Preparing correlated fermionic states on a quantum computer

Pierre-Luc Dallaire-Demers

Quantum computing and scientific research:
State of the art and potential impact in nuclear physics

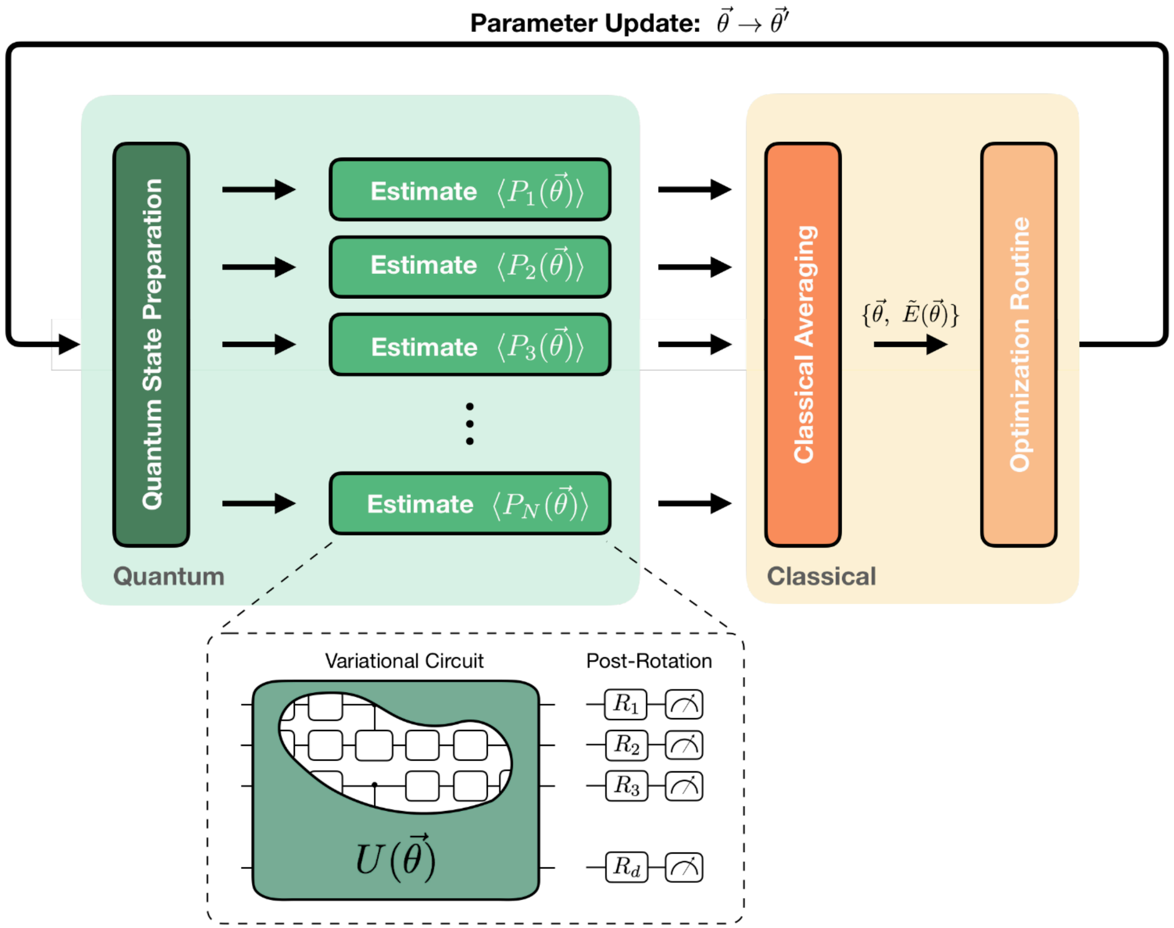
June 14th 2019

Content

- Ansatz for VQE
- Advanced variational state preparation methods
- Variational quantum machine learning

Cao, Yudong, et al. "Quantum Chemistry in the Age of Quantum Computing." *arXiv:1812.09976* (2018).

Variational quantum eigensolver



$$\langle H\rangle = \sum_{i_1\alpha_1} h^{i_1}_{\alpha_1}\langle\sigma^{i_1}_{\alpha_1}\rangle + \sum_{i_1\alpha_1 i_2\alpha_2} h^{i_1 i_2}_{\alpha_1\alpha_2}\langle\sigma^{i_1 i_2}_{\alpha_1\alpha_2}\rangle + \cdots$$

$$m = \left(\frac{1}{\epsilon}\sum_i^M |h_i|\sigma_i\right)^2 \leq \left(\frac{1}{\epsilon}\sum_i^M |h_i|\right)^2$$

VQE resilient to coherent (and some incoherent) errors!

Peruzzo, Alberto, et al. "A variational eigenvalue solver on a photonic quantum processor.”
Nature communications 5 (2014): 4213.

Hamiltonian variational ansatz

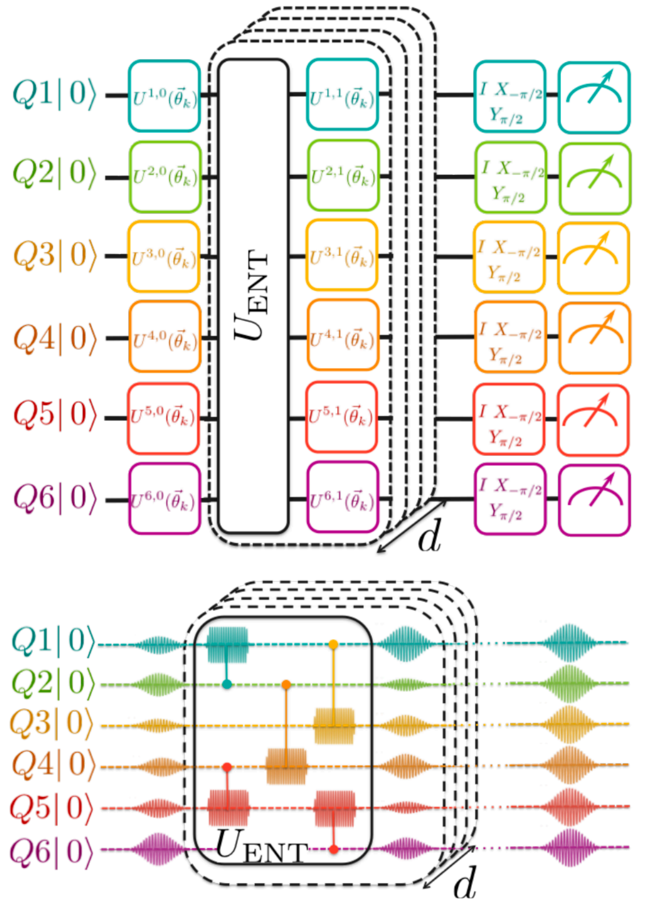
$$\Psi_T = \prod_{b=1}^{S} \Big(U_U(\frac{\theta_U^b}{2}) U_h(\theta_h^b) U_v(\theta_v^b) U_U(\frac{\theta_U^b}{2}) \Big) \Psi_I$$

