Overview SQMS Algorithms: attivita' italiana

- Leonardo Banchi – UniFi / INFN Firenze

- SQMS Algotithm Thrust
 - Simulation of condensed matter / quantum field theories
 - Device benchmarking
 - Control methods
 - Open source libraries

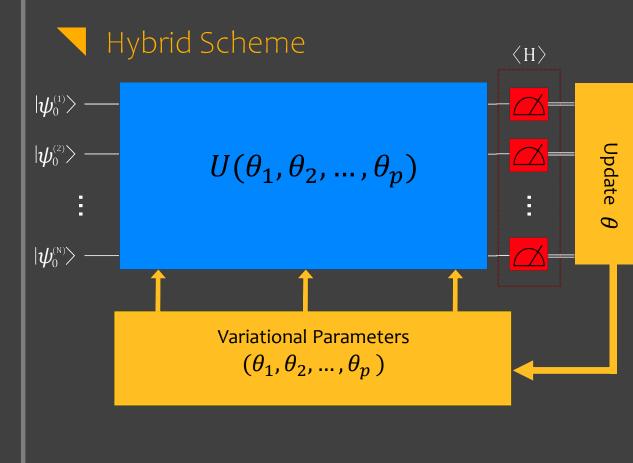
Florence:

- Quantum Simulations of Condensed Matter Systems
 - Slides coutesy of Laura Gentini
- Quantum Learning for Hardware Characterization
 - Slides courtesy of Paolo Braccia



Find ground state of an Hamiltonian, \widehat{H}

- Ansatz \rightarrow parametrize $|\psi(\theta)\rangle$
- Compute the energy $C(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle$
- Minimize $C(\theta) \to \text{find } \theta^{opt} \mid C(\theta^{opt}) = \min_{\theta} C(\theta)$
- $|\psi(\theta^{opt})\rangle$ best approximation of the ground state



Quantum

- $|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$
- $C(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle$

Classical

- Perform a optimization step
- Pass new parameters

as feedback



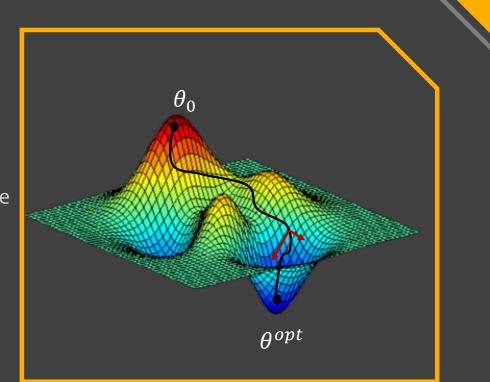
Find $\theta^{opt}!$

Exploring the landscape

- θ define a parameter space
- $C(\theta) \rightarrow \text{landscape}$
- At each optimization step we move a little

 $\theta^{(i+1)} = \theta^{(i)} - \alpha_i \nabla_\theta C(\theta^i)$

- Guided by the gradient
- The algorithm defines a *path*



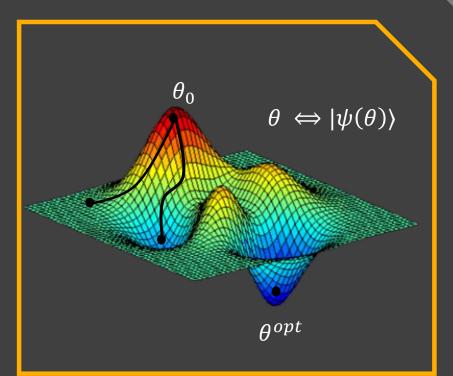
Exploring the landscape

- Path full of traps
- Local minima or Plateaus

 $\nabla_{\theta} C = 0$

- We can't take any step further
- but we do not have the solution

Stochastic outcomes & Noise \rightarrow useful?



Convergence Role of Noise and outcomes

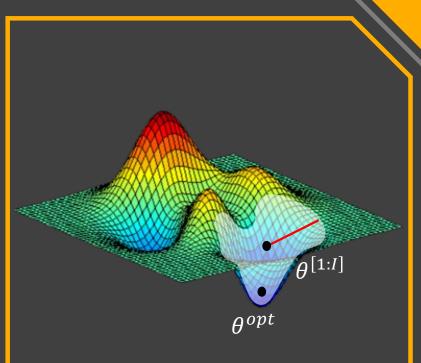
geometrical point of view?

On device gradient evaluation

 $\nabla C(\theta) = \left\langle \psi(\theta) \middle| \hat{F} \middle| \psi(\theta) \right\rangle$

 $\nabla C(\theta) = \mathbb{E}_{z \sim q(z|\theta)} [g(\theta, z)]$

 $g: \mathbb{R}^p \to \mathbb{R}^p \quad \text{sampling } z \text{ from } q(z|\theta) \neq p(y|\theta)$ $\theta^{(i+1)} = \theta^{(i)} - \alpha_i g(\theta^{(i)})$



If $\mathbb{E}[\|g(\theta)\|^2] \le G^2$

After *I* iterations $\rightarrow C(\theta^{[1:I]}) - C(\theta^{opt}) \leq R \frac{G}{\sqrt{I}}$

$$\alpha_i = \frac{R}{G\sqrt{I}} \qquad \theta^{[1:I]} = \frac{1}{I} \sum_{i}^{I} \theta_i$$

Taking Noise into account

CPTP map
$$|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle \rightarrow \rho(\theta) = \mathcal{E}(\theta)[\rho_0]$$

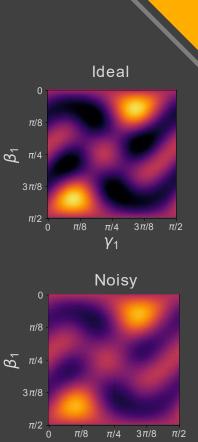
 $\rho(\theta) = \mathcal{E}_p^{\theta_p} \circ \dots \circ \mathcal{E}_1^{\theta_1}[\rho_0] \qquad \qquad \mathcal{E}_j^{\theta_j} \text{ CPTP map}$

