Title: Dimensional Expressivity Analysis for Quantum Circuits

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Collection: Tensor Networks: from Simulations to Holography III

Date: November 18, 2020 - 1:00 PM

URL: http://pirsa.org/20110027

Abstract: "Besides tensor networks, quantum computations (QC) as well use a Hamiltonian formulation to solve physical problems. Although QC are presently very limited, since only small number of qubits are available, they have the principal advantage that they straightforwardly scale to higher dimensions. A standard tool in the QC approach are Variational Quantum Simulations (VQS) which form a class of hybrid quantum-classical algorithms for solving optimization problems. For example, the objective may be to find the ground state of a Hamiltonian by minimizing the energy. As such, VQS use parametric quantum circuit designs to generate a family of quantum states (e.g., states obeying physical symmetries) and efficiently evaluate a cost function for the given set of variational parameters (e.g., energy of the current quantum state) on a quantum device. The optimization is then performed using a classical feedback loop based on the measurement outcomes of the quantum device.

In the case of energy minimization, the optimal parameter set therefore encodes the ground state corresponding to the given Hamiltonian provided that the parametric quantum circuit is able to encode the ground state. Hence, the design of parametric quantum circuits is subject to two competing drivers. On one hand, the set of states, that can be generated by the parametric quantum circuit, has to be large enough to contain the ground state. On the other hand, the circuit should contain as few quantum gates as possible to minimize noise from the quantum device. In other words, when designing a parametric quantum circuit we want to ensure that there are no redundant parameters.

In this talk, I will consider the parametric quantum circuit as a map from parameter space to the state space of the quantum device. Using this point of view, the set of generated states forms a manifold. If the quantum circuit is free from redundant parameters, then the number of parameters is precisely the dimension of the manifold of states. This leads us to the notion of dimensional expressivity analysis. I will discuss means of analyzing a given parametric design in order to remove redundant parameters as well as any unwanted symmetries (e.g., a gate whose only effect is a change in global phase). Time permitting, I may discuss the manifold of physical states as well since this will allow us to decide whether or not a parametric quantum circuit can express all physical states (thereby ensuring that the ground state can be expressed as well)."

Dimensional Expressivity Analysis for Quantum Circuits

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Variational Quantum Simulations

VQS Objective

Find a quantum state $|\psi\rangle$ that minimizes a given cost function Cost.

Example

Let H be a Hamiltonian. Find the ground state $|\psi_{\text{gs}}\rangle$ minimizing the energy

$$\text{Cost}(|\psi\rangle) := \langle\psi| H |\psi\rangle .$$

Acting on qubits

- Pauli gates, Hadamard gate

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- entanglement gates: e.g., CNOT:

$$\begin{aligned} &\mathrm{CNOT}(\alpha_{00}\,|00\rangle + \alpha_{01}\,|01\rangle + \alpha_{10}\,|10\rangle + \alpha_{11}\,|11\rangle) \\ =&\alpha_{00}\,|00\rangle + \alpha_{01}\,|11\rangle + \alpha_{10}\,|10\rangle + \alpha_{11}\,|01\rangle \end{aligned}$$

In general, CG applies G to target qubit(s) if control qubit is $|1\rangle$.

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  In general, CG applies G to target qubit(s) if control qubit is $|1\rangle$.

- parametric gates: e.g., rotation gates $R_G(\vartheta) = \exp\left(-\frac{i}{2}\vartheta G\right)$ for a gate G

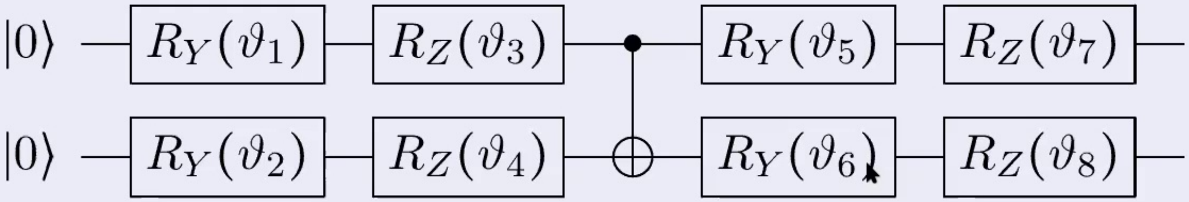
  Multi-qubit rotations: $R_{X_0 X_1}\left(\frac{\pi}{2}\right)|00\rangle = \cos\frac{\pi}{4}\,|00\rangle - i\sin\frac{\pi}{4}\,|11\rangle = \frac{|00\rangle - i|11\rangle}{\sqrt{2}}$.

