

A Unified Theory of Barren Plateaus for Deep Parametrized Quantum Circuits

Marco Cerezo CCS-3

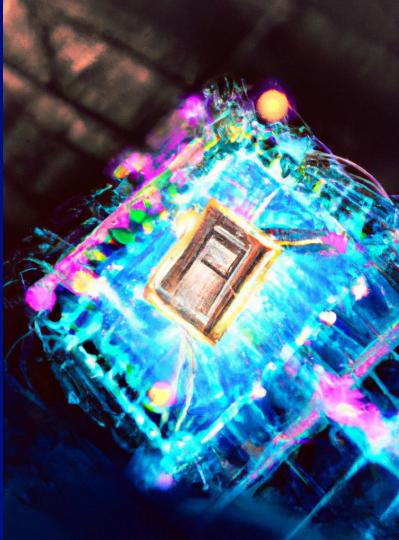
"A Unified Theory of Barren Plateaus for Deep Parametrized Quantum Circuits" arxiv 2309.09342 (2023) Michael Ragone, Bojko N. Bakalov, Frédéric Sauvage, Alexander F. Kemper, Carlos Ortiz Marrero, Martin Larocca, <u>MC</u> *"Showcasing a Barren Plateau Theory Beyond the Dynamical Lie Algebra"* this week on arxiv. N. L. Diaz, Diego García-Martín, Sujay Kazi, Martin Larocca, and <u>MC</u>

10/17/2023 @IPAM Workshop

Outline

- (Very brief) Introduction to variational quantum computing
- A casual stroll through the history of Barren Plateaus (BPs)
- A unified Dynamical Lie algebraic perspective to BPs
- Beyond the Dynamical Lie algebra BP Theory
- Outlook

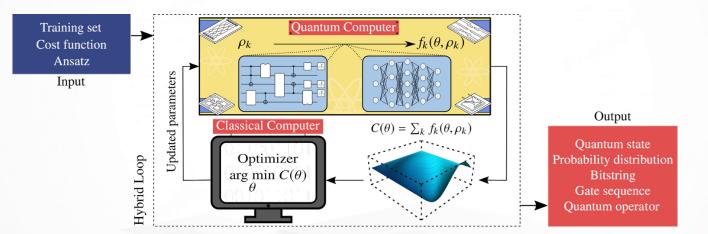




Variational Quantum Computing

Solve a problem of interest by encoding it as an optimization task.

These include Variational Quantum Algorithms (VQE, QAOA, etc), but also Quantum Machine Learning schemes. We will consider models passed on Parametrized Quantum Circuits, or, Quantum Neural Networks.



The loss function will take the form:

$\ell_{\boldsymbol{\theta}}(\rho, 0) = \operatorname{Tr}[U(\boldsymbol{\theta})\rho U^{\dagger}(\boldsymbol{\theta})0]$

We will assume (standard) $|O|_2^2 \le 2^n$



Review: Variational Quantum Algorithms, MC et al, Nature Reviews Physics 3, 625-644 (2021) Review: Noisy intermediate-scale quantum algorithms, K. Bharti et al, Rev. Mod. Phys. 94, 015004 (2022)

16/2023

How and when can this computational approach fail?

While NN are widely used today, their historical development saw periods of great stagnation (or winters).



Variational Quantum Computing holds tremendous the tremendous promise to achieve a quantum advantage – a computational speedup – we need to guarantee that our architectures will work when scaled up and applied to large, realistic problems.

Challenges and opportunities in quantum machine learning, MC et al, Nature Computational Science 2, 567–576 (2022)

os Alamos

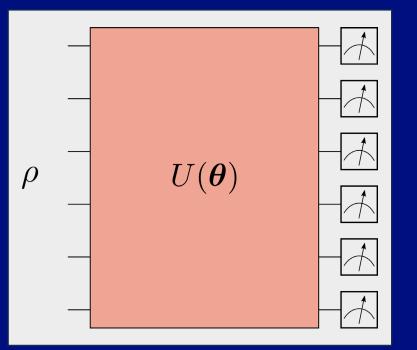
Two memes in a row? Oh, the humanity!



Z₂ symmetric Meme



A review of Barren Plateaus and their sources



Good practices that we have come to learn and love <?

- Global on all q
- Too mu
- Deep ci



We will study loss concentration, not partial derivative concentration. They can be shown to be equivalent.