S	ΔE^s	ΔE^f	P^s	P^f
	4			
3	0.24	1.00×10^{-8}	0.7180	1.0000
5	0.20	3.00×10^{-8}	0.76289	1.0000
7	0.17	2.00×10^{-8}	0.8021	1.0000
9	0.15	7.00×10^{-8}	0.8275	1.0000
11	0.13	2.00×10^{-8}	0.8460	1.0000
	8			
3	0.1	0.033	0.9790	0.9934
5	0.042	0.0046	0.9906	0.9983
7	0.031	0.0030	0.9930	0.9989
9	0.024	0.0013	0.9947	0.9995
11	0.019	0.00089	0.9960	0.9997
13	0.015	0.00038	0.9968	0.9999
15	0.013	0.00031	0.9973	0.9999
17	0.012	0.00022	0.9976	0.9999
19	0.010	0.00027	0.9978	0.9999

Hubbard, half filling, 4 and 8 spin orbitals

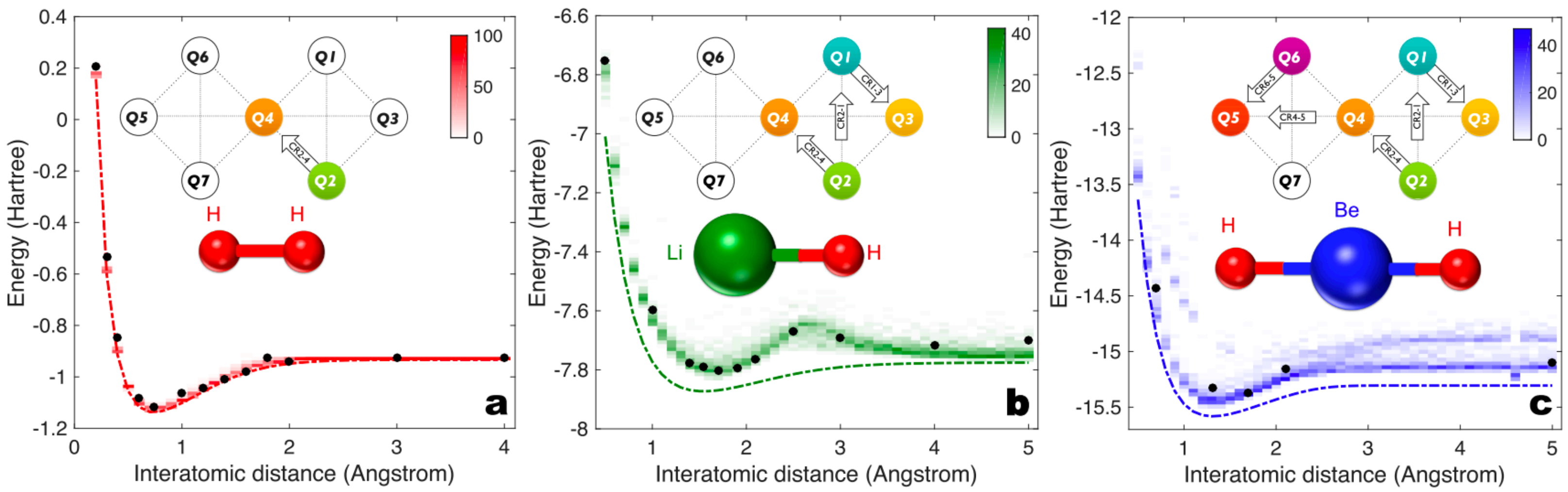
Wecker et al. "Progress towards practical quantum variational algorithms." *Physical Review A* 92.4 (2015): 042303.

Hardware efficient ansatz



$$|\Phi(\vec{\theta})\rangle = \prod_{q=1}^{N}\left[U^{q,d}(\vec{\theta})\right] \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N}\left[U^{q,d-1}(\vec{\theta})\right]$$

$$\cdots \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N}\left[U^{q,0}(\vec{\theta})\right]|00\ldots0\rangle.$$



d=1

Kandala, Abhinav, et al. "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets." *Nature* 549.7671 (2017): 242.

Low-depth circuit ansatz

Dallaire-Demers, Pierre-Luc, et al.
"Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer."
arXiv:1801.01053 (2018).

The traditional VQE subroutine

Jordan-Wigner transformation

$$a_k^\dagger = \left(\bigotimes_{j=1}^{k-1} \sigma_z\right) \otimes \sigma_+ \qquad \left\{a_k, a_l^\dagger\right\} = \delta_{kl}$$

$$a_k = \left(\bigotimes_{j=1}^{k-1} \sigma_z\right) \otimes \sigma_- \qquad \{a_k, a_l\} = \left\{a_k^\dagger, a_l^\dagger\right\} = 0$$

Hartree-Fock reference state

$$|\Phi_0\rangle = \prod_k a_k^\dagger |\text{vac}\rangle$$

Variational unitary coupled cluster

$$\min_\Theta E(\Theta) = \langle\Psi(\Theta)| H |\Psi(\Theta)\rangle \qquad |\Psi(\Theta)\rangle = e^{i\left(\mathcal{T}(\Theta) + \mathcal{T}^\dagger(\Theta)\right)} |\Phi_0\rangle$$