VQS Ansatz

- Quantum device starts initialized in some initial state $|\psi_{\text{init}}\rangle$.
- Apply a sequence of quantum gates G_j $(1 \le j \le N_G)$ to produce the state

$$|\psi\rangle = G_{N_G} \cdots G_1 |\psi_{\text{init}}\rangle .$$

- Some of these gates are depend on a parameter ϑ_k $(1 \le k \le N \le N_G)$, e.g.,



where $R_G(\vartheta_k) = \exp\left(-\frac{i}{2}\vartheta_k G\right)$ is a rotation gate.

VQS Algorithm

- A *Parametric Quantum Circuit* C (for us) is the map

$$C: \text{ parameter space } \mathcal{P} \to \text{quantum device state space } \mathcal{S};\ \vartheta \mapsto |\psi(\vartheta)\rangle\,,$$

  i.e., C contains both the gate sequence and the initial state $|\psi_{\text{init}}\rangle$.
- *VQS quantum part:* use quantum device to measure cost function $\text{Cost}(C(\vartheta))$ at a given parameter set ϑ.
- *VQS classical part:* use classical feedback loop optimizer to solve

$$\vartheta \mapsto \text{Cost}(C(\vartheta)) \to \min\,.$$

VQS Obstacles

Number of parameters N needs to be:

- *large* for solution to be reachable.
- *large* in order not to introduce artificial local optima.
- *small* to reduce quantum device noise.
- *small* for efficient use of many classical optimizers.

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Optimal VQS Circuit

- *maximally expressive:* be able to generate all (physically relevant) states
- *minimal:* not contain "unnecessary" parameters/gates

DEA assumptions

- Parameter space $\mathcal{P}$ is a compact manifold without boundary.
  For rotation gates only $\mathcal{P} = (\mathbb{R}/2\pi\mathbb{Z})^N$ (N-dim. flat torus w/ side length 2π).
- State space $\mathcal{S}$ is a compact submanifold of the quantum device state space (unit sphere $\partial B_{\mathcal{H}}$ of the complex $2^{\#\text{qubits}}$-dimensional Hilbert space $\mathcal{H}$) without boundary.
  This could be broken in practice but will be satsified if $\mathcal{S}$ is a quotient of $\partial B_{\mathcal{H}}$ with respect to continuous symmetries.
- The parametric quantum circuit $C: \mathcal{P} \to \mathcal{S}$ is continuously differentiable.
  Standard parametric gates are all analytic.
- The image of C is contained in $\mathcal{S}$; *circuit manifold* $\mathcal{M}$.
  $\mathcal{M}$ may not globally be a manifold but locally (with respect to $\mathcal{P}$) it is.

DEA Objectives

- *Primary Objective*
  Given a parametric quantum circuit C, which of the parameters $\vartheta_1, \ldots, \vartheta_N$ are not necessary to locally generate $\mathcal{M}$?
- *Secondary Objective*
  Given a set of "unwanted" symmetries, can we further remove parameters such that $\mathcal{M}$ does not obey these symmetries?
  E.g., removal of global phase generation.
- *Tertiary Objective*
  Given a state space $\mathcal{S}$, how to custom design a parametric quantum circuit that parametrizes $\mathcal{S}$ with the least number of parameters?

How to identify redundant parameters?

- The tangent space of $\mathcal{M}$ is locally spanned by the tangent vectors $\partial_j C(\vartheta)$.

$\Rightarrow$ ϑ_k is redundant iff $\partial_k C(\vartheta)$ is a linear combination of the $\partial_j C(\vartheta)$ with $j \neq k$.

