Understanding Variational Quantum Learning Models

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

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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.

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



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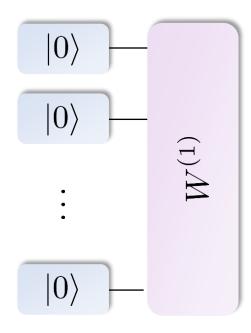
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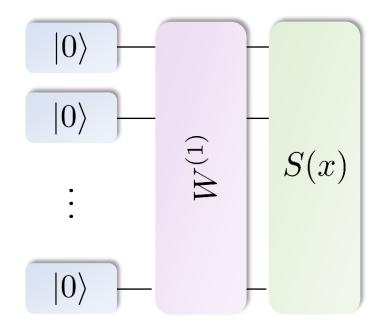
So we asked ourselves: What functions can such models learn?

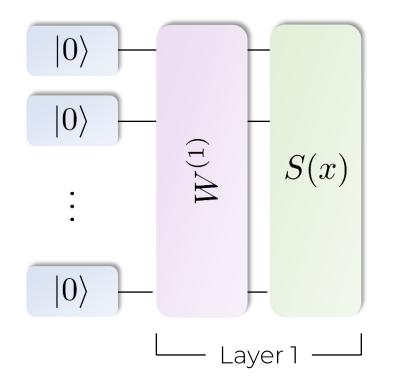


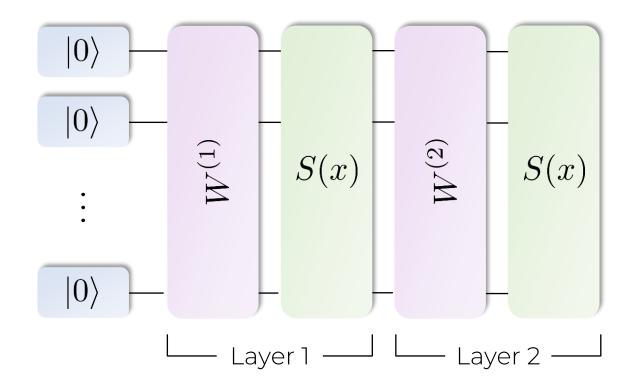


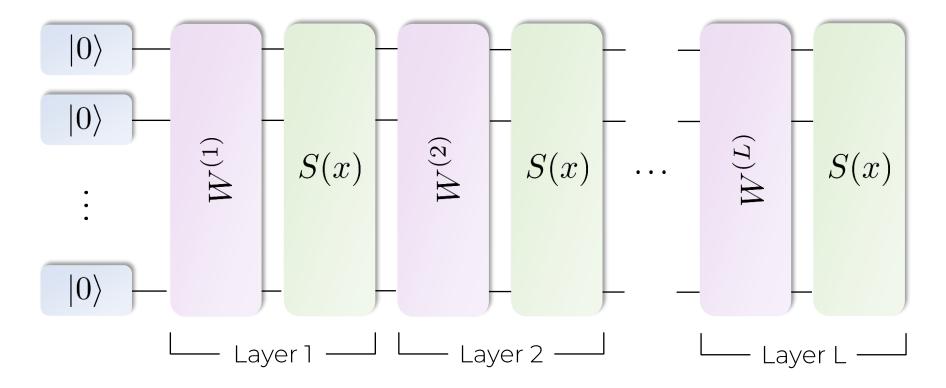
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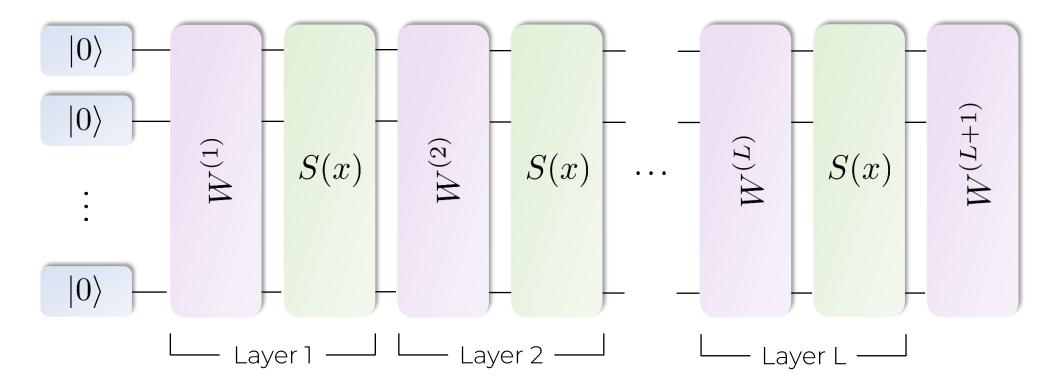


