[
\hat{M}_{\gamma}^{(t)} = \sum_\alpha \hat{\mathcal{M}}_{\gamma,\alpha}^{(t)} \langle \alpha_{\gamma}(t) | \langle \alpha_{\gamma}(t) | \tag{II.4}
\]

The time-independent Hermitian operators can be expressed as a series \([4]\):

\[
\hat{\mathcal{M}}_{\gamma}^{(t)} = \sum_{n=1}^{\infty} \hat{\mathcal{O}}_{\gamma,n}^{(t)} \tag{II.5}
\]

The first few terms are as follows:

\[
\hat{\mathcal{O}}_{\gamma,1}^{(t)} = -i \int_0^t dt_1 \hat{H}_{\gamma}(t_1) \tag{II.6}
\]

\[
\hat{\mathcal{O}}_{\gamma,2}^{(t)} = \frac{i}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [\hat{H}_{\gamma}(t_1), \hat{H}_{\gamma}(t_2)] \tag{II.7}
\]

\[
\ldots
\]

3. Haar Measure Accessibility

The simulated Haar subset contains the AQS unitary operators:

\[
\mathcal{U}_{\text{sim.}} \in \mathcal{U}_{\text{Haar}}. \tag{II.8}
\]

The expanded Haar subset contains the unitary operators whose expectation values can be determined with USER:

\[
\mathcal{U}_{\text{sim.}} \in \mathcal{U}_{\text{exp.}} \in \mathcal{U}_{\text{Haar}}. \tag{II.9}
\]

B. Analog Simulation Expansion

An intermediate unitary operator requires USER to evaluate its expectation values:

\[
\hat{U}_i \in \mathcal{U}_{\text{exp.}}, \quad \hat{U}_i \notin \mathcal{U}_{\text{sim}}. \tag{II.10}
\]

USER is applied in three stages:

I. Exponentiation: Parametrize the intermediate unitary operator.

II. Discretization: Identify an accessible discretization unitary.

III. Reconstruction: Reconstruct the intermediate expectation value.
1. Exponentiation

The intermediate unitary operator can be expressed in terms of the intermediate Hermitian operator:

$$\hat{U}_i = e^{i\pi \hat{A}} \quad (\text{II.11})$$

$$\hat{A} = \sum_\alpha \hat{A}_\alpha |\alpha\rangle \langle \alpha| \quad (\text{II.12})$$

$$|\hat{A}_\alpha| \leq 1 \quad (\text{II.13})$$

The intermediate multiplicative subset is the following:

$$\langle \hat{U}_i \rangle^\eta = e^{i\pi \eta \hat{A}} \quad (\text{II.14})$$

2. Discretization

The simulation discretization unitary is the following:

$$\hat{U}_{s,d} \in \mathcal{U}_{\text{sim.}} \quad (\text{II.15})$$

$$\hat{U}_{s,d} = e^{i\pi \lambda \hat{A}} \quad (\text{II.16})$$

$$\lambda < \frac{1}{2} \quad (\text{II.17})$$

3. Reconstruction

The intermediate expectation value is the following:

$$\langle \hat{O}_i \rangle = \hat{U}_i^\dagger \hat{O} \hat{U}_i \quad (\text{II.18})$$

The minimal intermediate eigenvalue gap is as follows:

$$\Delta A_{\text{min}} = |\hat{A}_\alpha - \hat{A}_\beta|_{\text{min}} \quad (\text{II.19})$$

The discrete sampling unitary operators are as follows:

$$\left[ \hat{U}_{s,d}^{-n_1}, \cdots, \hat{1}, \hat{U}_{s,d}, \cdots, \hat{U}_{s,d}^{n_1} \right] \quad (\text{II.20})$$

$$n_1 \gg \frac{2 + \Delta A_{\text{min}}}{\lambda \Delta A_{\text{min}}} \quad (\text{II.21})$$

The discrete multiplicative expectation values are as follows:

$$\left[ \langle \hat{O}_i(-n_1\lambda) \rangle, \cdots, \langle \hat{O}_i(0) \rangle, \cdots, \langle \hat{O}_i(n_1\lambda) \rangle \right] \quad (\text{II.22})$$

The discrete multiplicative expectation values are used to reconstruct the intermediate expectation value [5]:

$$\langle \hat{O}_i \rangle \approx \sum_{k=-n_1}^{n_1} \langle \hat{O}_i(k\lambda) \rangle \frac{1 - k\lambda}{\lambda} \quad (\text{II.23})$$

III. SIMULATED EXPECTATION-VALUE APPROXIMATE RECONSTRUCTION

Simulated Expectation-Value Approximate Reconstruction (SEAR), is a method for estimating the expectation value of an intermediate unitary operator.