Equivalence of quantum barren plateaus to cost concentration and narrow gorges, A. Arrasmith, et al, Quantum Sci. Technol. (2021)

Barren Plateaus

No Barren Plateau

Barren Plateau



Image Credits: Samson Wang

$\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] \in \Omega(1/\operatorname{poly}(n))$

$\operatorname{Var}_{\boldsymbol{\theta}}[\ell_{\boldsymbol{\theta}}(\rho, 0)] \in \mathcal{O}(1/b^n)$ with b > 1.

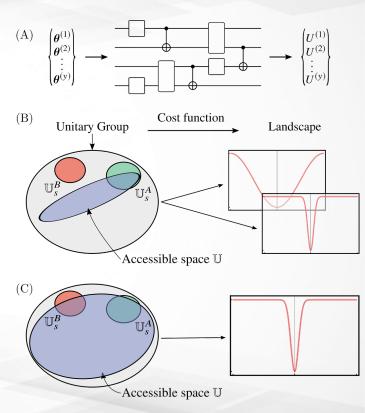
Expressiveness in the circuit, or, a general form of No-Free-Lunch theorem

The first, and perhaps, most studied source of BPs: Seminal Google paper: $U(\theta)$ forms a 2-design

 $|0\rangle - R_{Y}(\frac{\pi}{4}) - R_{P_{1,1}}(\theta_{1,1}) + R_{P_{1,2}}(\theta_{1,2}) + R_{Y}(\frac{\pi}{4}) - R_{P_{1,2}}(\theta_{1,2}) + R_{P_{1,3}}(\theta_{1,3}) + R_{P_{1,3}}(\theta_{1,3}) + R_{Y}(\frac{\pi}{4}) - R_{P_{1,4}}(\theta_{1,4}) + R_{P_{1,5}}(\theta_{1,5}) + R_{Y}(\frac{\pi}{4}) - R_{P_{1,5}}(\theta_{1,5}) + R_{P_{1,5}}(\theta_{$

 $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] = \frac{1}{4^{n} - 1} (\operatorname{Tr}[\rho^{2}] - 1/2^{n}) (\operatorname{Tr}[0^{2}] - \operatorname{Tr}[0]^{2}/2^{n})$

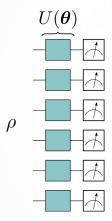
We have a BP for any ρ , and 0.



Locality of measurement operator

or, why comparing exponentially large objects is bound to fail

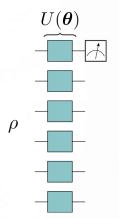
Let's take the most inexpressive imaginable circuit and a global measurement $O = Z^{\otimes n}$



Always has a BP:

 $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] \in \mathcal{O}(1/b^n)$ with b > 1 for any ρ .

What if we take a local measurement $O = Z_1$



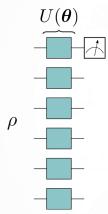
 $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] = \frac{2}{3} (\operatorname{Tr}[(\rho_{1})^{2}] - 1/2)$ If input is $\rho = |0\rangle \langle 0|^{\otimes n}$, then no BP.. But...

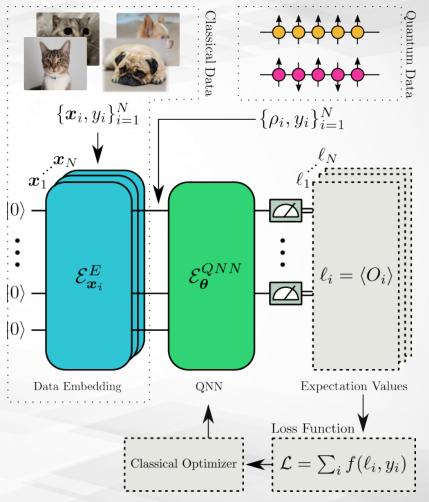
Cost Function Dependent Barren Plateaus in Shallow Parametrized Quantum Circuits, MC et al, Nat. Commun. (2020)

Entanglement in the initial state

or, why untamed entanglement can be bad

What if we take a local measurement $0 = Z_1$, but ρ follows a volume law of entanglement?