 $C_{noisy}(\theta) = Tr[\rho(\theta)H] \rightarrow C_{noisy}(\vartheta^{opt}) \text{ with } \vartheta^{opt} \neq \theta^{opt}$

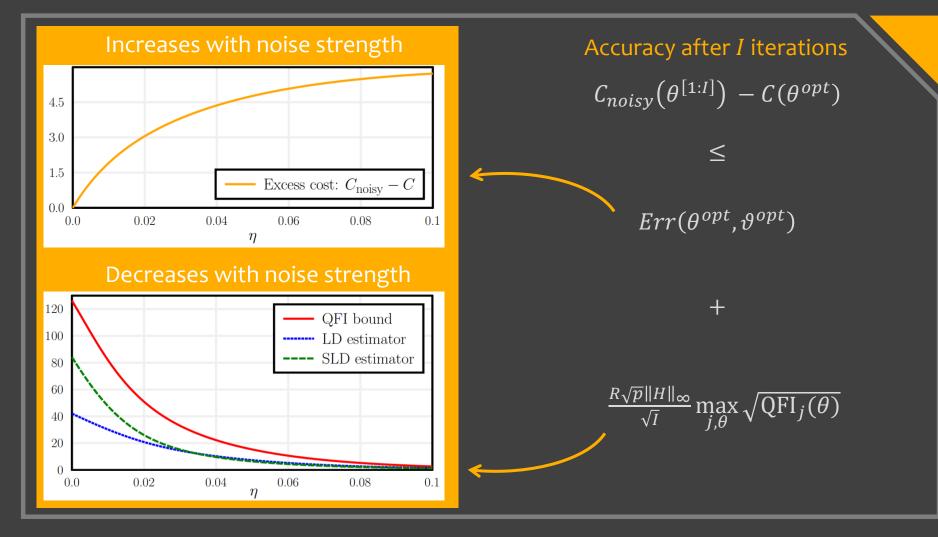
After *I* iterations $\rightarrow C_{noisy}(\theta^{[1:I]}) - C_{noisy}(\vartheta^{opt}) \leq R \frac{G_{noisy}}{\sqrt{I}}$

$$C_{noisy}(\theta^{[1:I]}) - C(\theta^{opt}) \le Err(\theta^{opt}, \vartheta^{opt}) + R \frac{G_{noisy}}{\sqrt{I}}$$

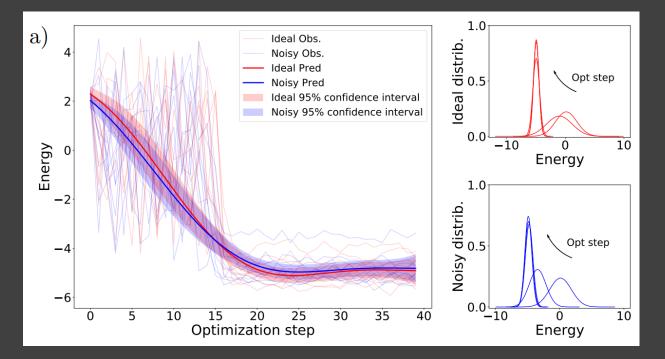
 $Err(\theta, \vartheta) \doteqdot C_{noisy}(\vartheta) - C(\theta)$



 γ_1



Numerical Experiment

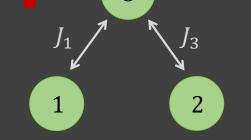


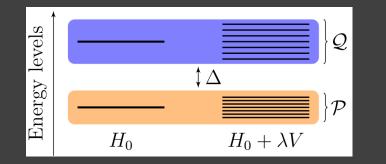
Noise Resilient Variational Quantum Classical Optimization

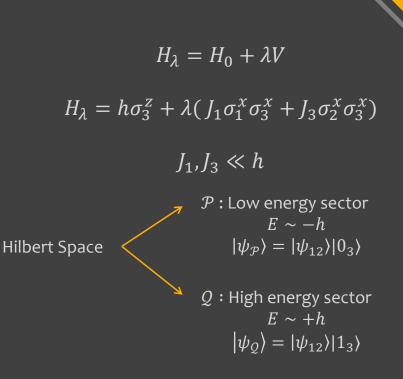
https://doi.org/10.1103/PhysRevA.102.052414 Gentini, Cuccoli, Pirandola, Verrucchi, Banchi Variational Approximation of Low-Energy Hamiltonians on Real Quantum Hardware

Gentini, Cuccoli, Banchi

Low energy approximation



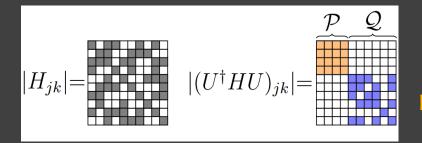




Effective interaction of qubits 1 and 2

Effective Hamiltonian $\langle \psi_{\mathcal{P}} | H_{eff} | \psi_{\mathcal{Q}} \rangle = 0$

Variational low energy approximation



Block diagonalize the Hamiltonian = Find a Low energy effective Hamiltonian

 $U^{\dagger} HU = D_{\mathcal{PQ}}$ $U(\theta) ?$

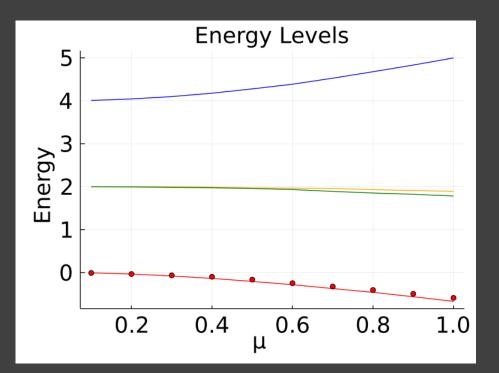
- No trivial cost function for "Block Diagonalization" (or even Diagonalization...)
- Very difficult to create a sufficiently complex ansatz