SEAR is applied in three stages:

I. Analog Simulation Expansion: Apply USER to approximate the intermediate expectation value.

II. Series Approximation: Repeat Stage I to generate a series of approximations for the intermediate expectation value.

III. Error Estimation: Approximate the average error in the intermediate expectation value.

1. Analog Simulation Expansion

The $\kappa^{\text{th}}$-order time-independent Hermitian operators are the following:

$$\hat{M}^{(t)}_{\gamma,\kappa} = \sum_{n=1}^{\kappa} \hat{\Omega}^{(t)}_{\gamma,n} \quad (\text{III.1})$$

A sequence of members of the Hamiltonian family is chosen that satisfies the following condition:

$$\sum_{\xi=1}^{n_\xi} \hat{M}^{(t)}_{\xi,\kappa} = \pi \lambda \hat{A}, \quad (\text{III.2})$$

$$\lambda < \frac{1}{2} \quad (\text{III.3})$$

The approximate simulation discretization unitary is the following:

$$\hat{U}_{s,d} = \prod_{\xi=1}^{n_\xi} e^{i\hat{M}^{(t)}_{\xi}} \quad (\text{III.4})$$

$$\approx e^{i\pi \lambda \hat{A}} \quad (\text{III.5})$$

Performing reconstruction yields the approximate intermediate expectation value:

$$\langle \hat{O}_{i,a} \rangle = \langle \hat{U}_{i,a}^\dagger \hat{O} \hat{U}_{i,a} \rangle \quad (\text{III.6})$$
2. Series Approximation

The expectation values for a series of approximate intermediate unitaries are obtained (Figure 2):

\[
\left\{ \hat{U}^{(1)}_{i,a}, \hat{U}^{(2)}_{i,a}, \ldots, \hat{U}^{(n_a)}_{i,a} \right\} \quad (III.7)
\]

3. Error Estimation

The mean approximate intermediate expectation value is the following:

\[
\langle \hat{O}_{i,a} \rangle_{\text{mean}} = \frac{1}{n_a} \sum_{k=1}^{n_a} \langle \hat{U}^{(k)}_{i,a} \hat{O} \hat{U}^{(k)}_{i,a} \rangle \quad (III.8)
\]

The error in this quantity can be approximated using quantum channel technology.

A. Quantum Channel Technology

1. Density Matrix Formalism

A density matrix describes an ensemble of quantum states \( |\psi_k\rangle \), each with observational probability \( p_k \) [6]:

\[
\rho = \sum_{k} p_k |\psi_k\rangle \langle \psi_k| \quad (III.9)
\]

Density matrices satisfy the following condition:

\[
\text{Tr}[\rho] = 1 \quad (III.10)
\]

Expectation values of density matrices are as follows:

\[
\langle \hat{O} \rangle = \text{Tr}[\rho \hat{O}] \quad (III.11)
\]

2. Quantum Channel Formalism

Quantum channels are a type of superoperator [7]:

\[
\hat{C} = \sum_{\mu} \hat{K}_{\mu} \otimes \hat{K}_{\mu}^\dagger \quad (III.12)
\]

They satisfy the following condition:

\[
\sum_{\mu} \hat{K}_{\mu} \hat{K}_{\mu}^\dagger = \mathbb{1} \quad (III.13)
\]

Quantum channels act on density matrices as follows:

\[
\rho' = \hat{C}[\rho] \quad (III.14)
\]

\[
= \sum_{\mu} \hat{K}_{\mu} \rho \hat{K}_{\mu}^\dagger \quad (III.15)
\]