Inductive procedure to identify redundant parameters

- ϑ_1 is never redundant (unless changing ϑ_1 has no impact at all).
- Check whether $\partial_{k+1} C(\vartheta)$ is a linear combination of $\partial_1 C(\vartheta)$, …, $\partial_k C(\vartheta)$.
  $\mathcal{P}$ is a *real* manifold, so linear combinations are with respect to *real* coefficients!
- Remove redundant parameters as necessary.
  Removal of parameters = setting them to a constant. This does not always imply removal of a gate!

How to check for linear independence?

- Define real partial Jacobian J_k of C

$$J_k = \begin{pmatrix} | & & | \\ \Re\partial_1 C & \cdots & \Re\partial_k C \\ | & & | \\ & & \\ | & & | \\ \Im\partial_1 C & \cdots & \Im\partial_k C \\ | & & | \end{pmatrix}$$

  and set $S_k := J_k^* J_k$.
- Assuming $\vartheta_1, \ldots, \vartheta_{k-1}$ are independent, then ϑ_k is dependent if and only if $\det S_k = 0$. Note $S_k \geq 0$, so we can check $\lambda_{\min} > \varepsilon$ to conclude $\det S_k \neq 0$.

Example: $C(\vartheta) = R_Z(\vartheta_2)R_X(\vartheta_1)\left|0\right\rangle$

$$C(\vartheta) = R_Z(\vartheta_2)R_X(\vartheta_1)\left|0\right\rangle = \begin{pmatrix} \cos\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} - i\cos\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} \\ -i\sin\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} + \sin\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} \end{pmatrix} \begin{pmatrix} \left|0\right\rangle \\ \left|1\right\rangle \end{pmatrix}$$

yields

$$J_1 = \frac{1}{2}\begin{pmatrix} -\sin\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} \\ \cos\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} \\ \sin\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} \\ -\cos\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} \end{pmatrix} \quad \text{and} \quad J_2 = \frac{1}{2}\begin{pmatrix} -\sin\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} & -\cos\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} \\ \cos\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} & \sin\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} \\ \sin\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} & -\cos\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} \\ -\cos\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} & \sin\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} \end{pmatrix}.$$

Hence

$$S_1 = J_1^* J_1 = \frac{1}{4} \quad \text{and} \quad S_2 = J_2^* J_2 = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}$$

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yields

$$J_2 = \frac{1}{2}\begin{pmatrix} -\sin\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} - \cos\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} & -\cos\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} - \sin\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} \\ 0 & 0 \\ 0 & 0 \\ -\cos\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} + \sin\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} & \sin\frac{\vartheta_1}{2}\sin\frac{\vartheta_2}{2} - \cos\frac{\vartheta_1}{2}\cos\frac{\vartheta_2}{2} \end{pmatrix}.$$

Hence

$$S_1 = J_1^* J_1 = \frac{1}{4} \quad \text{and} \quad S_2 = J_2^* J_2 = \frac{1}{4}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{with} \quad \sigma(S_2) = \left\{0, \frac{1}{2}\right\}.$$

Removing unwanted symmetries

- Suppose C has a continuous symmetry we wish to remove, i.e., for every $\vartheta \in \mathcal{P}$ there exists $\vartheta' \in \mathcal{P}$ such that $C(\vartheta)$ and $C(\vartheta')$ differ at most by an action of the unwanted symmetry.
  E.g., the symmetry might be a global phase factor, that is, $C(\vartheta) = e^{i\alpha}C(\vartheta')$.
- Suppose a parametric gate block $U(\varphi)$ generates this symmetry, that is, there exists a value φ_0 such that $U(\varphi_0)$ acts as the identity and insertion of U at a relevant point of C forces the unwanted symmetry.
  E.g., for a global phase we could consider $U(\varphi) = U_{\text{init}}^{*} R_Z(\varphi) U_{\text{init}}$ where $U_{\text{init}} |\psi_{\text{init}}\rangle = |0\dots0\rangle$ and R_Z acts on any qubit. U would be inserted as the first operation after initialization of the quantum device.
- Remove redundant parameters from the new circuit $\tilde{C}(\varphi, \vartheta)$ where φ acts as the new first parameter.