Need a physical motivated structure

Adiabatic Gauge Potential

Adiabatic state preparation $H_{\lambda} = H_0 + \lambda V$ $\mu \in [0 \dots \lambda]$ $H(\mu=0)=H_0$ $|g_0\rangle$ μ $H(\mu = \lambda) = H_{\lambda}$ $|g_{\lambda}\rangle$ Only ground state

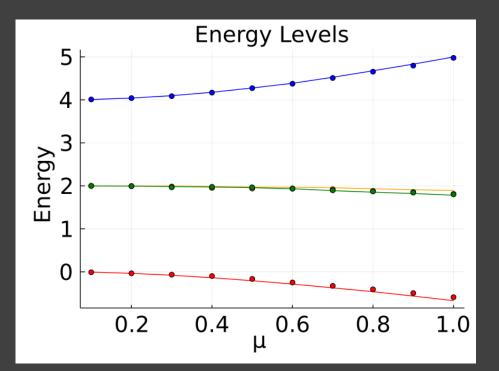
Level crossing \rightarrow Failure

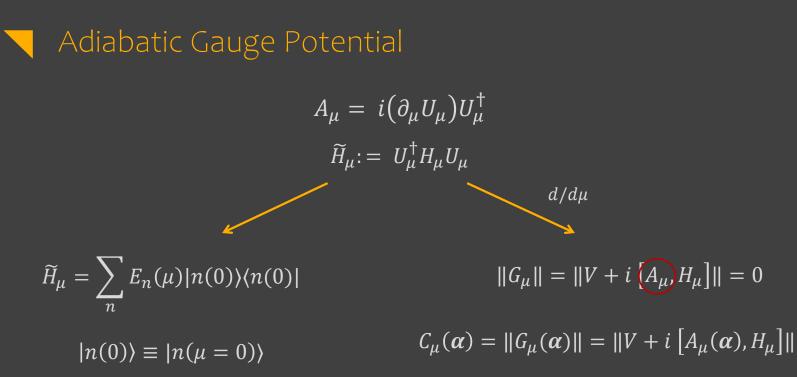


Adiabatic Gauge Potential

$$H_{\lambda} = H_{0} + \lambda V \qquad \mu \in [0 \dots \lambda]$$
$$U_{\mu} = \mathcal{T}_{\nu} e^{(-i \int_{0}^{\mu} A_{\nu} d\nu)}$$
$$A_{\mu} = i (\partial_{\mu} U_{\mu}) U_{\mu}^{\dagger}$$
$$\widetilde{H}_{\mu} := U_{\mu}^{\dagger} H_{\mu} U_{\mu}$$
$$\downarrow$$

 \widetilde{H}_{μ} is diagonal at every step In the eigenbasis of H_0





 $\boldsymbol{\alpha}^{opt} \mid C_{\mu}(\boldsymbol{\alpha}^{opt}) = \min_{\boldsymbol{\alpha}} C_{\mu}(\boldsymbol{\alpha})$

Approximating the AGF
$$A_{\mu}(\boldsymbol{\alpha}) = \sum_{i=1}^{L} \alpha_{i}^{\mu} B_{i}$$

 B_i 's are Local Operators \rightarrow Approximation!

Efficiently reproduce the EXACT AGP between sectors

Fail in reproducing the EXACT AGP inside each sector

 $\|\mathcal{P}\left(V+i\left[A_{\mu}(\boldsymbol{\alpha}),H_{\mu}\right]\right)\mathcal{Q}\| \coloneqq \|\mathcal{P}\left(G_{\mu}\right)\mathcal{Q}\| = 0$

 $\|\mathcal{P}\left(V+i\left[A_{\mu}(\boldsymbol{\alpha}),H_{\mu}\right]\right)\mathcal{P}\| \coloneqq \|\mathcal{P}\left(G_{\mu}\right)\mathcal{P}\| \neq 0$

 $\widetilde{H}_{\mu} = U_{\mu}^{\dagger}(\boldsymbol{\alpha})H_{\mu}U_{\mu}(\boldsymbol{\alpha})$ Block diagonalized the Hamiltonian

Variational Schrieffer-Wolff Transformations for Quantum Many-Body Dynamics J.Wurtz, P.W. Claeys, and A. Polkovnikov <u>10.1103/PhysRevB.101.014302</u>

Embedding in Quantum Computing framework

$$U_{\mu}(\boldsymbol{\alpha}) = \prod_{i=1}^{L} e^{-i\alpha_{i}^{\mu}B_{i}} \qquad g_{i}^{\mu} = e^{-i\alpha_{i}^{\mu}B_{i}}$$

$$\mu \in [0 \dots \lambda] \rightarrow \mu_t = \delta \mu t$$
$$\delta \mu = \frac{\lambda}{T}, \quad t \in [0, T] \in \mathbb{N}$$

$$C_{\mu}(\boldsymbol{\alpha}_t) \rightarrow C_t (\boldsymbol{\alpha}_{t+1} - \boldsymbol{\alpha}_t)$$

 $X_t \left(\frac{\boldsymbol{\alpha}_{t+1} - \boldsymbol{\alpha}_t}{\delta \mu} \right) = Y_t \qquad \begin{array}{c} \text{Analytic Minimization} \\ \text{solving a linear system} \end{array}$