B. SEAR Error Channel

The intermediate expectation value is the following:

\[
\langle \hat{O}_{i,a} \rangle = \text{Tr}[\rho_{i,a} \hat{O}] \quad (III.16)
\]

\[
\rho_{i,a} = \hat{U}_{i,a} \rho \hat{U}_{i,a}^\dagger \quad (III.17)
\]

The mean approximate intermediate expectation value is as follows:

\[
\langle \hat{O}_{i,a} \rangle_{\text{mean}} = \frac{1}{n_a} \sum_{k=1}^{n_a} \text{Tr}\left[ \hat{U}^{(k)}_{i,a} \rho_{i,a} \hat{U}^{(k)}_{i,a}^\dagger \hat{O} \right] \quad (III.18)
\]

This quantity can be written using the SEAR error channel:

\[
\langle \hat{O}_{i,a} \rangle_{\text{mean}} = \text{Tr}\left[ \hat{S} \rho_{i,a} \hat{O} \right] \quad (III.19)
\]

\[
\hat{S} = \sum_{\mu=1}^{n_a} \hat{S}_{\mu} \otimes \hat{S}_{\mu}^\dagger \quad (III.20)
\]

\[
\hat{S}_{\mu} = \frac{1}{n_a} \hat{U}^{(\mu)}_{i,a} \hat{U}_{i,a}^\dagger \quad (III.21)
\]
C. SEAR Error

1. Quantum Channel Averaging

Applying a similarity transformation to a quantum channel yields the following:

\[ \hat{\mathcal{C}}_u = \hat{U} \hat{C} \hat{U} \tag{III.22} \]

\[ = \sum_{\mu} \hat{U}^\dagger \hat{K}_\mu \hat{U} \otimes \hat{U}^\dagger \hat{K}_\mu^\dagger \hat{U} \tag{III.23} \]

Integrating over the Haar measure yields a depolarizing channel [8]:

\[ \hat{\mathcal{D}}_\epsilon = \int dU_{\text{Haar}} \hat{U}^\dagger \hat{C} \hat{U} \tag{III.24} \]

Depolarizing channels mix quantum states with the identity at noise strength \( \epsilon \):

\[ \hat{\mathcal{D}}_\epsilon [\rho] = (1 - \epsilon) \rho + \epsilon \frac{1}{\text{dim}(\mathcal{H})} \tag{III.25} \]

The SEAR depolarizing channel is the following:

\[ \hat{\mathcal{D}}_{\epsilon_s} = \int dU_{\text{Haar}} \hat{U}^\dagger \hat{S} \hat{U} \tag{III.26} \]

2. Expectation Value Error

The intermediate expectation value error is as follows:

\[ \Delta O^i = \left| \text{Tr} \left( (\rho_i - \hat{S} [\rho_i]) \hat{O} \right) \right| \tag{III.27} \]

The average intermediate expectation value error is the following:

\[ \Delta O^i_{\text{mean}} = \left| \text{Tr} \left( (\rho_i - \int dU_{\text{Haar}} \hat{S}_u [\rho_i]) \hat{O} \right) \right| \tag{III.28} \]

\[ = \left| \text{Tr} \left( (\rho_i - \hat{\mathcal{D}}_{\epsilon_s} [\rho_i]) \hat{O} \right) \right| \tag{III.29} \]

It can be expressed using the SEAR noise strength:

\[ \Delta O^i_{\text{mean}} = \epsilon_s \left| \langle \hat{O} \rangle - \frac{\text{Tr}[\hat{O}]}{\text{dim}(\mathcal{H})} \right| \tag{III.30} \]

D. Estimating the SEAR Error

1. Complementary SEAR Error Channel

The complementary SEAR error channels are the following:

\[ \hat{S}^{(k)} = \sum_{\mu=1}^{n_a} \hat{S}_\mu^{(k)} \otimes \hat{S}_\mu^{(k)\dagger} \tag{III.31} \]

\[ \hat{S}_\mu^{(k)} = \frac{1}{n_a} \hat{U}_{i,a}^{(\mu)} \hat{U}_{i,a}^{(\mu)\dagger} \tag{III.32} \]