Removing global phase from $C(\vartheta) = R_Y(\vartheta_3)R_Z(\vartheta_2)R_X(\vartheta_1)\,|0\rangle$

- The parameters ϑ_1, ϑ_2, and ϑ_3 are independent.
  $C:\ (\mathbb{R}/2\pi\mathbb{Z})^3 \to \partial B_{\mathbb{C}^2}$ is surjective.
- Consider

$$\tilde{C}(\varphi,\vartheta) = R_Y(\vartheta_3)R_Z(\vartheta_2)R_X(\vartheta_1)R_Z(\varphi)\,|0\rangle\,.$$

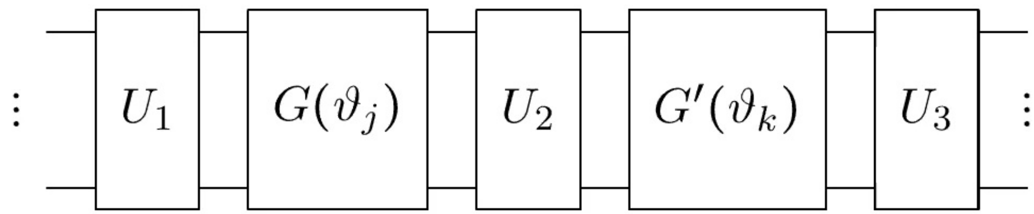
  4 parameters for 3-dim space $\Rightarrow$ there is a redundant parameter!
- DEA with φ acting as "ϑ_0" shows ϑ_3 to be redundant.
  Impact of ϑ_3 beyond ϑ_1 and ϑ_2 is only a global phase!
- *Minimal, maximally expressive single-qubit circuit:*

$$\check{C}(\vartheta) = R_Z(\vartheta_2)R_X(\vartheta_1)\,|0\rangle$$

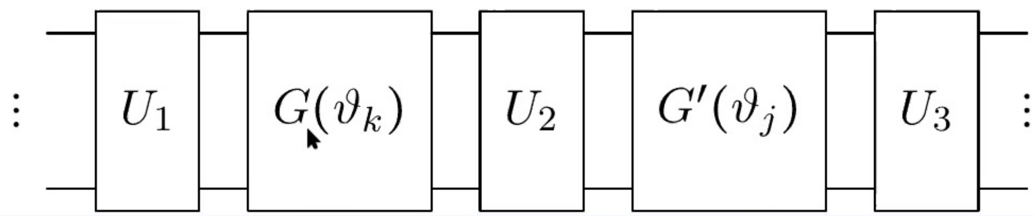
  can generate all single-qubit states up to a global phase factor.

Gate priority

- If ϑ_j and ϑ_k are mutually dependent and $j < k$, then DEA declares ϑ_j independent and ϑ_k dependent.
- For applications, keeping ϑ_k may be advantageous.
  E.g., G' lets us better prepare VQS initializations.

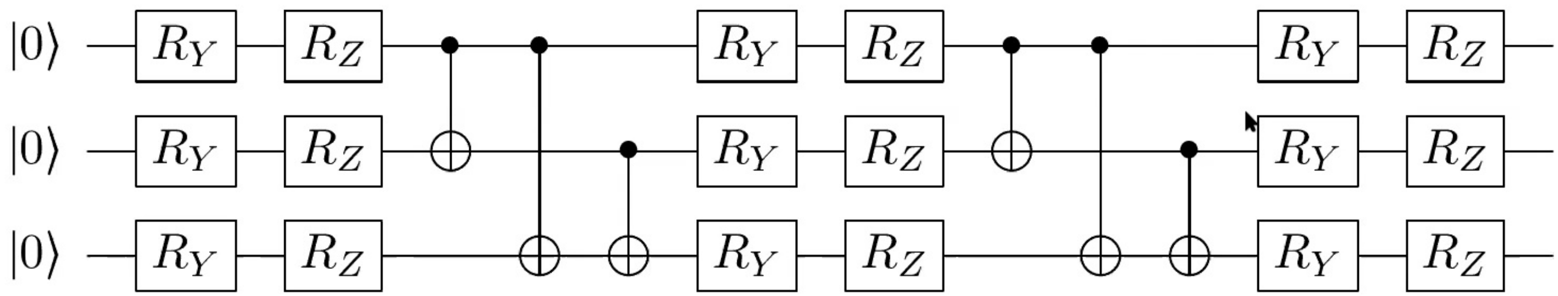


- Applying DEA with indices $j \leftrightarrow k$ swapped prioritizes G' over G.



