IOP QUANTUM 2020

What Functions can Quantum Models Learn?

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The effect of data encoding on the expressive power of variational quantum machine learning models

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(Dated: August 21, 2020)

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Disclaimer: After uploading to the arxiv we were notified of work by Vidal and Theis¹ that has significant overlap with ours.

¹Gil Vidal, Francisco Javier, and Dirk Oliver Theis. "Input Redundancy for Parameterized Quantum Circuits." *Frontiers in Physics* 8 (2020): 297.



Maria Schuld Xanadu



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Using quantum models for learning tasks is one of the key fields where NISQ devices are hoped to bring forth a quantum advantage

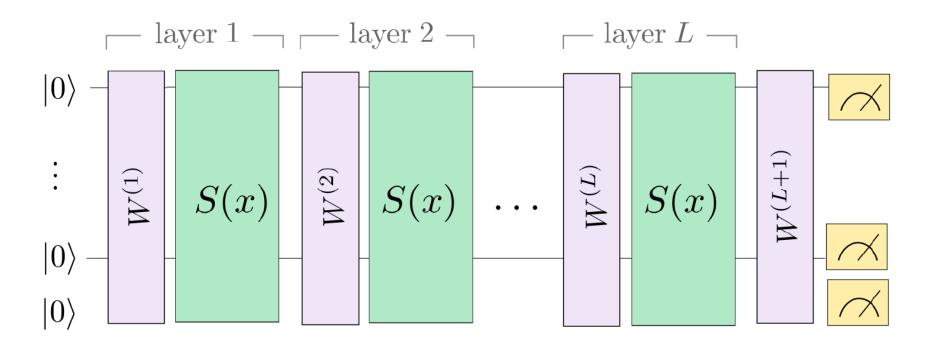
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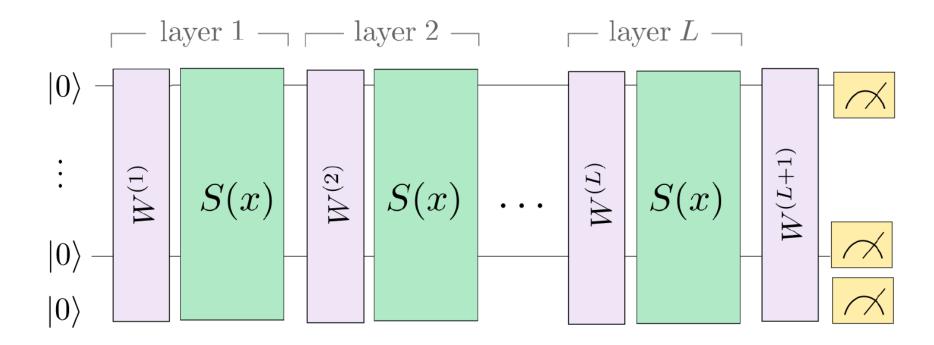
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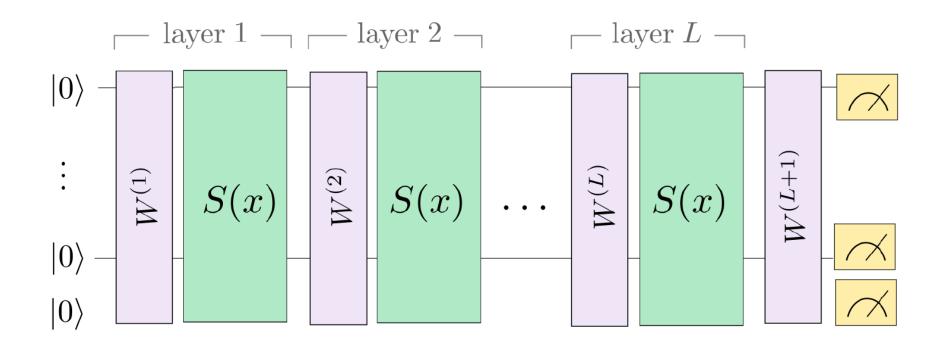
So we asked ourselves: What functions can such models learn?