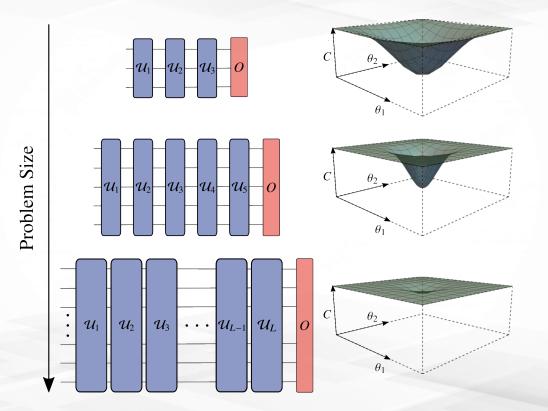




Has a BP: $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] \in \mathcal{O}(1/b^{n})$ Despite no expressiveness and local measurements Subtleties in the trainability of quantum machine learning models. S. Thanasilp et al. arxiv (2021).

And of course, Noise

or, why existence is pain



Previous understanding of BPs

or, yes this slide looks ugly, but it will get better soon.

Architecture Specific Analysis

Specific $U(\boldsymbol{\theta})$

Previous works:

Expressiveness

Entanglement

Locality

Sources of Barren Plateaus

Can we understand and unify all these sources of BPs?

Yes! We need to take a Lie algebraic perspective. Assume

$$U(\boldsymbol{\theta}) = \prod_{l=1}^{L} e^{-i \, \theta_l \, H_l}$$
 ,

Where $H_l \in \mathcal{G}$ (set of generators).

Then we need to construct the circuit's Dynamical Lie algebra (DLA):

 $\mathfrak{g} = \langle i\mathcal{G} \rangle_{Lie} \subseteq su(d)$

DLA = subspace spanned by the nested commutators of the generators

The DLA is important for 2 reasons:

1) $U(\theta) \in e^g$ for any θ , *L*.

2) Quantifies the ultimate expressiveness $U(\theta)$.

BCH Formula $e^A e^B = e^C$ with $C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{12}[B, [A, B]])$

Examples of DLA

Single qubit rotations:

Matchgate circuit:

Universal circuit:

 $\mathcal{G} = \{Z_i, Y_i\}_{i=1}^n$

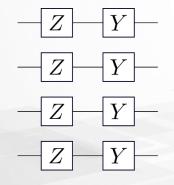
 $\mathcal{G} = \{Z_i\}_{i=1}^n \cup \{X_i X_{i+1}\}_{i=1}^{n-1}$

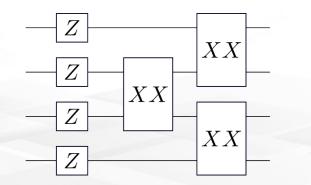
 $g = su(2)^{\bigoplus n}$

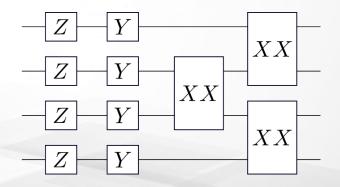
$$g = so(2n)$$

$$\mathcal{G} = \{Z_i, Y_i\}_{i=1}^n \cup \{X_i X_{i+1}\}_{i=1}^{n-1}$$

$$g = su(2^n)$$

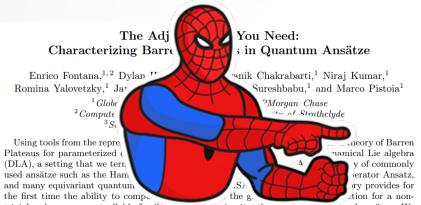






Enough math. Why is the DLA important?

The importance of the DLA was conjectured in our work [1], and recently proven to be central in the BP study. A classic QIP deadline induced rush:



trivial, subspace uncontrollable family or quantum circuits, the quantum compound ansätze. We rigorously prove that the variance of the gradient of the cost function, under Haar initialization, scales inversely with the dimension of the DLA, which agrees with existing numerical observations. Lastly, we include potential extensions for handling cases when the observable lies outside of the DLA and the implications of our results.