Example: QISKIT's Efficient $SU(2)$ 2-local circuit

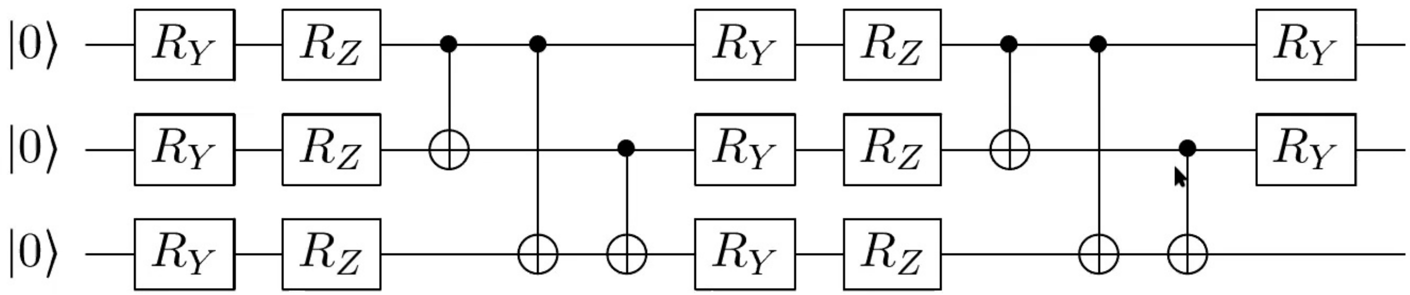
- EfficientSU2(3, reps=2)



- 18 parameters, 14-dimensional state space (3 qubits minus global phase) $\Rightarrow$redundant parameters

Example: QISKIT's EfficientSU2 - DEA naïve

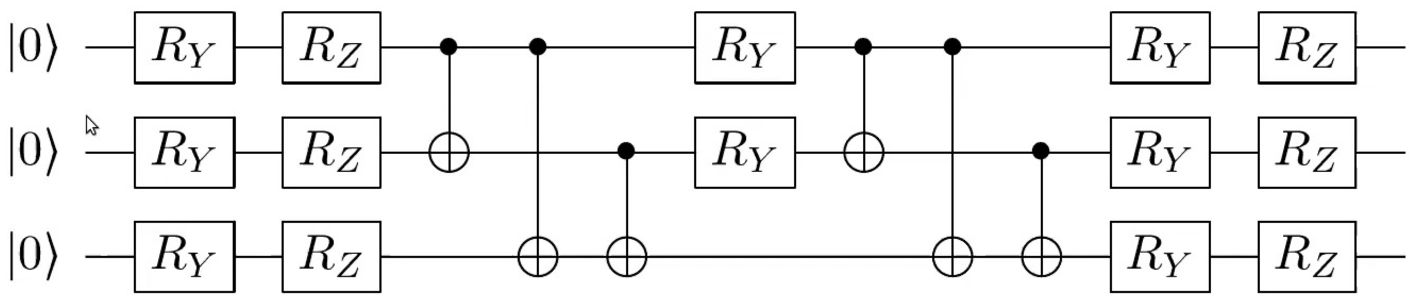
- Naïve application of DEA with global phase removal yields



- This circuit can generate arbitrary product states (e.g. necessary for VQS initialization).

Example: QISKIT's EfficientSU2 - DEA gate prioritized

- DEA with global phase removal and final layer prioritized yields



- Now it is easy to generate arbitrary product states for initialization.

Classical implementation of DEA

Requires storing the matrices J_k which have dimension $2^{\#\text{qubits}+1} \times k$

$\Rightarrow$ Exponential memory/CPU requirements in the number of qubits!

$\Rightarrow$ Doomed to failure

Hybrid quantum-classical implementation of DEA

- Use quantum device to measure matrices $S_k = J_k^* J_k = \begin{pmatrix} S_{k-1} & A_k \\ A_k^* & c_k \end{pmatrix}$.
- Check classically for invertibility of all S_k $(2 \le k \le N)$.