Single qubit or two qubit parametrized gate

$$t = 0, \mu = 0, H = H_0 \text{ is diagonal}$$

$$t = 0 \qquad C_0 (\alpha_1 - \mathbf{0}) \longrightarrow X_0 \left(\frac{\alpha_1}{\delta\mu}\right) = Y_0$$

$$t = 1 \qquad C_1 (\alpha_2 - \alpha_1^{opt}) \longrightarrow X_1 \left(\frac{\alpha_2}{\delta\mu}\right) = Y_1$$

$$t = 2 \qquad C_1 (\alpha_3 - \alpha_2^{opt}) \qquad \dots$$

$$t = T \quad (\mu = \lambda) \qquad \alpha_T^{opt}$$

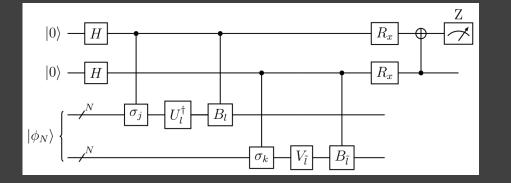
Embedding in Quantum Computing framework

$$X_t\left(\frac{\boldsymbol{\alpha}_{t+1}}{\delta\mu}\right) = Y_t$$

$$X_{\tilde{l}l} = \sum_{jk} h_j h_k Tr(i[U_l B_l U_l^{\dagger}, \sigma_j] i[U_{\tilde{l}} B_{\tilde{l}} U_{\tilde{l}}^{\dagger}, \sigma_k])$$

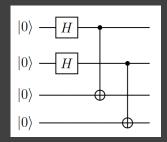
 $p(0) \propto X_{\tilde{l}l}$ Re

Repeat *S* times



$$H_{\mu} = \sum_{k} h_{k} \sigma_{k}$$
$$T_{l}(\boldsymbol{\alpha}[1:l]) = \prod_{i=1}^{l} e^{-i\alpha_{i}B_{i}}$$

$$|\phi_N\rangle \rightarrow Tr(AB) = 2^N \langle \phi_N | A^T \otimes B | \phi_N \rangle$$

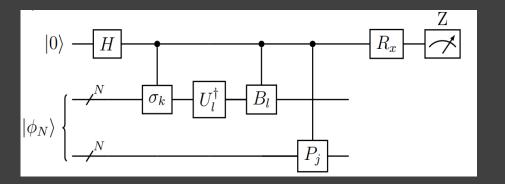


Embedding in Quantum Computing framework

$$X_t\left(\frac{\boldsymbol{\alpha}_{t+1}}{\delta\mu}\right) = Y_t$$

$$Y_{l} = -\sum_{jk} v_{j} h_{k} Tr(P_{j} i[U_{l} B_{l} U_{l}^{\dagger}, \sigma_{k}])$$

$$p(0) \propto Y_{l} \qquad \text{Repeat } S \text{ times}$$

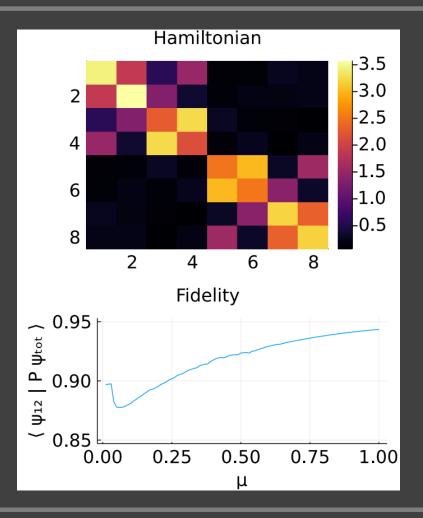


$$H_{\mu} = \sum_{k} h_{k} \sigma_{k}$$
$$l(\boldsymbol{\alpha}[1:l]) = \prod_{i=1}^{l} e^{-i\alpha_{i}B_{i}}$$

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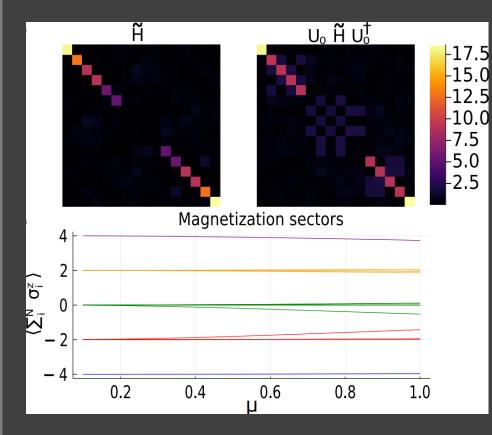
 $V = \sum_{k} v_k P_k$

 $\mathcal{O}(N^{2\gamma}L^2T)$ $\gamma = 1$ H_{μ} is 1-local or 2-local $\gamma = 2$ H_{μ} all couples interactions



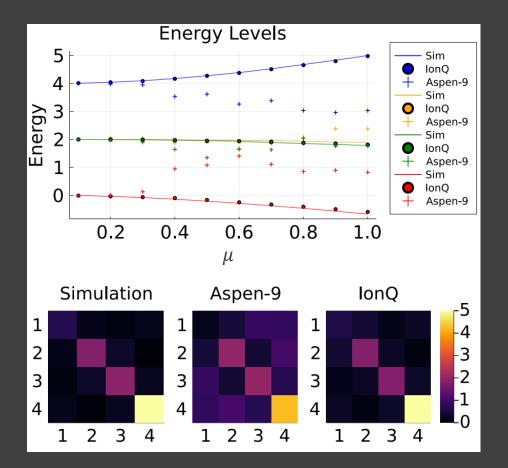
$H_{\lambda} = H_0 + \lambda V$
$H_{\lambda} = h\sigma_3^z + \lambda(J_1\sigma_1^x\sigma_3^x + J_3\sigma_2^x\sigma_3^x)$
$J_1 = J_3 = 1$, $h = 4.5$
T = 100, $L = 54$
$\left \widetilde{H}_{\lambda}\right = \left U_{\lambda}^{\dagger}H_{\lambda}U_{\lambda}\right $
$ a _{i}$ $(t = 1)$ $= a^{-i\mathcal{P}\widetilde{H}_{i}\mathcal{P}} a _{i}$ $(t = 0)$