A Unified Theory of Barren Plateaus for Deep Parametrized Quantum Circuits

Michael Ragone,^{1,*} Bojko N. Bakalov,^{2,*} Frédéric Sauvage,³ Alexander F. Kemper,⁴ Carlos Ortiz Marrero,^{5,6} Martín Larocca,^{3,7} and M. Cerezo^{8,†} ¹Department of Mathematics, University of California Davis, Davis, California 95616, USA ²Department of Mathematics, North Carolina State University, Raleigh, North Carolina 27695, USA Theoretical Division, Los Alamos National Jaboratory, Los Alamos, New Mexico 87545, USA partment of Physics, North Cor ⁴niversity, Raleigh, North Carolina 27695, USA ata Analytics Division, Pe Vational Laboratory, Richland, WA 99354, USA ⁶Departme Computer Engineering. North Carolina Sta gh, North Carolina 27607, USA onlinear Studies. Los aboratory, Los Alamos, New Mexico 87545, USA Sciences, Los Ala atory, Los Alamos, New Mexico 87545, USA ntum computing ad considerable attention due to their high tial to make pre--quantum devices. At their core, these vers modě parametrized quantum circuit, and evalua vtput. Despite their promise, the trainablit bd by the expressiveness of the parametrize e locality of the observable, or the presence of hard a plateaus have been regarded as independent and have ires. In this work, we present a general Lie algebraic theory that variance of the loss function of sufficiently deep parametrized qu f certain noise models. Our results unify under one single frame ren plateaus by leveraging generalized (and subsystem indepen erator locality, as well as generalized notions of algebraic deco. leap resolves a standing on of the Lie algebra of conjecture about a connection between the generators of the parametrized circu

arXiv:2309.07902

arXiv:2309.09342

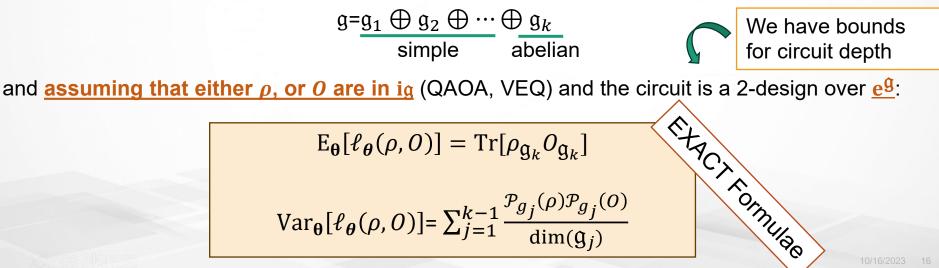
[1] Diagnosing Barren Plateaus with tools from quantum optimal control, M. Larocca, et al, Quantum. (2022).

Exact variance formula for states or observables in the DLA

Given an arbitrary subalgebra $\mathfrak{t} \subseteq su(2^n)$ with Hermitian basis $\{B_j\}_{j=1}^{\dim(\mathfrak{t})}$, we define the \mathfrak{t} -purity of an operator H as

$$\mathcal{P}_{\mathfrak{F}}(H) = \mathrm{Tr}[H_{\mathfrak{F}}^2] = \sum_{j=1}^{\dim(\mathfrak{F})} \mathrm{Tr}\left[B_j^{\dagger}H\right]^2.$$

Then, recalling that any DLA



A Unified Theory of Barren Plateaus for Deep Parametrized Quantum Circuits, M. Ragone et al, arxiv (2023)

What can we learn from here?

Assume g is simple

$$E_{\theta}[\ell_{\theta}(\rho, O)] = 0$$
$$Var_{\theta}[\ell_{\theta}(\rho, O)] = \frac{\mathcal{P}_{g}(\rho)\mathcal{P}_{g}(O)}{\dim(\mathfrak{g})}$$

If either dim(g), $1/\mathcal{P}_g(\rho)$, $1/\mathcal{P}_g(0) \in \Omega(b^n)$ with b > 2, one has a BP!



Proves a conjecture in [1]!

- 1. The circuit expressiveness, measured through dim(g).
- 2. The generalized entanglement in ρ , measured through $\mathcal{P}_{q}(\rho)$.
- 3. The generalized locality of 0, measured through $\mathcal{P}_{g}(0)$.

[1] Diagnosing Barren Plateaus with tools from quantum optimal control, M. Larocca, et al, Quantum (2022) Generalizations of entanglement based on coherent states and convex sets, H. Barnum et al, Phys. Rev. A (2003) A subsystem-independent generalization of entanglement, H. Barnum et al, Phys. Rev. Lett. (2004)

Maximized for O in DLA

Maximized for a HWS.