$\Rightarrow$ Memory: $O(N^2)$
CPU calls: $O(N^4)$
QPU calls: $O(N^2 \varepsilon^{-2})$ where ε is the acceptable noise level for S_k

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$\Rightarrow$ Polynomial in #parameters N and independent of #qubits!

How to measure S_k?

- The (m,n)-element of S_k is given by $\Re\langle \partial_m C, \partial_n C\rangle$.
- Assume all parametric gates are rotations $R_G(\vartheta_j) = \exp\left(-\frac{i}{2}\vartheta_j G\right)$.
  Note: G could be a multi-qubit gate, e.g., $\sum_q X_q X_{q+1}$ or even CNOT.

$\Rightarrow$ $\partial_j C = -\frac{i}{2}\gamma_j$ where γ_j is a quantum circuit with an additional gate.
E.g., $C(\vartheta) = R_Z(\vartheta_2)R_X(\vartheta_1)|0\rangle$ implies $\gamma_1 = R_Z(\vartheta_2)XR_X(\vartheta_1)|0\rangle$ and $\gamma_2 = ZR_Z(\vartheta_2)R_X(\vartheta_1)|0\rangle$.

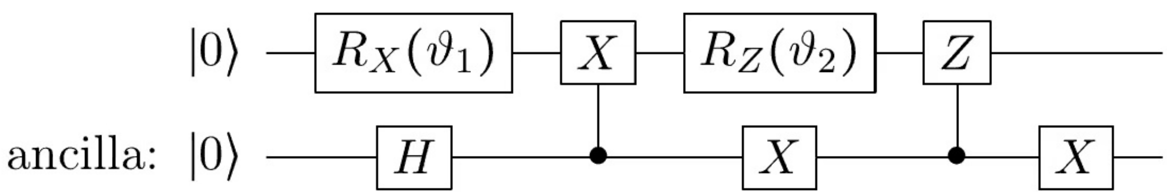
$\Rightarrow$ The (m,n)-element of S_k is given by $\frac{1}{4}\Re\langle\gamma_m,\gamma_n\rangle$.

How to measure $\Re\langle\gamma_m, \gamma_n\rangle$?

- Construct the state

$$|\varphi_{m,n}\rangle = \frac{|0\rangle \otimes |\gamma_m\rangle + |1\rangle \otimes |\gamma_n\rangle}{\sqrt{2}}.$$

- Requires 1 ancilla qubit, and two controlled gates CG. Controlled gate for ϑ_m is conditioned to ancilla = $|0\rangle$, controlled gate for ϑ_n is conditioned to ancilla = $|1\rangle$.
  E.g., for $C(\vartheta) = R_Z(\vartheta_2)R_X(\vartheta_1)\,|0\rangle$, $|\varphi_{2,1}\rangle$ is obtained from



How to measure $\Re\langle\gamma_m, \gamma_n\rangle$?

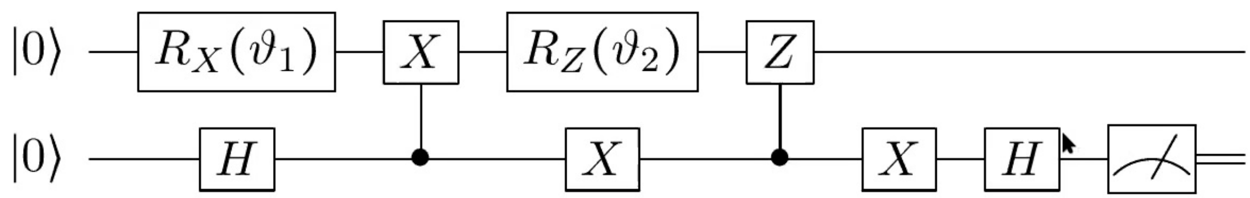
- Given $|\varphi_{m,n}\rangle$, apply a Hadamard gate to the ancilla

$$H_{\mathrm{anc}}\,|\varphi_{m,n}\rangle = \frac{|0\rangle \otimes (|\gamma_m\rangle + |\gamma_n\rangle) + |1\rangle \otimes (|\gamma_m\rangle - |\gamma_n\rangle)}{2}$$