The complementary SEAR depolarizing channels are as follows:

\[ \hat{\mathcal{D}}_{\epsilon_s}^{(k)} = \int dU_{\text{Haar}} \hat{U}^\dagger \hat{S}^{(k)} \hat{U} \tag{III.33} \]

\[ \epsilon_s^{(k)} \approx \epsilon_s \tag{III.34} \]

2. Discrete Quantum Channel Averaging

The approximate complementary SEAR depolarizing channels are as follows:

\[ \hat{B}_{\epsilon_s}^{(k)} = \frac{1}{n_t} \sum_{m=1}^{n_t} \hat{U}_m^{(\mu)} \hat{S}^{(k)} \hat{U}_m \tag{III.35} \]

\[ \hat{U}_m \in U_{\text{sim.}} \tag{III.36} \]

Shown explicitly:

\[ \hat{B}_{\epsilon_s}^{(k)} = \sum_{\mu=1}^{n_a} \sum_{m=1}^{n_t} \hat{B}_{\mu,m}^{(k)} \otimes \hat{B}_{\mu,m}^{(k)\dagger} \tag{III.37} \]

\[ \hat{B}_{\mu,m}^{(k)} = \frac{1}{n_\alpha n_t} \hat{U}_{i,a}^{(\mu)} \hat{U}_{i,a}^{(\mu)\dagger} \hat{U}_m \tag{III.38} \]

\[ = \frac{1}{n_\alpha n_t} \hat{U}_{i,a}^{(\mu)} \hat{U}_{i,a}^{(\mu)\dagger} \hat{U}_m \tag{III.39} \]

3. Evaluating the Approximate Complementary SEAR Depolarizing Channels

The approximate complementary SEAR depolarizing expectation value is the following:

\[ \langle \hat{O}^{(k)} \rangle_{\text{comp.}} = \text{Tr} \left[ \hat{B}_{\epsilon_s}^{(k)} [\rho] \hat{O} \right] \tag{III.40} \]
Universalizing Analog Quantum Simulators

IV. NUMERICAL IMPLEMENTATION

This quantity can be expressed using the partial SEAR depolarizing expectation values:

\[
\langle \hat{O}^{(k)} \rangle_{\text{comp.}} = \frac{1}{n_a n_t} \sum_{\mu, m=1}^{n_a, n_t} \langle \hat{O}_{\mu, m}^{(k)} \rangle \\
= \frac{1}{n_a n_t} \sum_{\mu, m=1}^{n_a, n_t} \text{Tr} \left[ \hat{U}_{\mu, m}^{(k)} \rho \hat{U}_{\mu, m}^{(k)\dagger} \hat{O} \right]
\]  

(III.41)

(III.42)

4. Estimating the Approximate Complementary SEAR Depolarizing Expectation Value

The discrete approximate intermediate unitaries are the following:

\[
\hat{U}_{i,a,d}^{(k)} = \left[ \hat{U}_{s,d}^{(k)} \right]^{(i)}
\]

(III.43)

\[
\tau^{(k)} = \text{round} \left( \frac{1}{\lambda^{(k)}} \right)
\]

(III.44)

The approximate partial SEAR depolarizing expectation values are the following:

\[
\langle \hat{O}_{\mu, m}^{(k)} \rangle_{\text{comp.}} = \text{Tr} \left[ \hat{U}_{\mu, m}^{(k)} \rho \hat{U}_{\mu, m}^{(k)\dagger} \hat{O} \right]
\]

(III.45)

(III.46)

5. Estimating the SEAR Noise Strength

The discrete complementary SEAR noise strength is as follows:

\[
\epsilon_{s,d}^{(k)} = \left[ \langle \hat{O}_{\mu, m}^{(k)} \rangle_{\text{comp.}} - \text{Tr} \left[ \rho \hat{O} \right] \right] \left[ \text{Tr} \left[ \hat{O} \right] / \text{dim}(\mathcal{H}) - \text{Tr} \left[ \rho \hat{O} \right] \right]^{-1}
\]

(III.47)

(III.48)

(III.49)