 $su(2^n)$

 $su(2^n)$

. . .

 X_1

 X_1X_2

 $X_{1}X_{2}$

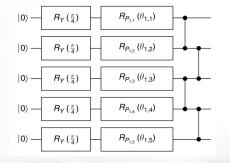
Revisiting previous examples

Google's result:

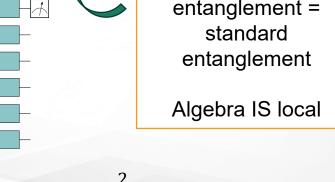
$$g = su(2^{n}); \quad \dim(g) = 4^{n} - 1$$

$$\mathcal{P}_{g}(\rho) = \operatorname{Tr}[\rho^{2}] - 1/2^{n} \ (\rho = \rho_{g} - I/2^{n})$$

$$\mathcal{P}_{g}(O) = \operatorname{Tr}[O^{2}] \ (0 = O_{g} - \operatorname{Tr}[O] I/2^{n})$$



 $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] = \frac{1}{4^{n} - 1} (\operatorname{Tr}[\rho^{2}] - 1/2^{n}) (\operatorname{Tr}[0^{2}] - \operatorname{Tr}[0]^{2}/2^{n})$



 $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] = \frac{2}{3} (\operatorname{Tr}[(\rho_{1})^{2}] - 1/2^{n})$

An important lesson learnt

The previous examples led the community to developing a series of good practice guidelines such as:

- Global observables (acting
- Too much entanglement le
- Deep circuits are have BPs

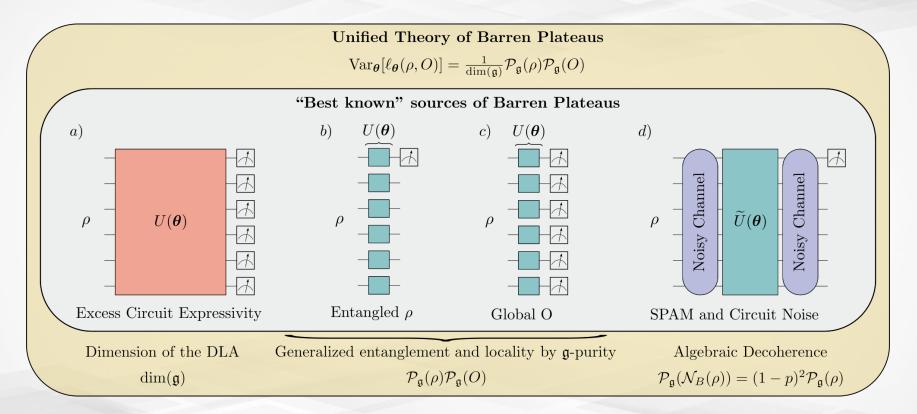


We show that generalized entanglement in ρ is relative to the DLA, generalized locality of 0, is relative to the DLA.

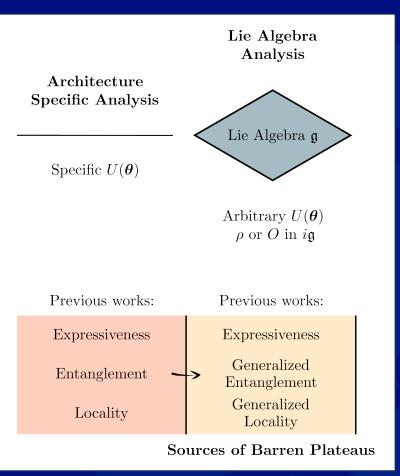
Hence, it is entirely possible for a circuit to be trained on highly entangled initial states using highly nonlocal measurements (i.e., acting on all qubits) as long as they are well aligned with the underlying DLA of the circuit.

A Unified Theory of Barren Plateaus for Deep Parametrized Quantum Circuits, M. Ragone et al, arxiv (2023)

Summary







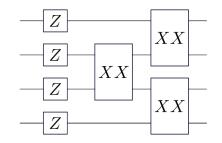
Can we go beyond the DLA?

Yes! We need to take (at least for now) an architecture specific analysis.