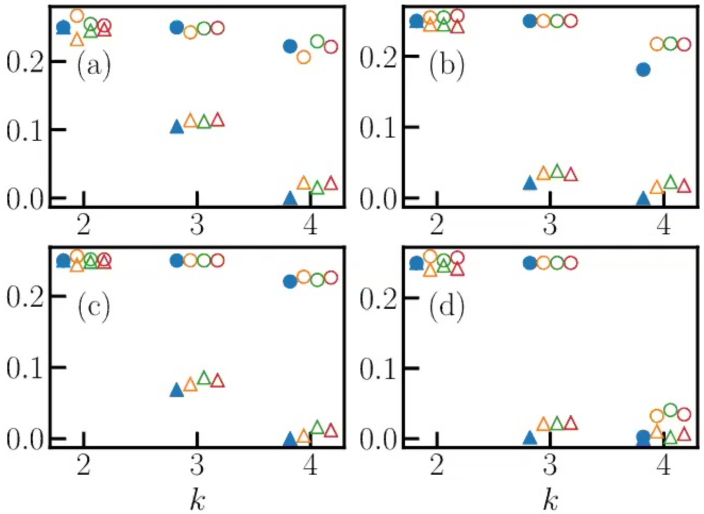
- Measuring the ancilla yields

$$\mathrm{prob}(\mathrm{anc} = |0\rangle) = \frac{1 + \Re\langle\gamma_m, \gamma_n\rangle}{2}.$$

- Complete circuit to measure $\Re\langle\gamma_2, \gamma_1\rangle$ for $C(\vartheta) = R_Z(\vartheta_2) R_X(\vartheta_1)\,|0\rangle$



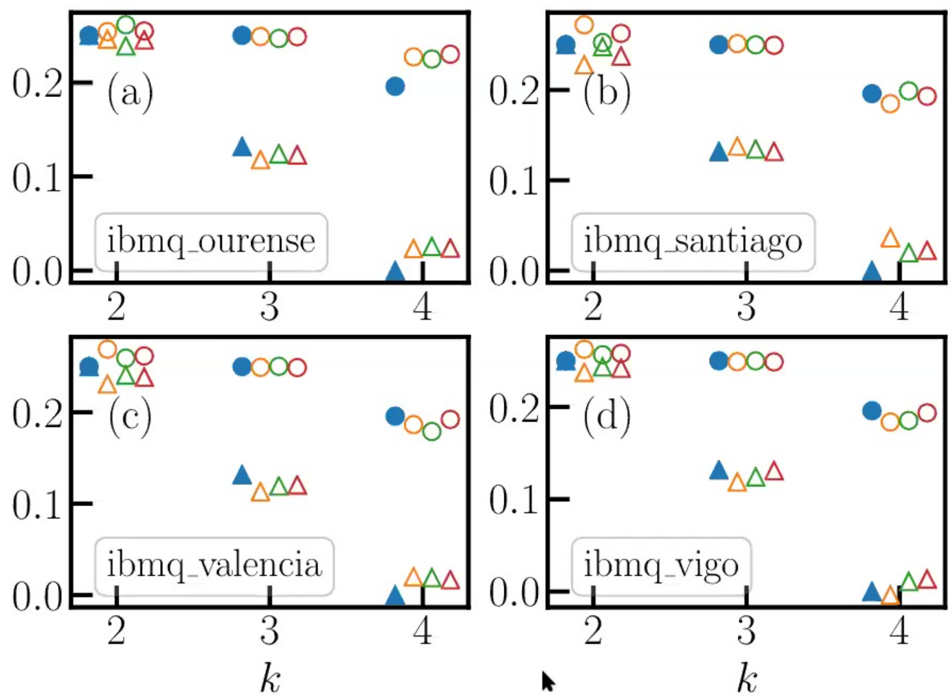
$C(\vartheta) = R_Y(\vartheta_4)R_Z(\vartheta_3)R_X(\vartheta_2)R_Z(\vartheta_1)|0\rangle$ on IBMQ Vigo



- Smallest (triangles) and 2nd smallest (dots) eigenvalues of the matrices S_k, $k \geq 2$.
- The different panels each correspond to a different, randomly drawn parameter set ϑ.
- The filled markers indicate the exact solution, the open markers the results obtained from ibmq_vigo with 1000 measurements (orange markers), 4000 measurements (red markers) and 8000 measurements (green markers).