Hamiltonian

$$
\begin{aligned}
H \quad = \quad & \sum_{pq} \left(t_{pq} a_p^\dagger a_q + \Delta_{pq} a_p^\dagger a_q^\dagger + \Delta_{pq}^* a_q a_p \right) \\
& + \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r \\
& + \sum_{pqrstu} w_{pqrstu} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s
\end{aligned}
$$

The Bogoliubov transformation

Most general linear transformation

$$\begin{aligned} \beta^\dagger_{p'} &= \sum_p \left(U_{pp'} a^\dagger_p + V_{pp'} a_p\right) \\ \beta_{p'} &= \sum_p \left(U^*_{pp'} a_p + V^*_{pp'} a^\dagger_p\right) \end{aligned}$$

$$\mathcal{U} = \begin{pmatrix} \mathbf{U}^* & \mathbf{V}^* \\ \mathbf{V} & \mathbf{U} \end{pmatrix}$$

Anti-commutation relations

$$\left\{\beta_k, \beta^\dagger_l\right\} = \delta_{kl} \qquad \{\beta_k, \beta_l\} = \left\{\beta^\dagger_k, \beta^\dagger_l\right\} = 0$$

Reference state: Quasiparticle vacuum

$$|\Phi_0\rangle = C \prod_{k=1}^{\mathrm{rank}(V)} \beta_k \, |\mathrm{vac}\rangle \qquad \beta_j \, |\Phi_0\rangle = 0$$

Covariance matrix notation

The Majorana transformation

$$\begin{aligned} \gamma_j &= a_j^\dagger + a_j \\ \gamma_{j+M} &= -i\left(a_j^\dagger - a_j\right) \end{aligned}$$

$$\{\gamma_k, \gamma_l\} = 2\delta_{kl}$$

$$\gamma_k^2 = 1$$

$$\Omega = \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ i\mathbf{1} & -i\mathbf{1} \end{pmatrix}$$

The real and complex covariance matrices (Gaussian states)

$$\Gamma_{kl} = \frac{i}{2}\mathrm{tr}\left(\rho\left[\gamma_k, \gamma_l\right]\right) \Rightarrow \Gamma_c = \frac{1}{4}\Omega^\dagger \Gamma \Omega^* = \begin{pmatrix} \mathbf{Q} & \mathbf{R} \\ \mathbf{R}^* & \mathbf{Q}^* \end{pmatrix} \Rightarrow$$

$$\varrho \equiv \frac{1}{2}\mathbf{1} - i\mathbf{R}^\top$$

$$\kappa \equiv -i\mathbf{Q}$$

The single-particle density matrix (Bloch-Messiah form)

$$\mathcal{M} = \begin{pmatrix} \varrho & \kappa^\dagger \\ \kappa & \mathbf{1} - \varrho^\top \end{pmatrix}$$

$$\mathcal{E} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}$$

$$\mathcal{M}\mathcal{U}^\dagger = \mathcal{E}\mathcal{U}^\dagger$$

Bloch and Messiah (1962)

Generalized Hartree-Fock

$$H = i\sum_{pq} T_{pq}\gamma_p\gamma_q + \sum_{pqrs} V_{pqrs}\gamma_p\gamma_q\gamma_s\gamma_r + i\sum_{pqrstu} W_{pqrstu}\gamma_p\gamma_q\gamma_r\gamma_u\gamma_t\gamma_s$$

Assuming Wick's theorem:

$$h(\Gamma) = T + 6\mathrm{tr}_B(V\Gamma) + 45\mathrm{tr}_C(W\Gamma\Gamma)$$

where

$$\mathrm{tr}_B(V\Gamma)_{ij} = \sum_{kl} V_{ijkl}\Gamma_{lk}$$

$$\mathrm{tr}_C(W\Gamma\Gamma)_{ij} = \sum_{klmn} W_{ijklmn}\Gamma_{kn}\Gamma_{ml}$$

Imaginary time evolution

$$\Gamma(\tau) = O(\tau)\Gamma(0)O(\tau)^{\top}$$

$$O(\tau) = \mathbb{T}e^{2\int_0^{\tau} d\tau' [h(\Gamma(\tau')),\Gamma(\tau')]}$$

$$[h(\Gamma),\Gamma] = 0$$

Fixed point method

$$\Gamma = \lim_{\beta\to\infty} \tanh[2i\beta h(\Gamma)]$$

Kraus and Cirac (2010)

Bogoliubov unitary coupled clusters

Coupled cluster operators

$$\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \ldots$$

$$\mathcal{T}_1 = \sum_{k_1 k_2} \theta_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2}$$

$$\theta_{k_1 k_2 \ldots} \in \mathbb{C}$$

$$\mathcal{T}_2 = \sum_{k_1 k_2 k_3 k_4} \theta_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$

$$\mathcal{T}_3 = \sum_{k_1 k_2 k_3 k_4 k_5 k_6} \theta_{k_1 k_2 k_3 k_4 k_5 k_6} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} \beta^\dagger_{k_5} \beta^\dagger_{k_6}$$

Parametrized state

$$|\Psi(\Theta)\rangle = e^{i\left(\mathcal{T}(\Theta) + \mathcal{T}^\dagger(\Theta)\right)} |\Phi_0\rangle$$

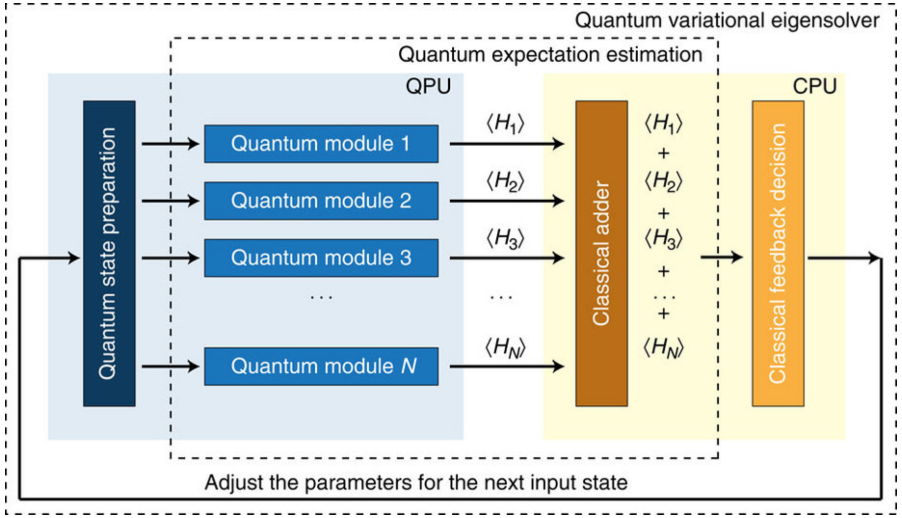
Constrained optimization $\min_{\Theta} E(\Theta) = \langle \Psi(\Theta)| H |\Psi(\Theta)\rangle$