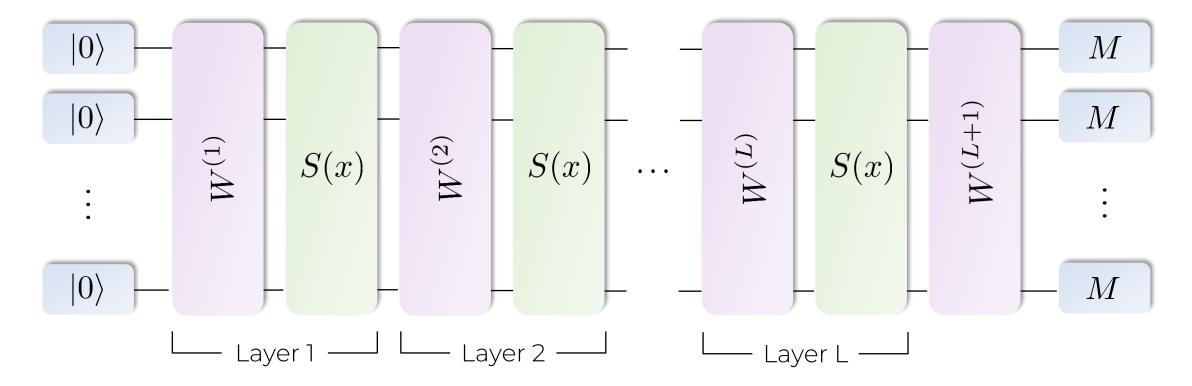


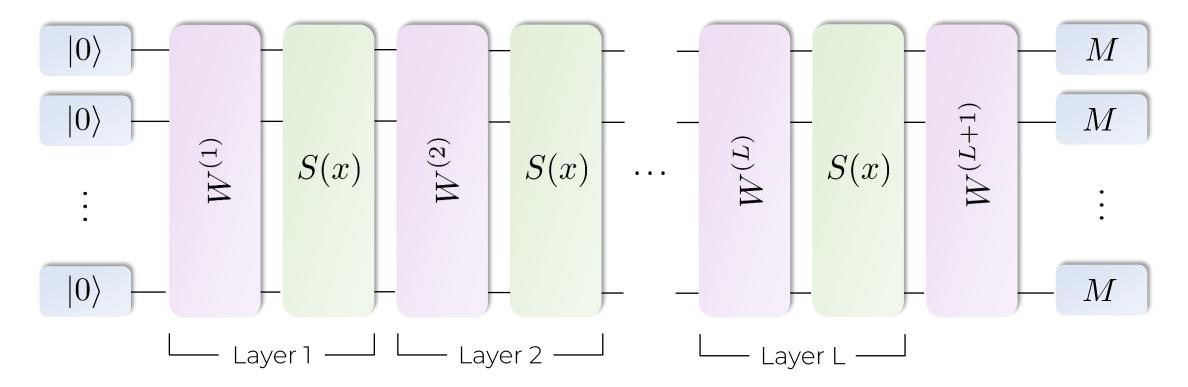






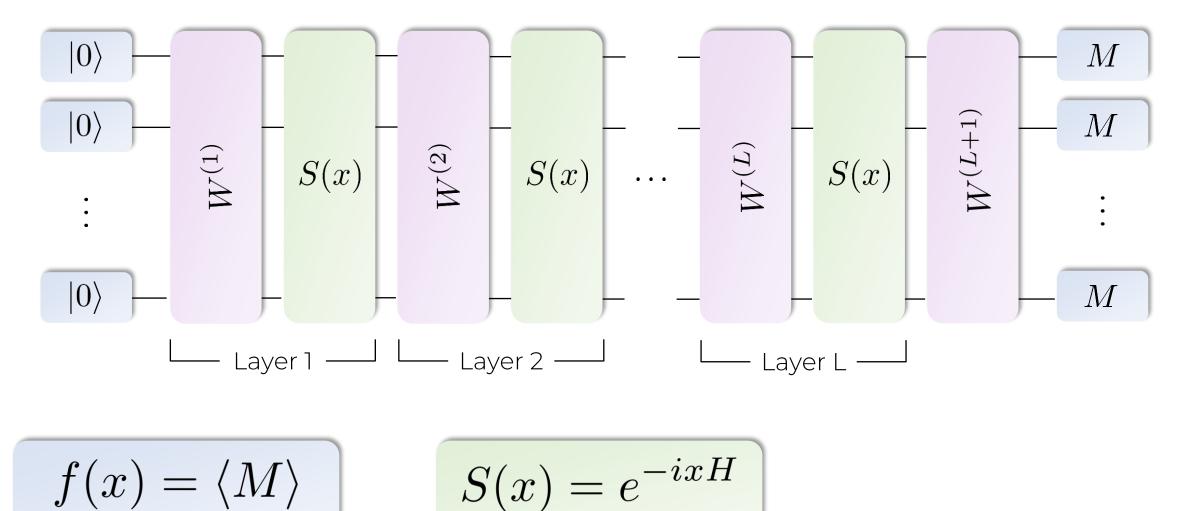






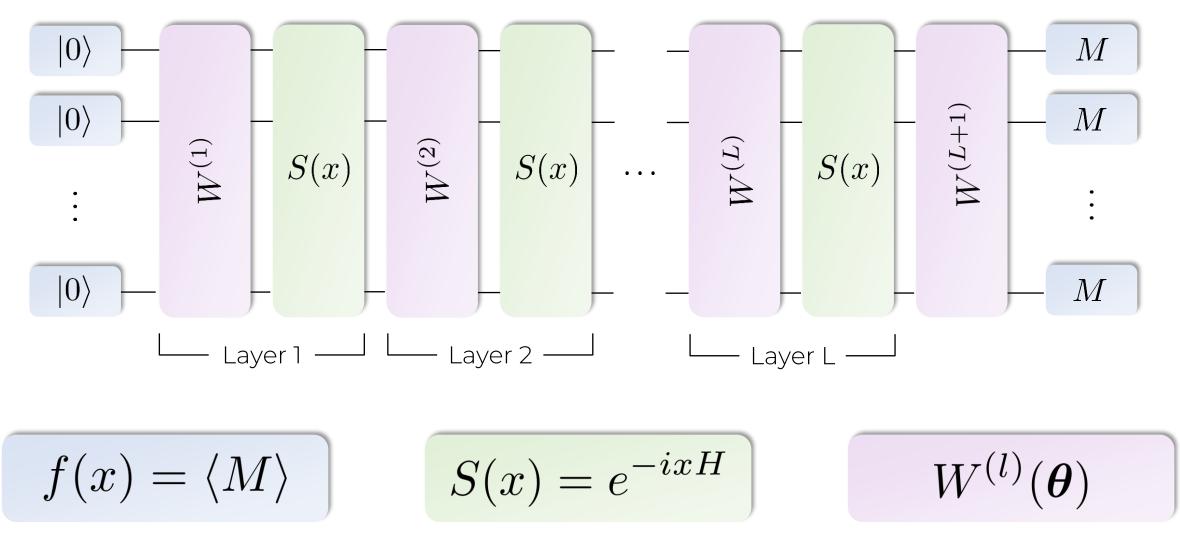
$$f(x) = \langle M \rangle$$

Model Output



Model Output

Hamiltonian Evolution



Model Output

Hamiltonian Evolution

Trainable Blocks

The eigenvalues of the generator determine the frequencies

 $H|\boldsymbol{\lambda}\rangle = \boldsymbol{\lambda}|\boldsymbol{\lambda}\rangle$ $S(x)|\boldsymbol{\lambda}\rangle = e^{-ix\boldsymbol{\lambda}}|\boldsymbol{\lambda}\rangle$

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 $|\psi\rangle = \sum |\psi_{\lambda}|\rangle$

and the frequencies accumulate between layers:

The output state contains all possible sums of frequencies

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

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

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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

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

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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

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

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

$$S(x) = R_Z(x) = e^{-ixZ/2}$$

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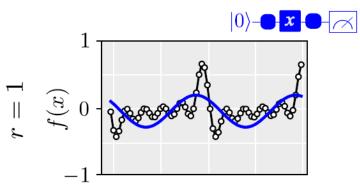
But for general encodings the dependence can be exponential:

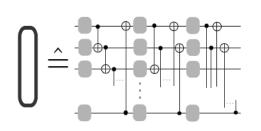
$$\#(\text{frequencies}) \le \frac{d^{2L}}{2} - 1$$

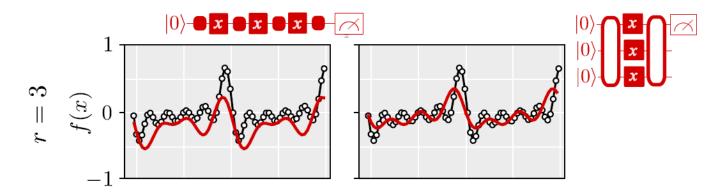
d System dimension*L* Number of layers

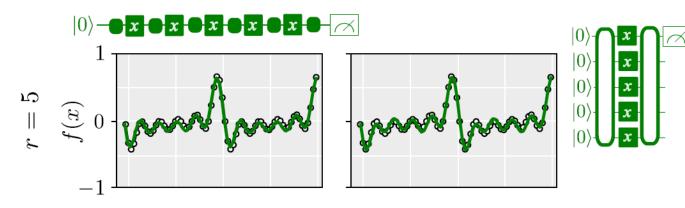
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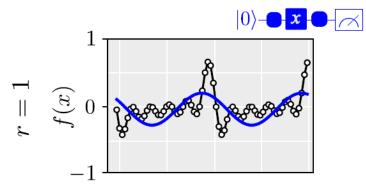


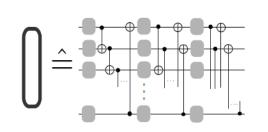




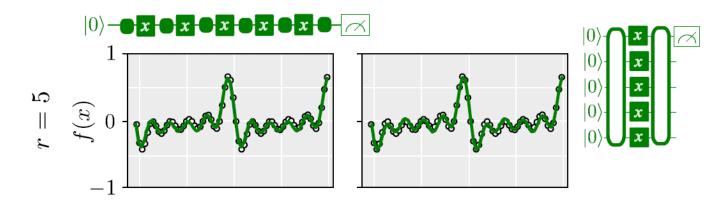


Consequences for Learning Tasks





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You can reproduce all figures from the paper at home!



arXiv:2106.03880

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Encoding-dependent generalization bounds for parametrized quantum circuits

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 ²Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany
 ³Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany
 ⁴QMATH, Department of Mathematical Sciences, University of Copenhagen, 2100 Copenhagen, Denmark
 ⁵Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany
 (Dated: June 9, 2021)