$$f(x) = \langle M \rangle$$

Model Output

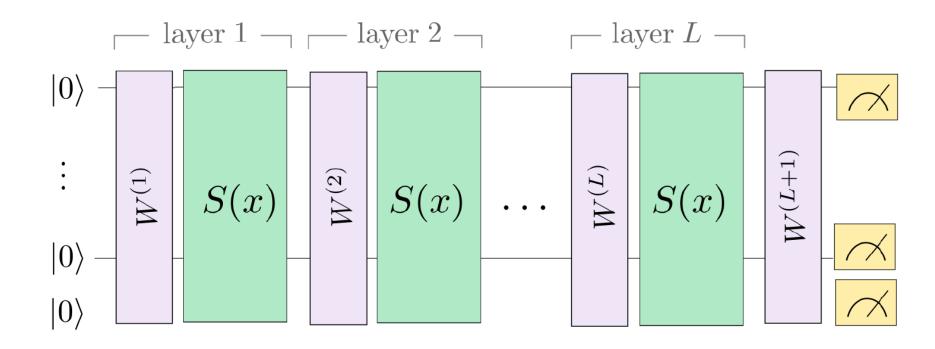


$$f(x) = \langle M \rangle$$

$$S(x) = e^{-ixH}$$

Model Output

Hamiltonian Evolution



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 $W^{(l)}(oldsymbol{ heta})$

Model Output

Hamiltonian Evolution

Trainable Blocks

The eigenvalues of the generator determine the frequencies

$$H|\lambda\rangle = \lambda|\lambda\rangle$$

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$$H|\lambda\rangle = \lambda|\lambda\rangle$$

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and the frequencies accumulate between layers:

$$|\psi\rangle = \sum_{\lambda} \psi_{\lambda} |\lambda\rangle \qquad \text{contains}$$

$$S(x)|\psi\rangle = \sum_{\lambda} \psi_{\lambda} e^{-ix\lambda} |\lambda\rangle$$

$$WS(x)|\psi\rangle = \sum_{\lambda'\lambda} W_{\lambda'\lambda} \psi_{\lambda} e^{-ix\lambda} |\lambda'\rangle$$

$$S(x)WS(x)|\psi\rangle = \sum_{\lambda'\lambda} W_{\lambda'\lambda} \psi_{\lambda} e^{-ix(\lambda+\lambda')} |\lambda'\rangle$$

The output state contains all possible sums of frequencies

Output is expectation value and therefore contains a complex conjugation

$$f_{M,\theta}(x) = \langle \psi_{\theta}(x) | M | \psi_{\theta}(x) \rangle = \sum_{\omega \in \Omega} c_{\omega}(M, \theta) e^{i\omega x}$$

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For one layer of encoding

$$\Omega = \{\lambda_j - \lambda_k \mid \lambda_j, \lambda_k \in \operatorname{spec}(H)\}\$$

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For L layers of encoding

$$\Omega = \{\lambda_{j_1} + \dots + \lambda_{j_L} - \lambda_{k_1} - \dots - \lambda_{k_L} \mid \lambda_{j_l}, \lambda_{k_l} \in \operatorname{spec}(H)\}$$

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The accessible spectrum consists of all sums of differences of eigenvalues of the generator of the data encoding

Take-Home Message #1

Quantum learning models output Fourier series, repeating data encoding gives access to higher frequencies

Pauli rotations are the most popular encoding strategy, e.g.

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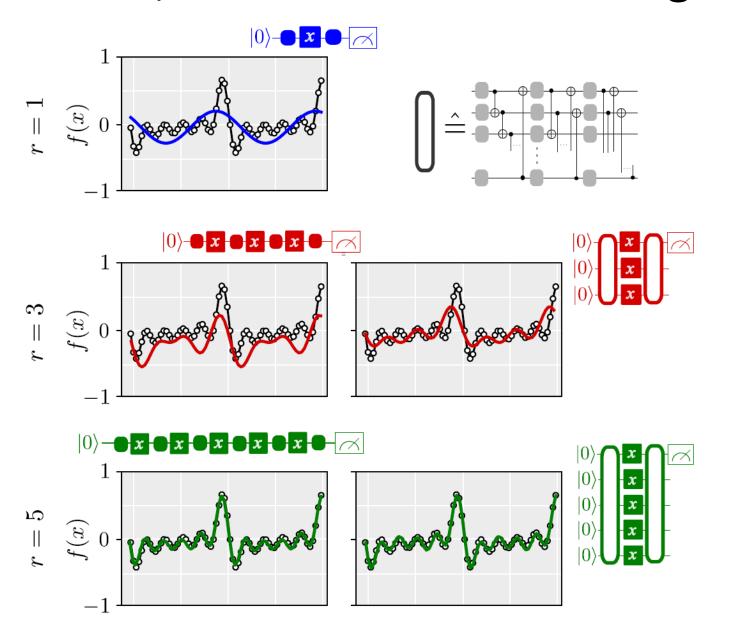
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For general encodings the dependence can be exponential:

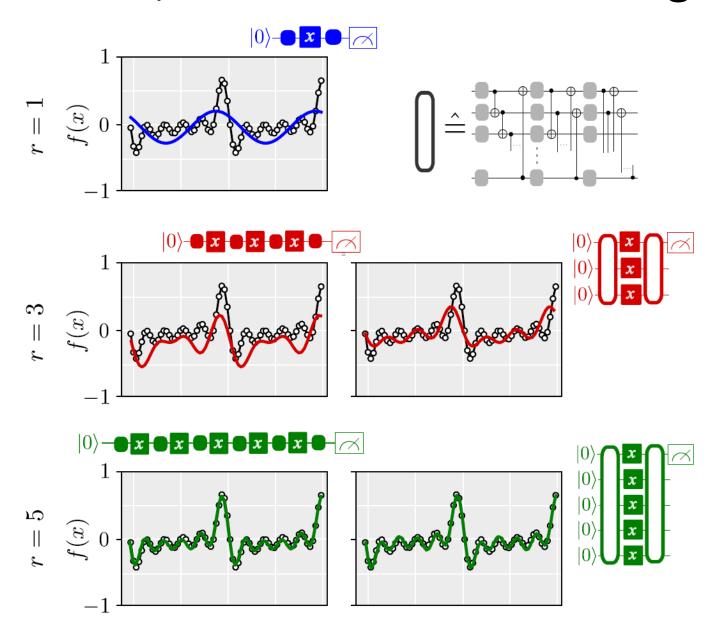
$$\#(\text{frequencies}) \leq \frac{d^{2L}}{2} - 1 \qquad \qquad \frac{d}{L} \quad \text{Number of layers}$$

Consequences for Learning Tasks

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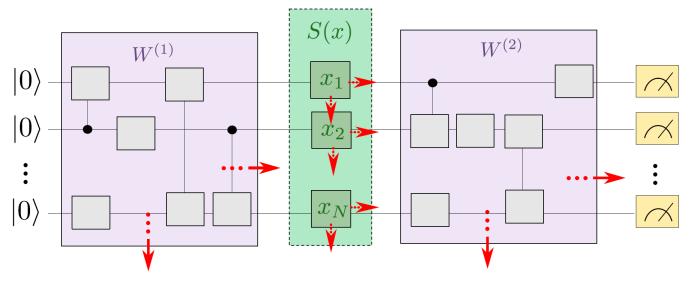
You can reproduce all figures from the paper at home!



Universality of Quantum Models

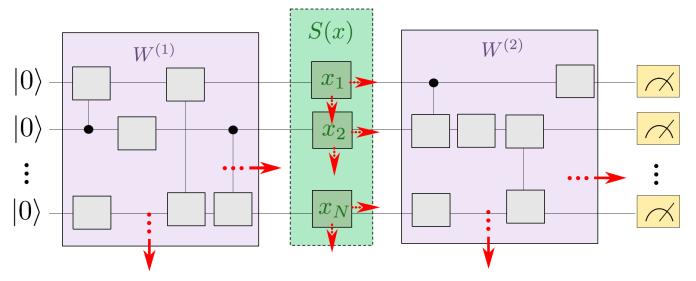
Universality of Quantum Models

A model with one layer of data encodings generated by a *universal* Hamiltonian family and arbitrary unitaries is a universal function approximator



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A model with one layer of data encodings generated by a *universal* Hamiltonian family and arbitrary unitaries is a universal function approximator



A universal Hamiltonian family asymptotically has access to all integer frequencies. Repeated single-qubit Pauli rotation encodings are a universal Hamiltonian family!

Take-Home Message #2

Quantum learning models are universal function approximators

1. Know your data encoding, it fundamentally limits what you can learn!

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- 2. Powerful quantum computers can make stupid models

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- 3. Rescale your data wisely
- 4. Classical pre-processing can alter the model's output dramatically
- 5. Make your observables trainable

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- 2. Can we link specific ansatz classes for the trainable blocks to the output Fourier coefficients?
- 3. Is universal approximation possible with fixed qubit numbers?
- 4. Are quantum models good for signal processing?

Thank you for your attention!



Paper



Demo



Slides