$$N(\Theta) = \langle \Psi(\Theta)| N |\Psi(\Theta)\rangle$$

Jordan-Wigner

$$\beta^\dagger_p = \left(\bigotimes_{j=1}^{p-1} \sigma_z\right) \otimes \sigma_+$$

$$\beta_p = \left(\bigotimes_{j=1}^{p-1} \sigma_z\right) \otimes \sigma_-$$



Signoracci, Angelo, et al.
"Ab initio Bogoliubov coupled cluster theory for open-shell nuclei." *Physical Review C* 91.6 (2015): 064320.

Fermionic linear optics and matchgates

Reversing the Bogoliubov transformation

$$\mathcal{C}\gamma_j\mathcal{C}^\dagger = \sum_{k=1}^{2M} \mathcal{R}_{kj}\gamma_k$$

$$\mathcal{R} = \begin{pmatrix} \mathrm{Re}\,(\mathbf{U}+\mathbf{V}) & -\mathrm{Im}\,(\mathbf{U}-\mathbf{V}) \\ \mathrm{Im}\,(\mathbf{U}+\mathbf{V}) & \mathrm{Re}\,(\mathbf{U}-\mathbf{V}) \end{pmatrix}$$

Matchgates

$$\mathcal{G}\,(A,B) = \begin{pmatrix} p & 0 & 0 & q \\ 0 & w & x & 0 \\ 0 & y & z & 0 \\ r & 0 & 0 & s \end{pmatrix}$$

$$A = \begin{pmatrix} p & q \\ r & s \end{pmatrix}$$

$$B = \begin{pmatrix} w & x \\ y & z \end{pmatrix}$$

$$\det A = \det B$$

Fermionic SWAP

$$\mathcal{S} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

6 generators

$$\{\sigma_x\otimes\sigma_x, \sigma_x\otimes\sigma_y, \sigma_y\otimes\sigma_x, \sigma_y\otimes\sigma_y, \sigma_z\otimes\mathbb{I}, \mathbb{I}\otimes\sigma_z\}$$

Natural gates for SC qubits!

DiVincenzo and Terhal (2005)

Bogoliubov unitary coupled clusters

$$|\Psi(\Theta)\rangle = e^{i\left(\mathcal{T}(\Theta)+\mathcal{T}^\dagger(\Theta)\right)}|\Phi_0\rangle$$

$$|\Phi_0\rangle = C\prod_{k=1}^{M}\beta_k|\text{vac}\rangle$$

$$\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \dots$$

$$\mathcal{T}_1 = \sum_{k_1k_2}\theta_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2}$$

$$\mathcal{T}_2 = \sum_{k_1k_2k_3k_4}\theta_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4}$$

Note: Must constrain particle number!

Jordan-Wigner -> Matchgates

$$\gamma_j = \gamma_j^A = a_j^\dagger + a_j$$

$$\gamma_{j+M} = \gamma_j^B = -i\left(a_j^\dagger - a_j\right)$$

$$\sigma_x^j \otimes \sigma_x^{j+1} = -i\gamma_j^B\gamma_{j+1}^A$$

$$\sigma_x^j \otimes \sigma_y^{j+1} = -i\gamma_j^B\gamma_{j+1}^B$$

$$\sigma_y^j \otimes \sigma_x^{j+1} = i\gamma_j^A\gamma_{j+1}^A$$

$$\sigma_y^j \otimes \sigma_y^{j+1} = i\gamma_j^A\gamma_{j+1}^B$$

$$\sigma_z^j \otimes \mathbb{I}^{j+1} = -i\gamma_j^A\gamma_j^B$$

$$\mathbb{I}^j \otimes \sigma_z^{j+1} = -i\gamma_{j+1}^A\gamma_{j+1}^B$$

$$H = i\sum_{pq}T_{pq}\gamma_p\gamma_q + \sum_{pqrs}V_{pqrs}\gamma_p\gamma_q\gamma_s\gamma_r$$