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Elies Gil-Fuster FU Berlin



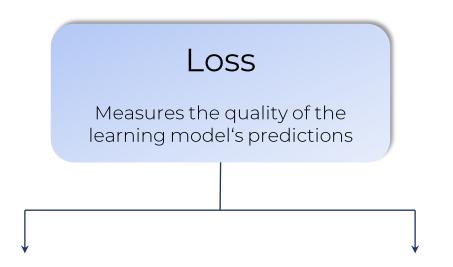
Jens Eisert FU Berlin

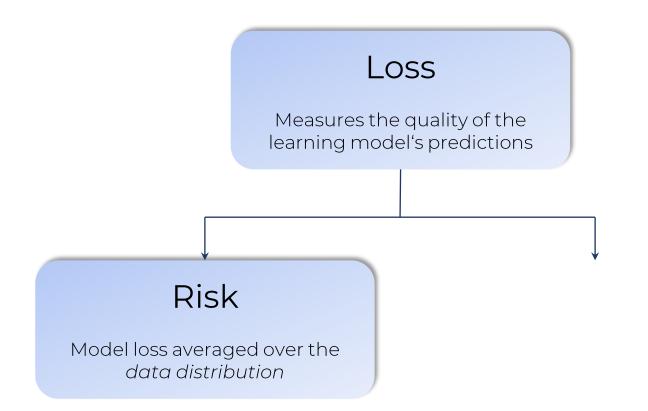


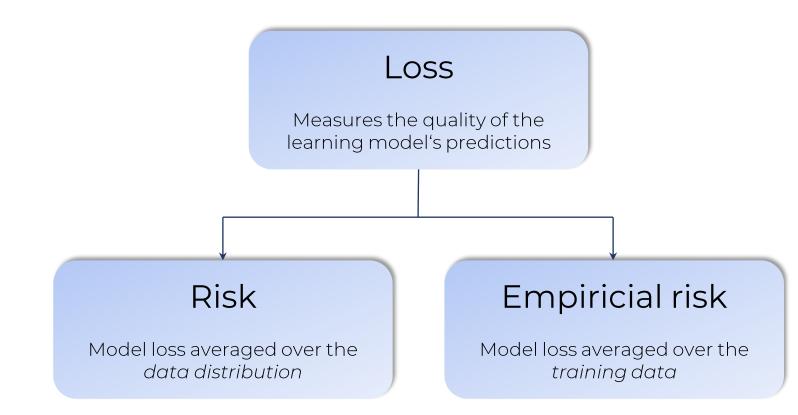
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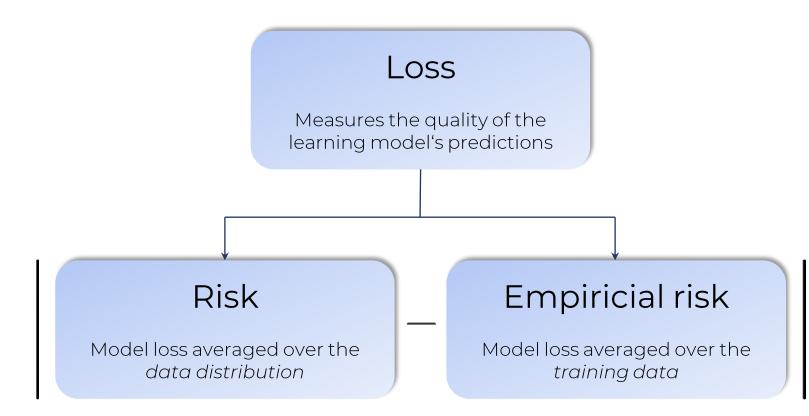


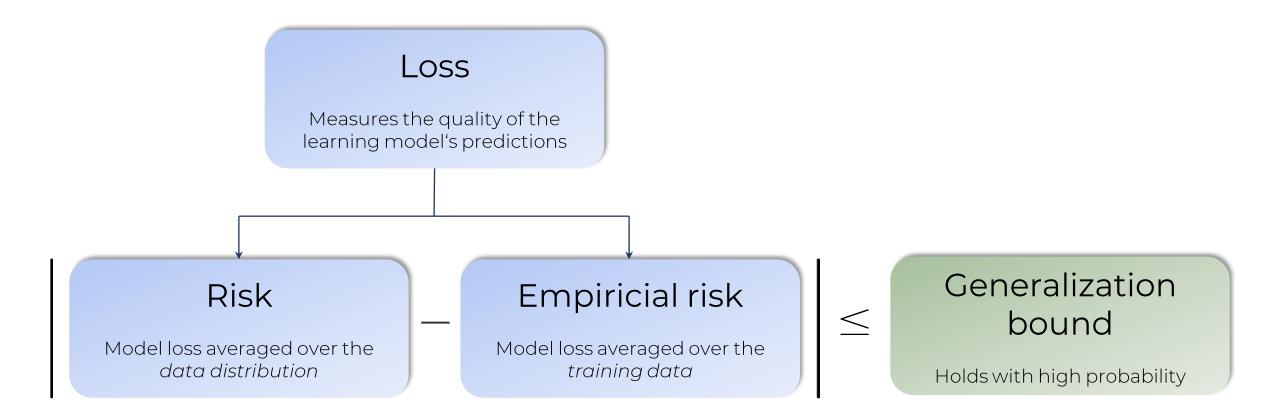












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The more different functions the model can learn, the more training data we need

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Can be made explicit via covering numbers: How many points do I need such that any possible output of the learning model is ϵ -close to at least one point?

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Can be made explicit via covering numbers: How many points do I need such that any possible output of the learning model is ϵ -close to at least one point?

We exploit the Fourier representation to derive covering numbers that depend explicitly on the data-encoding strategy

Results

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Models that use fixed Hamiltonians have a generalization bound that scales **polynomially** in the number of gates, guaranteeing efficient learning

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Models that use fixed Hamiltonians have a generalization bound that scales **polynomially** in the number of gates, guaranteeing efficient learning

Models using arbitrary Hamiltonians can have a generalization bound that scales exponentially

Take-Home Message

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Quantum learning models with fixed Hamiltonians can learn efficiently

Thank you for your attention!









Paper Data-encoding and Fourier series Paper Generalization bounds Slides

Demo