Parametrized Matchgate circuits: $\mathcal{G} = \{Z_i\}_{i=1}^n \cup \{X_iX_{i+1}\}_{i=1}^{n-1}$ Free fermion DLA:

$$g = \operatorname{span}_{R}\{Z_{i}, \widehat{X_{i}X_{j}}, \widehat{X_{i}Y_{j}}, \widehat{Y_{i}X_{j}}, \widehat{Y_{i}Y_{j}}\}_{1 \le i < j \le n} \simeq so(2n)$$

Where $\widehat{A_{i}B_{i}} = A_{i}Z_{i+1} \cdots Z_{j-1}B_{j}$



Before we needed ρ or 0 in ig. The DLA was the central element. Now we need to work with group modules.

$$\mathcal{B} = \bigoplus_{\kappa=0}^{2n} \mathcal{B}_{\kappa}; \dim(\mathcal{B}_{\kappa}) = \binom{2n}{\kappa}$$

Use Jordan-Wigner, and define Majorana operators

 $\mathbf{P} = \mathbf{Z}^{\otimes n} = (-i)^n \overline{c_1 \cdots c_{2n}}$

$$c_1 = XI \cdots I, c_3 = ZXI \cdots I, c_5 = Z \cdots ZX$$
$$c_2 = YI \cdots I, c_3 = ZYI \cdots I, c_5 = Z \cdots ZY$$

 $\forall M_{\kappa} \in \mathcal{B}_{\kappa}$, then $UM_{\kappa}U^{\dagger} \in \mathcal{B}_{\kappa}$ for any $U \in e^{\mathfrak{g}}$

Moar exact variance formulae,

/môar/ - adj - A way of asking for more of something you want very badly

$$E_{\theta}[\ell_{\theta}(\rho, 0)] = \sum_{\kappa=0,2n} \langle \rho_{\kappa}, O_{\kappa} \rangle_{I+P}$$
$$ar_{\theta}[\ell_{\theta}(\rho, 0)] = \sum_{j=1}^{k-1} \frac{\mathcal{P}_{\kappa}(\rho)\mathcal{P}_{\kappa}(0) + \mathcal{C}_{\kappa}(\rho)\mathcal{C}_{\kappa}(0)}{\dim(\mathcal{B}_{\kappa})}$$

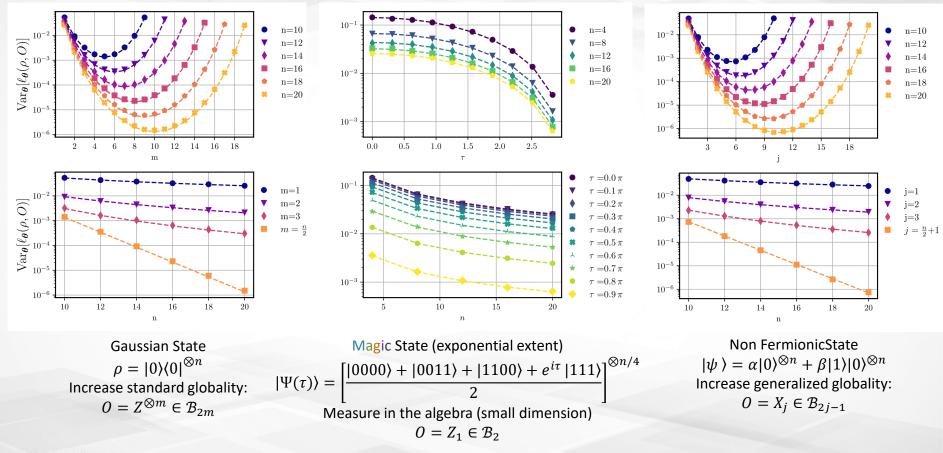
 $0 \in \mathcal{B}_{\kappa}$, then $\mathbb{E}_{\theta}[\ell_{\theta}(\rho, 0)] = 0$, and $\operatorname{Var}_{\theta}[\ell_{\theta}(\rho, 0)] = \frac{\mathcal{P}_{\kappa}(\rho)\mathcal{P}_{\kappa}(0)}{\dim(\mathcal{B}_{\kappa})}$

 $\mathcal{P}_{\kappa}(M) = \langle M_{\kappa}, M_{\kappa} \rangle_{I}, \, \mathcal{C}_{\kappa}(M) = i^{\kappa \, mod \, 2} \langle M_{\kappa}, M_{\kappa} \rangle_{P}, \, \text{and} \, \langle M_{1}, M_{2} \rangle_{\Gamma} = \text{Tr}[\Gamma M_{1}^{\dagger} M_{2}]$