Preparing fermionic Gaussian states

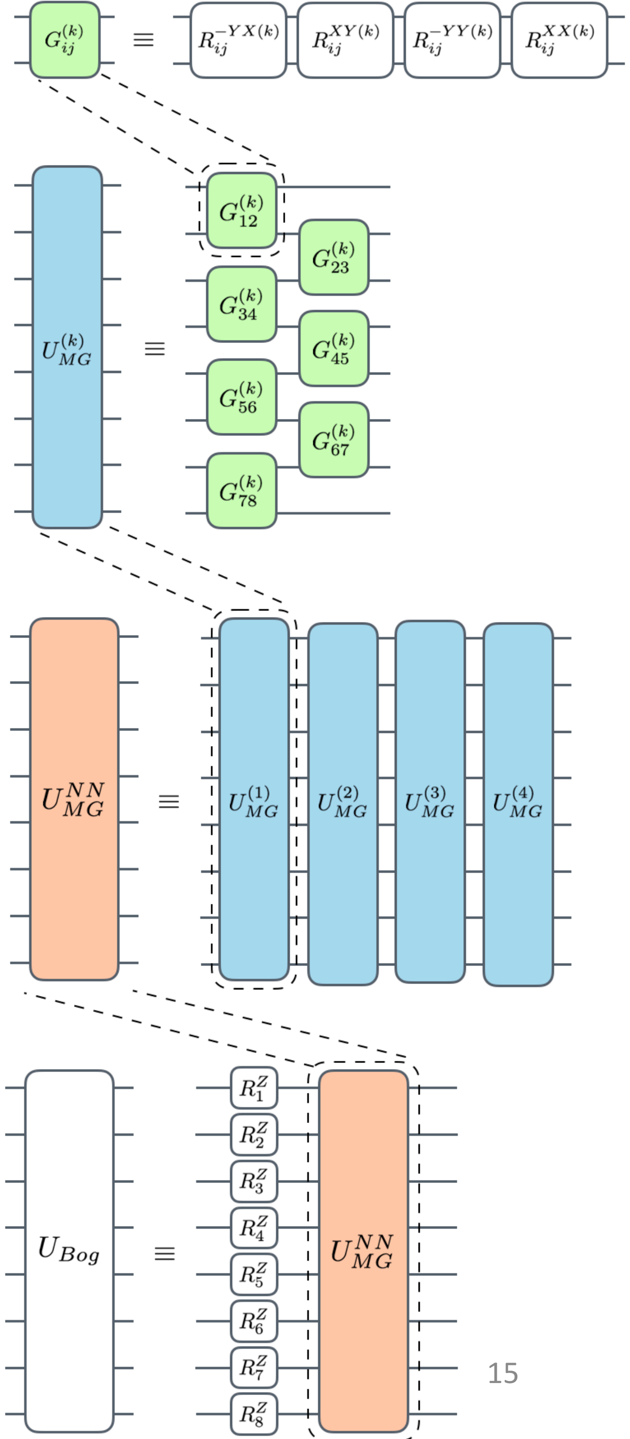
$$\Gamma_{kl} = \frac{i}{2}\mathrm{tr}\left(\rho\left[\gamma_k, \gamma_l\right]\right)$$ -> Generalized Hartree-Fock

$$U_{\mathrm{Bog}}\gamma_j U_{\mathrm{Bog}}^{\dagger} = \sum_{k=1}^{2M} \mathcal{R}_{kj}\gamma_k$$

$$\mathcal{R} = \begin{pmatrix} \mathrm{Re}\left(\mathbf{U}+\mathbf{V}\right) & -\mathrm{Im}\left(\mathbf{U}-\mathbf{V}\right) \\ \mathrm{Im}\left(\mathbf{U}+\mathbf{V}\right) & \mathrm{Re}\left(\mathbf{U}-\mathbf{V}\right) \end{pmatrix}$$

Number of parameters

$2M(M-1)$	$SO(4)$	Rotations
M	$SO(2)$	Rotations
$2M^2-2$	$SO(2M)$	Total



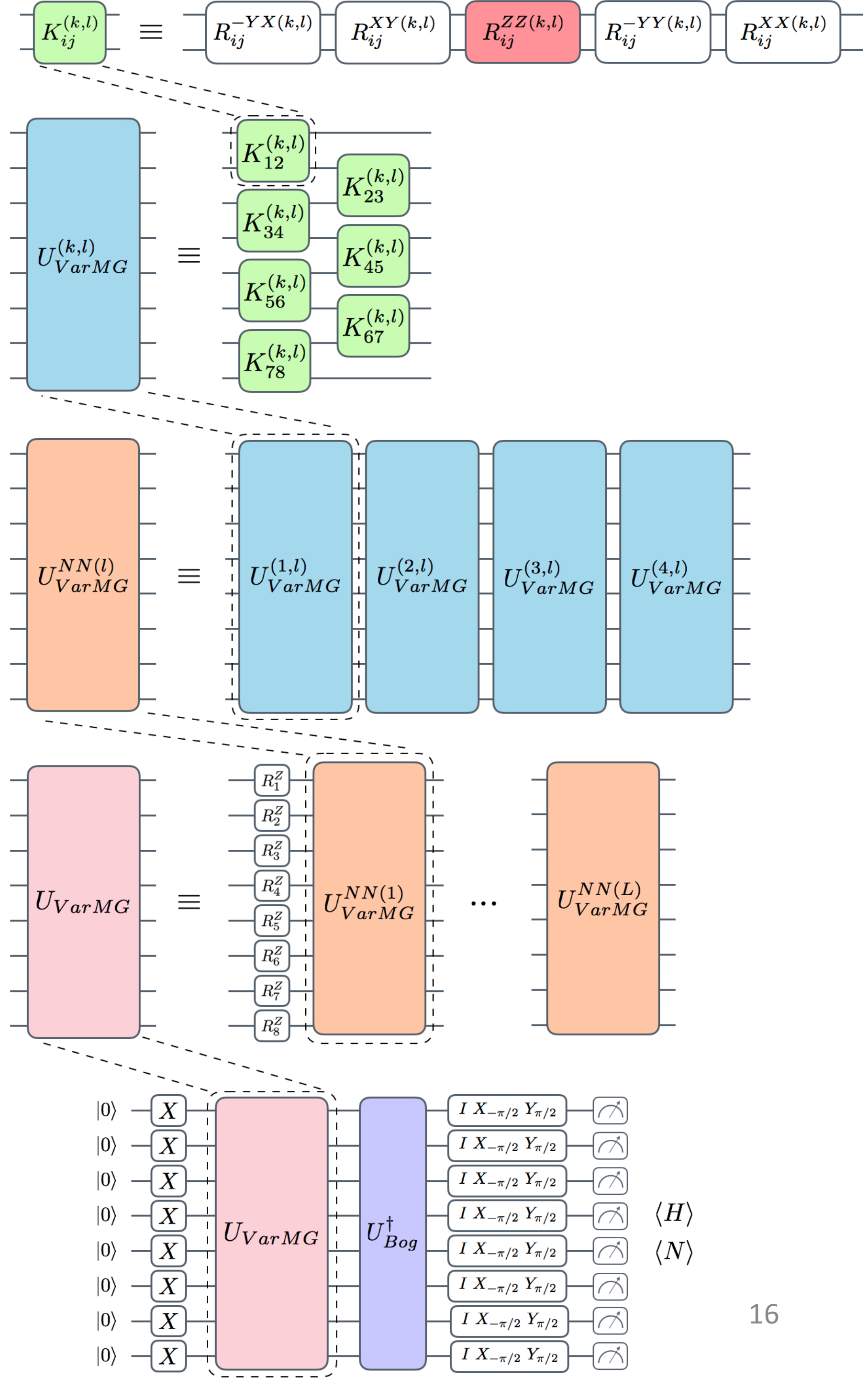
Non-Gaussian ansatz

$$|\Psi(\Theta)\rangle = U_{\mathrm{Bog}}^{\dagger} U_{\mathrm{VarMG}}(\Theta) \prod_{i=1}^{M} X_i |0\rangle^{\otimes M}$$