 $\begin{aligned} |\psi_{12}(t=1)\rangle &= e^{-t\mathcal{P}H_{\mu}\mathcal{P}}|\psi_{12}(t=0)\rangle \\ \mathcal{P} |\psi_{tot}(t=1)\rangle &= \mathcal{P} e^{-i\tilde{H}_{\mu}} |\psi_{12}(t=0)\rangle \otimes |0_{3}\rangle \end{aligned}$



 $H_{\lambda} = \sum_{i=1}^{\infty} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + h \sigma_i^z)$ $+\lambda \sum_{i=1}^{N} \sigma_{i}^{x}$ $m = \langle \sum_{i}^{n} \sigma_{i}^{z} \rangle$ N = 4, T = 100, $L = 210, h = 4.5, \lambda = 1$

 $\left|\widetilde{H}_{\lambda}\right| = \left|U_{\lambda}^{\dagger}H_{\lambda}U_{\lambda}\right|$



 $H_0 = 2\mathbb{I} + \sigma_1^z + \sigma_2^z$ $V = v_1 \sigma_1^x + v_2 \sigma_2^x + v_3 \sigma_1^y +$ $+ v_4 \sigma_2^y + v_5 \sigma_1^x \otimes \sigma_2^x + v_6 \sigma_1^x \otimes \sigma_2^y$ $+ v_7 \sigma_1^y \otimes \sigma_2^x + v_8 \sigma_1^y \otimes \sigma_2^y$

 $v_i \in (0, 1)$ randomly chosen

 $T = 100, \qquad S = 100, \qquad L = 15$

No sectors & Universal Ansatz ↓ Diagonalization

Noise Resilient Variational Quantum Classical Optimization

- convergence speed of variational hybrid quantum-classical optimization algorithms
- Bounded by two competing terms
- Accuracy may actually be higher in some noisy regimes
- Open question: obtain Fisher efficient estimators of the optimal parameters

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- Diagonalization or Block diagonalization
- Scalable and NISQ suitable
- Tested it on 3 models, one of them on quantum Hardware, concluding that connectivity is crucial
- Outcomes: Apply this method to complex many body Hamiltonians

Gentini, Cuccoli, Banchi

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Gentini, Cuccoli, Banchi

Enhancing **Quantum Generative Adversarial Networks** for Noise Sensing Applications

Outline

- Generative Adversarial Networks
- Quantum Generative Adversarial Networks
- Training QGANs with noisy information
- SuperQGANs for noise-sensing

"How to enhance quantum generative adversarial learning of noisy information." Braccia, Caruso, Banchi *New Journal of Physics* 23.5 (2021): 053024. "Quantum Noise Sensing by generating Fake Noise." Braccia, Banchi, Caruso. *arXiv* preprint arXiv:2107.08718.

Generative Adversarial Networks (GANs)



Generative Adversarial Networks (GANs)



https://thispersondoesnotexist.com/

How do GANs work?



Generator (Counterfeiter)

- Generator (G) and Discriminator (D) play a turn based game against each other.
- Each turn G produces a fake copy of some target object (say an image), and D compares it to the real one deciding the probability of it being actually real.
- After each turn G uses D's feedback to improve its counterfeiting ability, and D uses G's fake samples to improve its discrimination strategy
 Nash's game theory ensures this process will end with G being able to completely fool D



Discriminator (Detective)

Each turn G produces a fake copy of some target object (say an image), and D compares it to the real one deciding the probability of it being actually real.

After each turn G uses D's feedback to improve its counterfeiting ability, and D uses G's fake samples to improve its discrimination strategy

Nash's game theory ensures this process will end with G being able to completely fool D



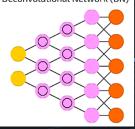
Real Data





Deconvolutional Network (DN)



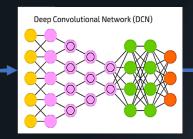


ê ê Fake Data

Discriminator's output is a continuous function of the agents' parameters, use it to build a score function

We can differentiate w.r.t. them and apply backpropagation algorithms.

Discriminator



p(Fake|data) = 1 - p(Real|data)

p(Real|data)

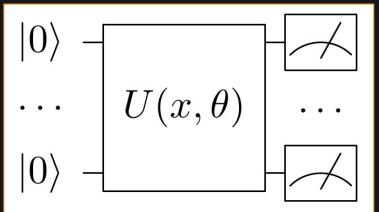
Real

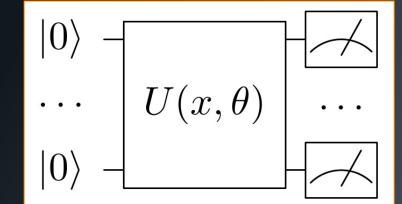
Fake



Quantum GANs (QGANs)

PQCs









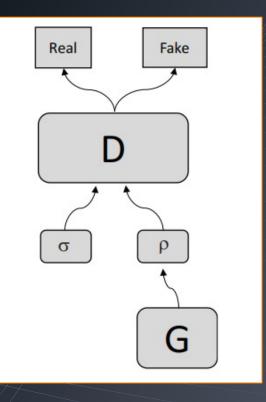
Quantum Generative Adversarial Games

- D: two-outcomes POVM $\{T, F = I T\}$
- G: quantum state generator $\rho = \rho_F$
- Real data: quantum state $\sigma = \rho_R$