The mean discrete complementary SEAR noise strength is the following:

\[
\tau_{s,d} = \frac{1}{n_d} \sum_{k=1}^{n_a} \epsilon_{s,d}^{(k)}
\]

(III.50)

6. Estimating the Expectation Value Error

The average intermediate expectation value error can be approximated as follows:

\[
\Delta O_{\text{mean}}^{i} \approx \tau_{s,d} \left| \langle \hat{O}_{i} \rangle - \frac{\text{Tr} [\hat{O}]}{\text{dim}(\mathcal{H})} \right|
\]

(III.51)

The observable is the following:

\[
\hat{O} = \sum_{\sigma} \omega_{\sigma} |\sigma\rangle \langle \sigma|\]

(III.52)

The observable eigenvalue spread is the following:

\[
\Delta \omega = |\omega_{\text{max}} - \omega_{\text{min}}|
\]

(III.53)

The approximate average intermediate expectation value error is as follows:

\[
\Delta O_{\text{mean}}^{i} = \tau_{s,d} \Delta \omega
\]

(III.54)

E. SEAR Result

SEAR gives the following estimate for the intermediate expectation value:

\[
\langle \hat{O}_{i} \rangle \sim \langle \hat{O}_{i, a} \rangle_{\text{mean}} \pm \Delta O_{\text{mean}}^{i}
\]

(III.55)

IV. NUMERICAL IMPLEMENTATION

The Hamiltonian family is the following:

\[
\hat{H}_{\gamma}(t) = -\frac{1}{2m} \left[ \frac{e^{-i\gamma a} - e^{i\gamma a}}{2a} \right]^{2} + a \ddot{x} \sin (\omega_{\gamma} t)
\]

(IV.1)

SEAR is used to perform quantum simulation of the target Hamiltonian:

\[
\hat{H}_{t} = -\frac{1}{2m} \left[ \frac{e^{-i\gamma a} - e^{i\gamma a}}{2a} \right]^{2} + b \ddot{x} + K(\dot{p})
\]

(IV.2)

1. Unitary Sampling

The AQS is used to compute the discrete multiplicative expectation values (Figure 3).

2. Reconstruction

The approximate intermediate expectation values are reconstructed (Figure 4).
Universalizing Analog Quantum Simulators

3. Noise Strength Estimation

The AQS is used to estimate the SEAR noise strength (Figure 5).

4. SEAR Result

The SEAR observable estimate is computed (Figure 6).

V. APPENDIX

If the approximate intermediate unitaries meet certain criteria, they can be used to recover the intermediate expectation value [9].

VI. ACKNOWLEDGEMENTS

He was oppressed and treated harshly, yet he never said a word.
He was led like a lamb to the slaughter.
And as a sheep is silent before the shearsers, he did not open his mouth.

-Isaiah 53:7

—AMDG—

[1] A. Haar, The standard in the theory of continuous groups, Annals of Mathematics 34, 147 (1933).
[2] H. Nyquist, Certain topics in telegraph transmission theory, Transactions of the American Institute of Electrical Engineers 47, 617 (1928).
[3] R. P. Feynman, Simulating physics with computers, International Journal of Theoretical Physics 21, 467 (1982).
[4] W. Magnus, On the exponential solution of differential equations for a linear operator, Communications on Pure and Applied Mathematics 7, 649 (1954).
[5] E. Whittaker, On the functions which are represented by the expansions of the interpolation-theory, Proceedings of the Royal Society of Edinburgh 35, 181 (1915).
[6] L. Landau, The damping problem in quantum mechanics, in Collected Papers of L.D. Landau (Pergamon, 1927) Chap. 2, pp. 8–18.
[7] M.-D. Choi, Completely positive linear maps on complex matrices, Linear Algebra and its Applications 10, 285 (1975).
[8] M. A. Nielsen, A simple formula for the average gate fidelity of a quantum dynamical operation, Physics Letters A 303, 219 (2002).
[9] A. Shaw, Classical-Quantum Noise Mitigation for NISQ Hardware, arXiv e-prints , arXiv:2105.08701 (2021), arXiv:2105.08701 [quant-ph].