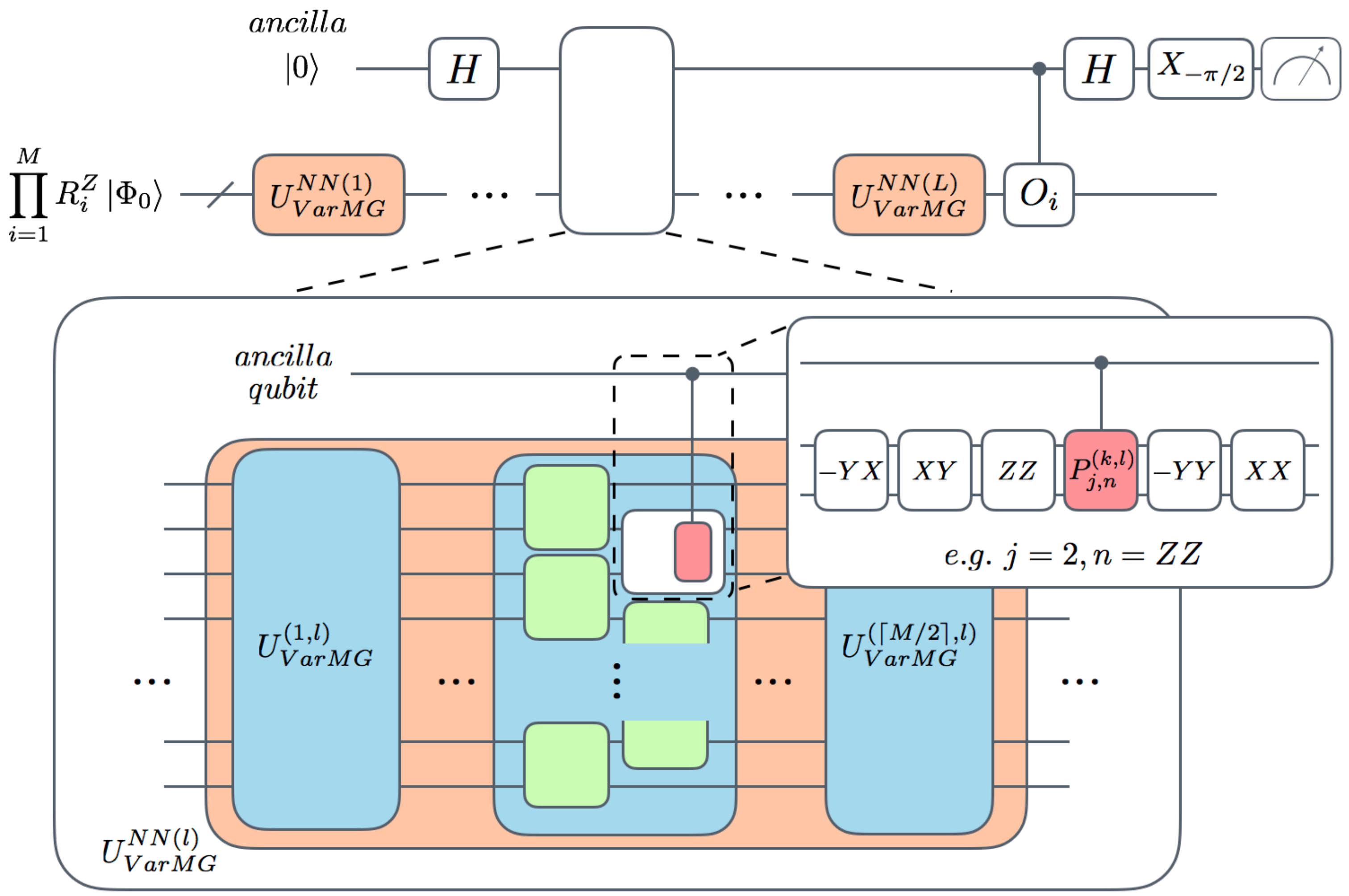
Layers/cycles: $\left\lceil \frac{M}{2} \right\rceil$