Strategies

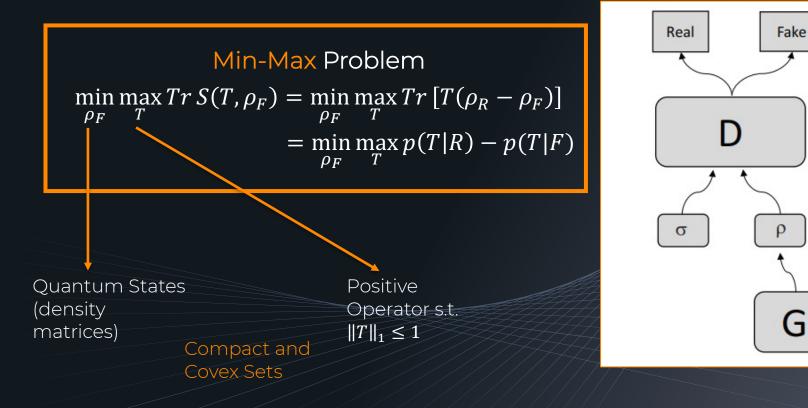
- D: maximize $p(T|R) p(T|F) = Tr[T(\rho_R \rho_F)]$
- G: maximize $p(T|F) = Tr[T\rho_F]$

 $\begin{aligned} & \underset{\rho_F}{\min} \max S(T,\rho_F) = \min_{\substack{\rho_F}} \max_T Tr\left[T(\rho_R - \rho_F)\right] \\ & = \min_{\rho_F} \max_T p(T|R) - p(T|F) \end{aligned}$



"Quantum Generative Adversarial Learning" S. Lloyd, C. Weedbrook. Physical review letters, 121(4), 040502

Quantum Generative Adversarial Games



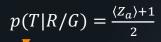
"Quantum Generative Adversarial Learning" S. Lloyd, C. Weedbrook. Physical review letters, 121(4), 040502

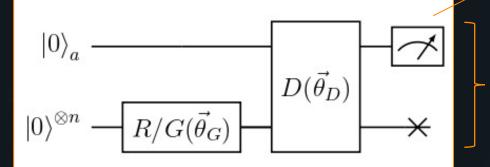
Possible Quantum Advantages

 Quantum processors can compress N dimensional feature vectors over log N qubits If the classical optimization algorithm takes
 O(poly(N)) time to run, the quantum version would ideally require only O(poly(log(N))) so.

 For classical models such as neural networks, learning quantum distributions of data is exponentially costly, whereas quantum ones can learn them natively.

Pure states QGAN





POVM measurement via Naimark Theorem

$$T = Tr_a \Big[|0\rangle_a \langle 0| \otimes I_S [D(|0\rangle_a \langle 0| \otimes I_S)D^{\dagger}] \Big]$$
$$|0\rangle_a \langle 0| = \frac{Z_a + I_a}{2}$$

Two-outcomes POVM, single ancilla qubit!

$$f(\theta) = \left\langle 0 \left| U^{\dagger}(\theta) \hat{O} U(\theta) \right| 0 \right\rangle$$
$$\partial_{\theta} f = \frac{f\left(\theta + \frac{\pi}{2}\right) - f\left(\theta - \frac{\pi}{2}\right)}{2}$$

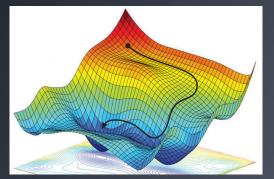
Gradient Descent (GD)

s.t. all gates appearing in U are generated by Pauli matrices

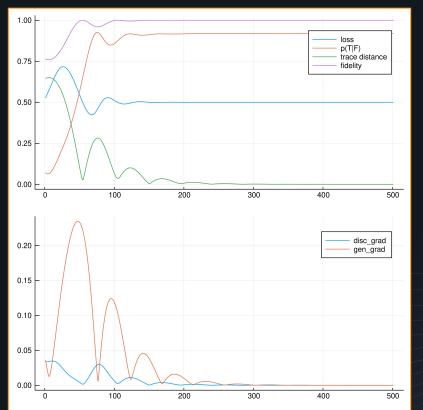
Parameter Shift Rule

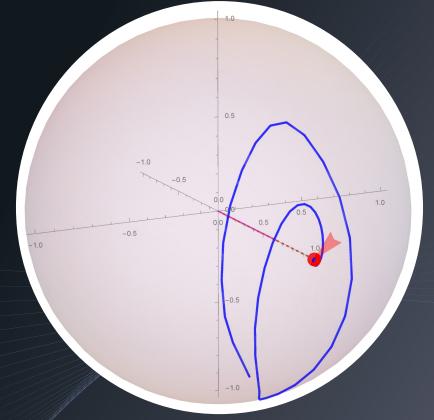
Schuld, Maria, et al. "Evaluating analytic gradients on quantum hardware." *Physical Review A* 99.3 (2019): 032331.

$$\vec{\theta} \leftarrow \vec{\theta} - \eta \nabla_{\vec{\theta}} f$$



Everything goes fine!





What is up with mixed states?

Recall mixed states are described by density matrices $|\psi\rangle \rightarrow \rho \in Lin^+(H) \ s.t. \ Tr(\rho) = 1$

Qubit: the interior of the Bloch ball is accessible

$$\rho = \frac{1}{2}(I + \vec{r} \cdot \vec{\sigma}), \qquad 0 \le |\vec{r}| \le 1$$

POVM elements can be described analogously $\Pi_D = \frac{1}{2} (d^0 I + \vec{d} \cdot \vec{\sigma}), \qquad d^0 \ge |\vec{d}|$

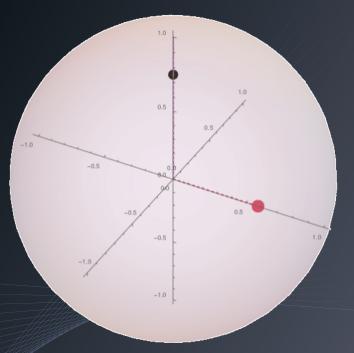
QGAN Score Function reads:

 $S(\Pi_D, \rho_G) = \frac{\vec{d} \cdot (\vec{r} - \vec{g})}{2}$

Quadratic function of Bloch vectors



"How to enhance quantum generative adversarial learning of noisy information." Braccia, Caruso, Banchi *New Journal of Physics* 23.5 (2021): 053024.