- 1. The (local) expressiveness measure $\dim(g)$ is replaced by the (global) expressiveness $\dim(\mathcal{B}_{\kappa})$. The conjecture in [1] is then not generally true. <u>*Trainability is module dependent*</u>.
- 2. We can define a notion of generalized globality, product of Majoranas: $\kappa \mod n \in \Theta(1)$ no BP but $\kappa \mod n \in \Theta(n)$ then BP! Remember, we have qubits!
- 3. For $\kappa = 2$ ($\mathcal{B}_2 = \mathfrak{g}$), operational meaning to $\mathcal{P}_{\kappa}(\rho)$ as a Fermionic entanglement measure.
- 4. The covariances are forms of generalized-coherences between isomorphic modules (related to the parity sectors).

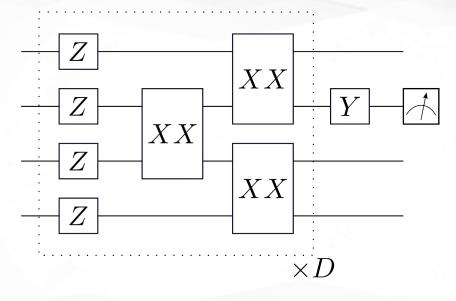
Showcasing a Barren Plateau Theory Beyond the Dynamical Lie Algebra, NL Diaz et al, to appear on arxiv this week. Entanglement in fermion systems, N. Gigena et al, Physical Review A (2015).

I do theory, but... here are some cool numerics:



Showcasing a Barren Plateau Theory Beyond the Dynamical Lie Algebra, NL Diaz et al, to appear on arxiv this week. *Classical simulation of non-gaussian fermionic circuits*, B. Dias arXiv (2023).

Enough is enough Marco! Ok, just one more cool result



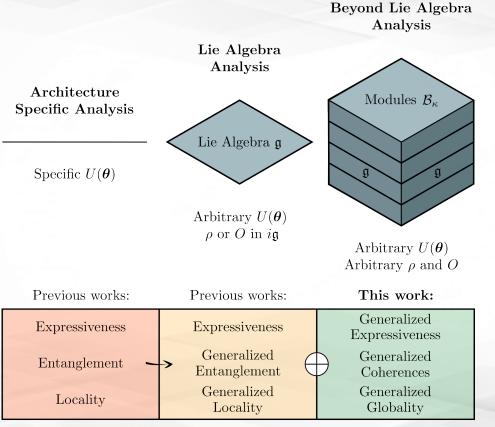
 $Z_{n/2} \to X_{n/2}$

$$\in \mathcal{B}_2 \quad \in \mathcal{B}_{n-2}$$

Showcasing a Barren Plateau Theory Beyond the Dynamical Lie Algebra, NL Diaz et al, to appear on arxiv this week. Classical simulation of non-gaussian fermionic circuits, B. Dias arXiv (2023).

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Towards a super duper, unified mega complete BP theory



Sources of Barren Plateaus

Showcasing a Barren Plateau Theory Beyond the Dynamical Lie Algebra, NL Diaz et al, to appear on arxiv this week.

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Phew.. That was a lot... What did we learn?

IMHO: Our understanding of BPs underwent a recent transformative shift. We can use these results to guide our model's design.

Here are some open questions:

In the Matchgate case, we can relate trainability to fermionic entanglement (a computational resource that can promote matchgates to universal circuits). We see that <u>e-v-e-r-y trainable model, is also (somehow*) classically simulable.</u>

We even propose a simulation method for exponential magic states that are non-simulable via Wick theorem simulation-based techniques!)

Is this connection more general?

- What about noise?
- What about shallow depth?
- Non-expectation value-based models (generative)?

This guy is amazing and looking for a job. HIRE HIM. Like NOW. No really, DO IT. DO IT NOW! JUST He's in the audience rn! DO IT!

Thanks for your attention!







Frederic Sauvage



Martin Larocca LANL



Bojko Bakalov NCU



Lex Kemper NCU

os Alamos



LANL

Carlos Ortiz Marrero Diego Garcia Martin PNNL

LANL

Nahuel Diaz LANL





LANL's 2024 Quantum Computing Summer School Applications opening soon! cerezo@lanl.gov