Number of parameters: $(10L + 8)\left\lceil \frac{M}{2} \right\rceil + 4$

Circuit depth: $5L(M-1)\left\lceil \frac{M}{2} \right\rceil + M$



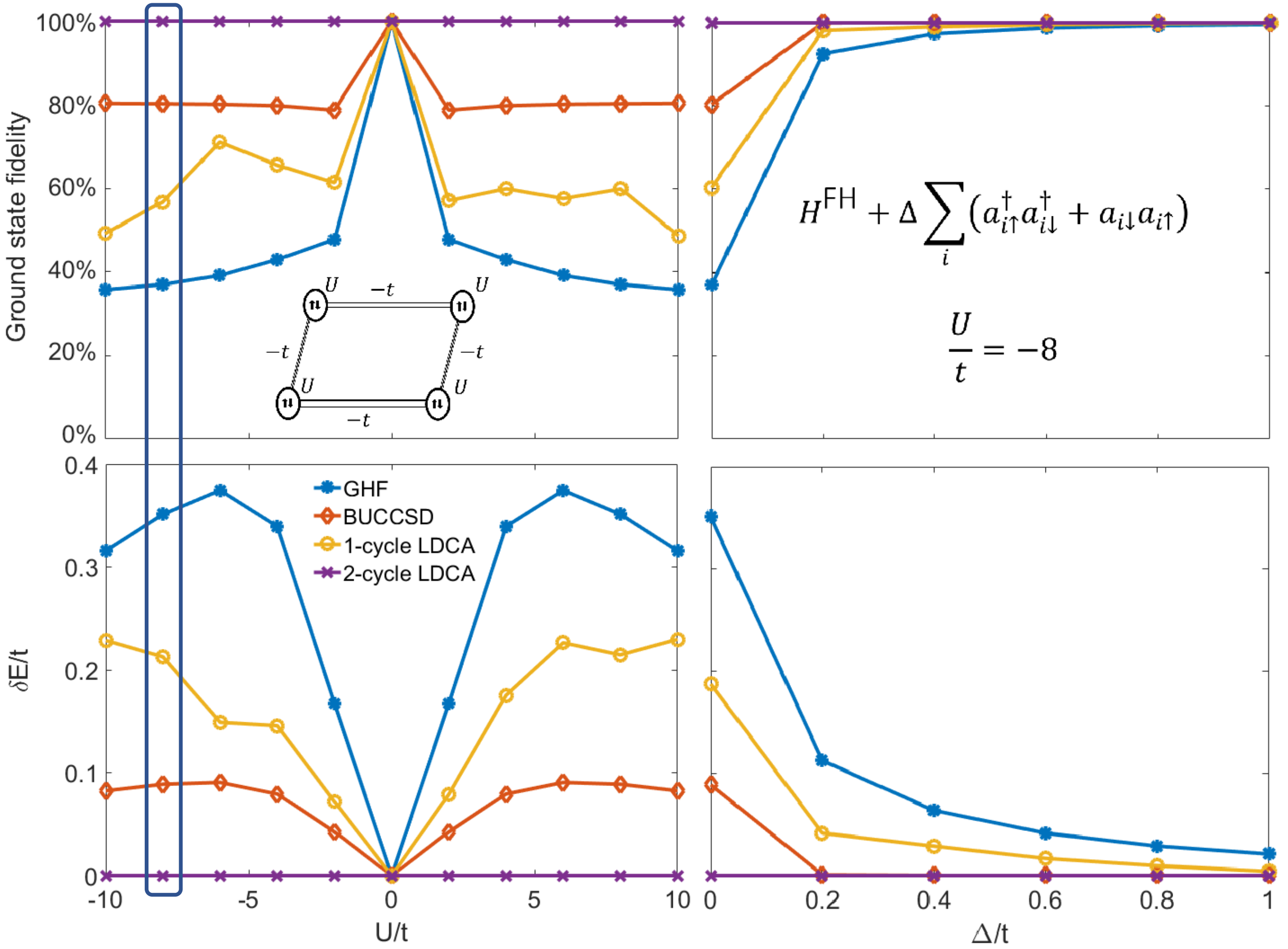
Gradients



$$\frac{\partial E(\Theta)}{\partial \theta_{j,n}^{(k,l)}} = 2\sum_i h_i \, \mathrm{Im}\Big(\langle \Phi_0 | V_{j,n}^{(k,l)\dagger}(\Theta) O_i U(\Theta) | \Phi_0 \rangle\Big)$$

Fermi-Hubbard model

$$H^{\mathrm{FH}} = -t\sum_{\langle p,q\rangle}\sum_{\sigma=\uparrow,\downarrow}\left(a^\dagger_{p\sigma}a_{q\sigma}+a^\dagger_{q\sigma}a_{p\sigma}\right) -\mu\sum_p\sum_{\sigma=\uparrow,\downarrow}\left(n_{p\sigma}-\frac{1}{2}\right) +U\sum_p\left(n_{p\uparrow}-\frac{1}{2}\right)\left(n_{p\downarrow}-\frac{1}{2}\right)$$