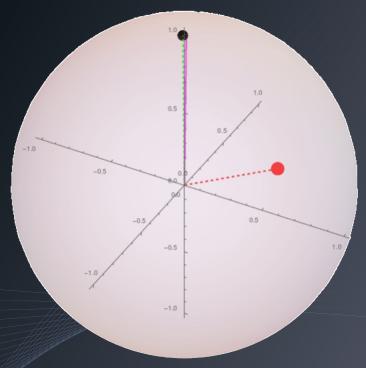


All we lack is some OPTIMISM!

Optimistic Mirror Descent (OMD) Players exploit knowledge of foe's strategy

$$\vec{\theta}^{t+1} \leftarrow \vec{\theta}^t - 2\eta \nabla_{\vec{\theta}}^t S + \eta \nabla_{\vec{\theta}}^{t-1} S$$

Daskalakis, Constantinos, et al. "Training gans with optimism." *arXiv:1711.00141* (2017).



No more convergence issues!

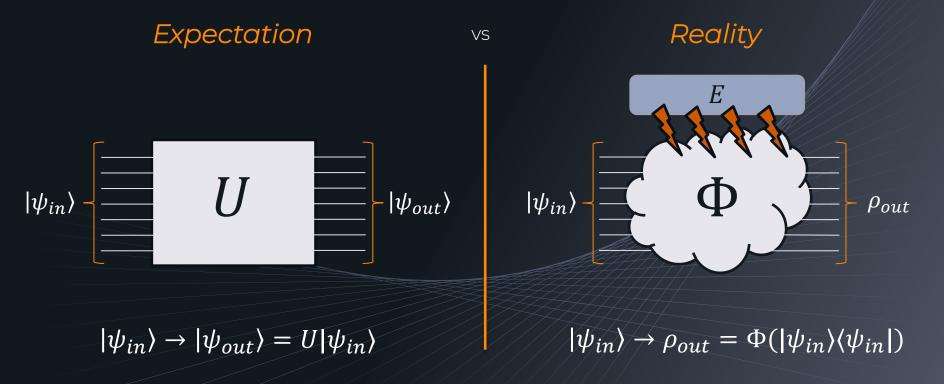
"How to enhance quantum generative adversarial learning of noisy information." Braccia, Caruso, Banchi New Journal of Physics 23.5 (2021): 053024.

SuperOGANs for Noise Sensing



NISQ devices

Nowadays quantum processors are Noisy (and Small)...



Quantum Channels

CPTP maps Φ

- Linear: $\sum_i p_i \rho_i \rightarrow \sum_i p_i \Phi(\rho_i)$
- Trace Preserving
- Positive (preserve positivity of ρ)

Stinespring representation

$$\Phi(\rho) = \mathrm{Tr}_E[U_{SE}(\rho_S \otimes \omega_E)U_{SE}^{\dagger}]$$

Kraus representation

Φ

Φ

Φ

$$\rho) = \sum_{i} K_{i} \rho K_{i}^{\dagger}, \qquad \sum_{i} K_{i}^{\dagger} K_{i} =$$

One would expect

$$= \Phi \otimes \cdots \otimes \Phi = \Phi^{\otimes n}$$

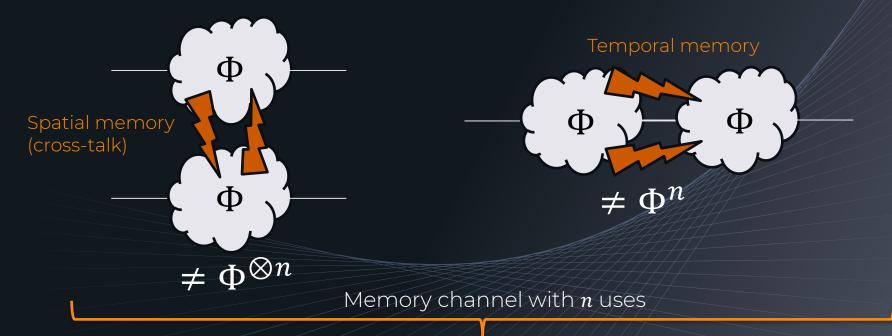
$$- = \Phi \circ \cdots \circ \Phi = \Phi^n$$

Composition of channels:

- «Parallel», different systems pass through n copies of the channel
- «Series», the same system is processed ntimes by the channel

Quantum Memory Channels

Most often instead



 $\Phi^{(n)}$

Pauli Channels

Knill, Emanuel. "Quantum computing with realistically noisy devices." *Nature* 434.7029 (2005): 39-44.

Random Unitary Channels

 $\Phi(\rho) = \sum_{i} p_{i} U_{i} \rho U_{i}^{\dagger}$ System undergoes evolution U_{i} with probability p_{i} Pauli Channels

Pauli Channels are exceptionally good at describing realistic noise models

$$\Phi^{(n)}(\rho) = \sum_{\vec{k}} p_{\vec{k}} \sigma_{\vec{k}} \rho \sigma_{\vec{k}} \qquad \qquad \sigma_{\vec{k}} = \sigma_{k_0} \otimes \sigma_{k_1} \otimes \cdots \otimes \sigma_{k_n} \\ \sigma_{\vec{k}} = \sigma_{k_0} \circ \sigma_{k_1} \circ \cdots \circ \sigma_{k_n}$$

 $\begin{array}{l} p_{\vec{k}} = p_{k_0} p_{k_1} \cdots p_{k_n} \rightarrow "memoryless \ channel" \\ p_{\vec{k}} \neq p_{k_0} p_{k_1} \cdots p_{k_n} \rightarrow "memory \ (correlated) \ channel" \end{array}$

This is the most common scenario, we want to characterize correlations!