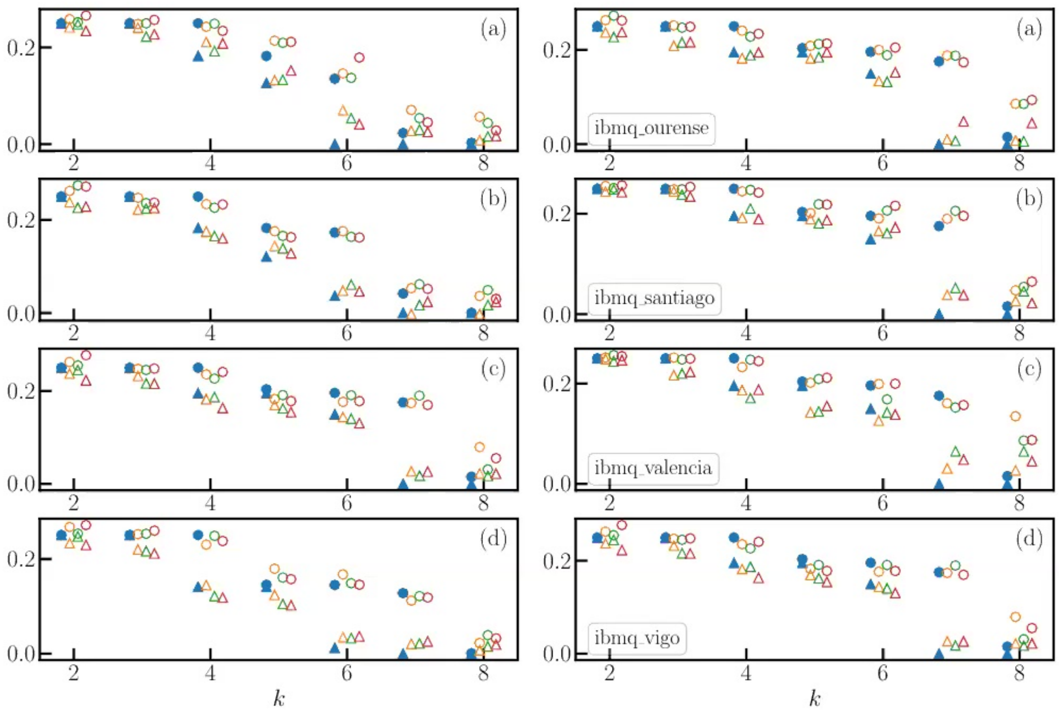
⇒ Independent parameters can be identified relatively well (in most cases).

⇒ Sometimes we may exclude an independent parameter as "dependent" for we cannot positively conclude independence.



⇒ All tested chips perform similarly well.

2 Qubits: EfficientSU2(2,reps=1) (8 parameters, 1 redundant)



- S_6 and S_7 often have eigenvalues with order of magnitude 10^{-4}.
- QPU noise with 8000 shots has order of magnitude 10^{-2}.

$\Rightarrow$ Harder to unambiguously identify all independent parameters.

What have we got? [arXiv:2011.03532]

- DEA can identify redundant parameters in parametric quantum circuits.
- DEA provides a measure of expressivity:
  - max. expressive if $\dim \mathcal{M} = \dim \mathcal{S}$, minimal circuit if $\dim \mathcal{S} = \#\text{parameters}$
  - deficiency $\operatorname{codim} \mathcal{M} = \dim \mathcal{S} - \dim \mathcal{M} \rightsquigarrow$ possible artificial local minima
- DEA can ensure a quantum circuit does not contain "unwanted" symmetries
- DEA can be used to guide custom circuit design
- DEA can be implemented efficiently using a hybrid quantum-classical algorithm (capable of on-the-fly circuit construction/reduction)

What do we need?

- Better quantum hardware!
  - Hardware noise currently greatest obstacle for large circuits on many qubits.
- Only parametric gate reduction currently included.
  - Methods for non-parametric gates reduction use entirely different techniques. $\Rightarrow$ not easily compatible