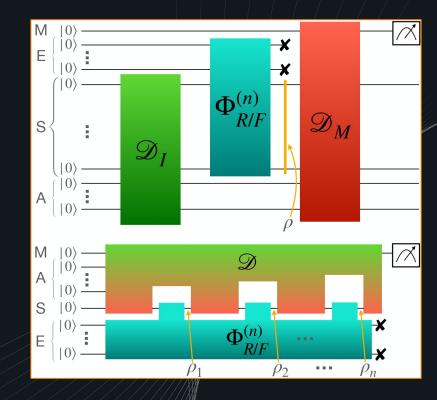
SuperQGANs setup

Spatially Correlated Noise:

- D_I prepares a probe state
- Real or Fake noisy channel $\Phi_{R/F}$ is applied
- D_M implements measuring POVM

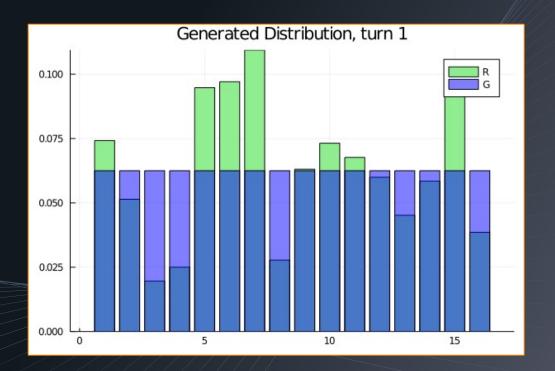
Temporally Correlated Noise:

- General Quantum Comb scheme is applied
- Comb *D* interacts with noisy Real/Fake channel at each of the *n* intermediate times
- A final map entangles **D**'s comb with the measurement ancilla qubit



SuperQGANs performance

- Since channel outputs are mixed, Optimistic strategy comes in handy
- Great advantage in using QCNN for the POVMimplementing PQC
- Method does not use any approximation, there is room for tweakings and speedups!

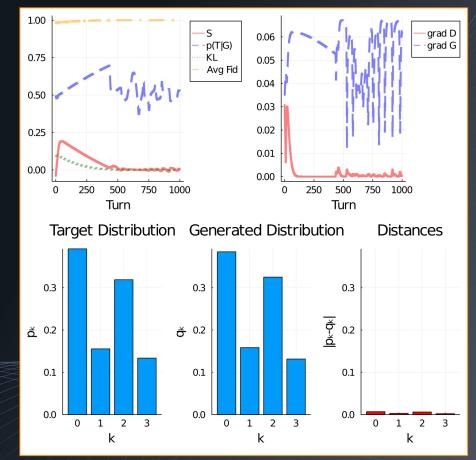


SuperQGANs tackling correlations

Correlation model

$$p_{ij}^{(2)} = (1 - \mu)p_i^{(1)}p_j^{(1)} + \mu p_i^{(1)}\delta_{ij}$$

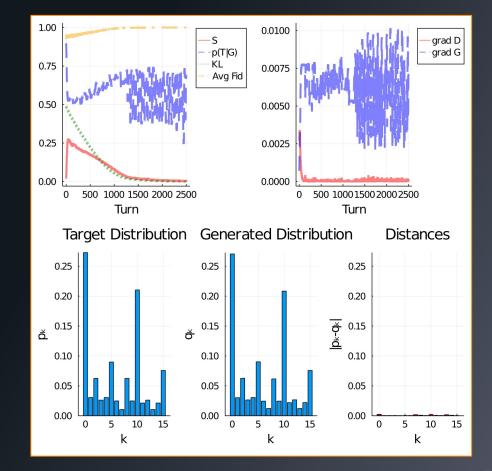
First, learn single use channel $\Phi^{(1)}$



SuperQGANs tackling correlations

Correlation model $p_{ii}^{(2)} = (1 - \mu)p_i^{(1)}p_i^{(1)} + \mu p_i^{(1)}\delta_{ij}$

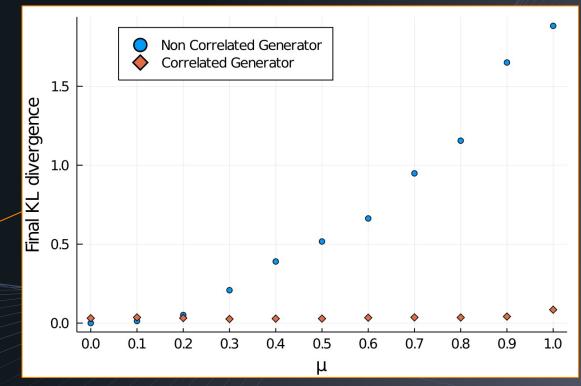
Then, use learnt «prior» $p_i^{(1)}$ to check wether $\Phi^{(2)} = \Phi^2$ (temporal), or $\Phi^{(2)} = \Phi^{\otimes 2}$ (spatial)



SuperQGANs tackling correlations

Constraining G to control only factorized error-rates and monitoring convergence failure is another way to check for correlations

$$D_{KL}(P||Q) = \sum_{x \in \mathbf{X}}^{P} P(x) \log(\frac{P(x)}{Q(x)})$$



Outlooks

Adversarial game paradigm can be shaped to perform implicit state/process tomography, what next?

- Find clever ways to exploit previously known structure of target state/noise
- Part from exact reconstruction and make QGAN/SuperQGAN scalable, e.g. by using Tensor Network representation of states/channels

Thank you for your attention!