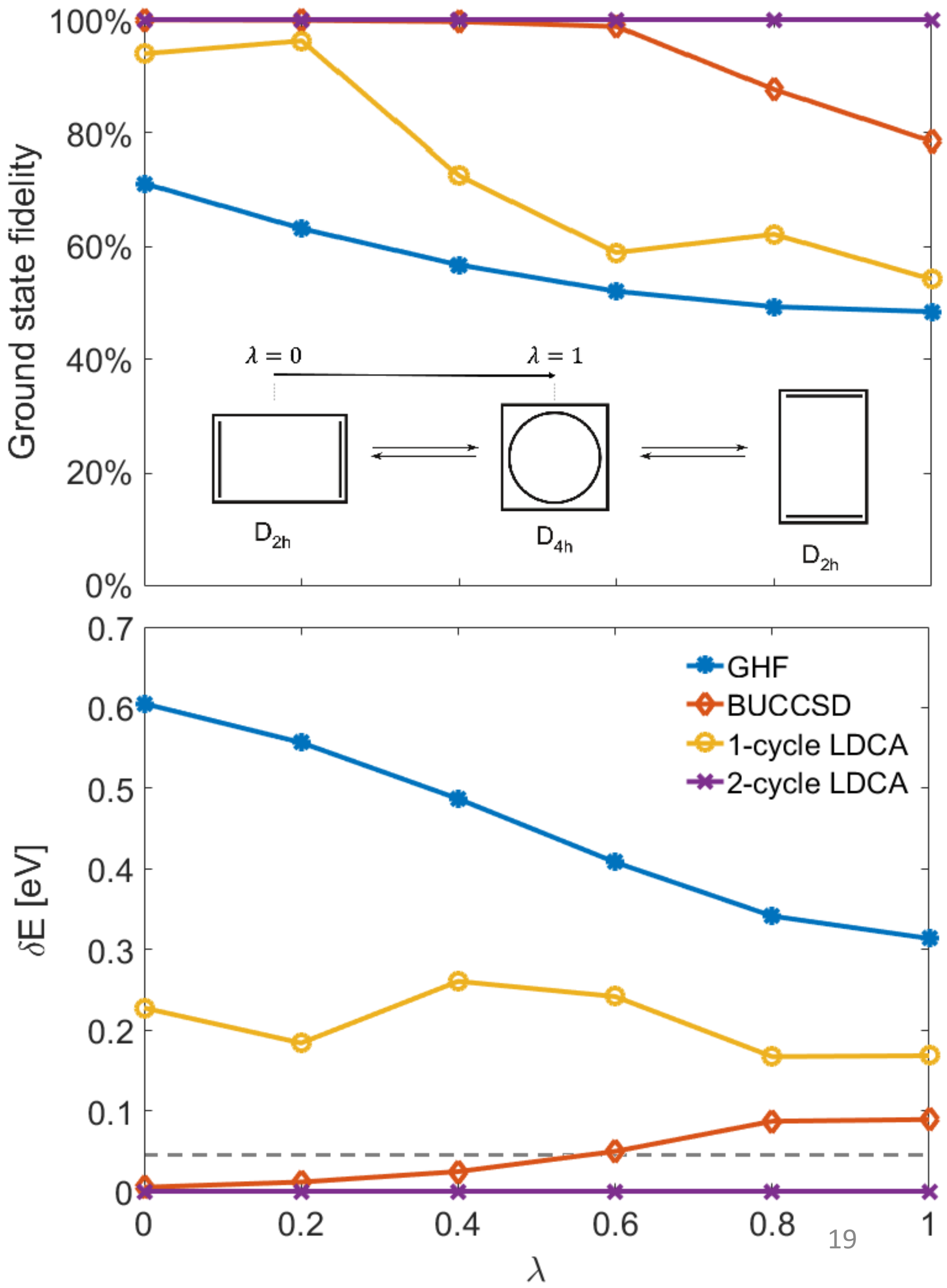
Cyclobutadiene

$$H^{\mathrm{PPP}} = \sum_{i<j} t_{ij} E_{ij} + \sum_i U_i n_{i\alpha} n_{i\beta} + V_c + \frac{1}{2} \sum_{ij} \gamma_{ij} (n_{i\alpha} + n_{i\beta} - 1)(n_{j\alpha} + n_{j\beta} - 1)$$

where $E_{ij} = \sum_{\sigma=\alpha,\beta} a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma}$

Dimensionless parameter:

$$\gamma_{ij}(r_{ij}) = \frac{1}{1/U + r_{ij}}$$

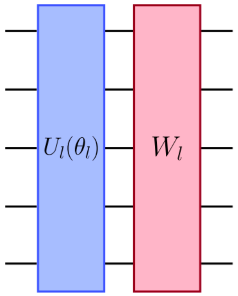


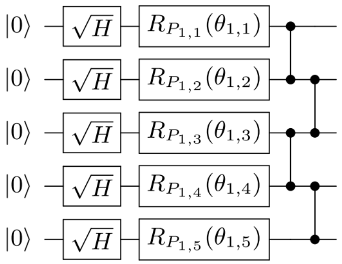
Advanced VQE

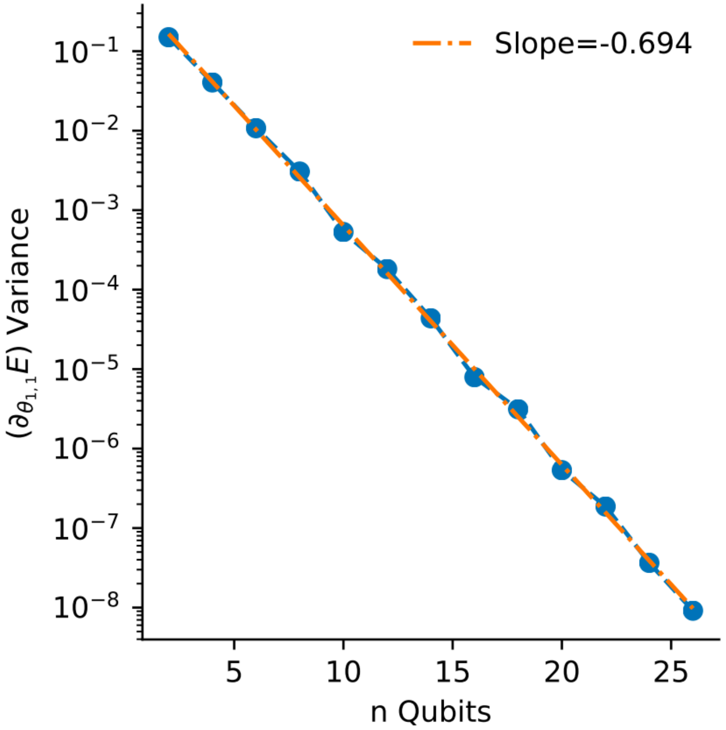
- Barren plateaus
- Variational imaginary time evolution
- Partial phase estimation

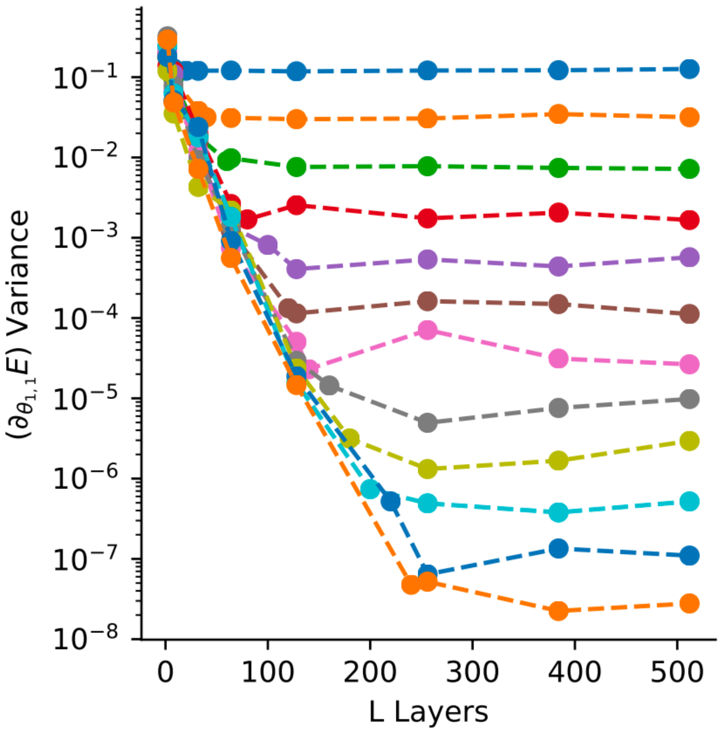
Barren plateaus

$$\langle \partial_k E \rangle = \int dU p(U) \partial_k \langle 0 | U(\vec{\theta})^\dagger H U(\vec{\theta}) | 0 \rangle$$









McClean, Jarrod R., et al. "Barren plateaus in quantum neural network training landscapes.”
Nature communications 9.1 (2018): 4812.

Imaginary time evolution

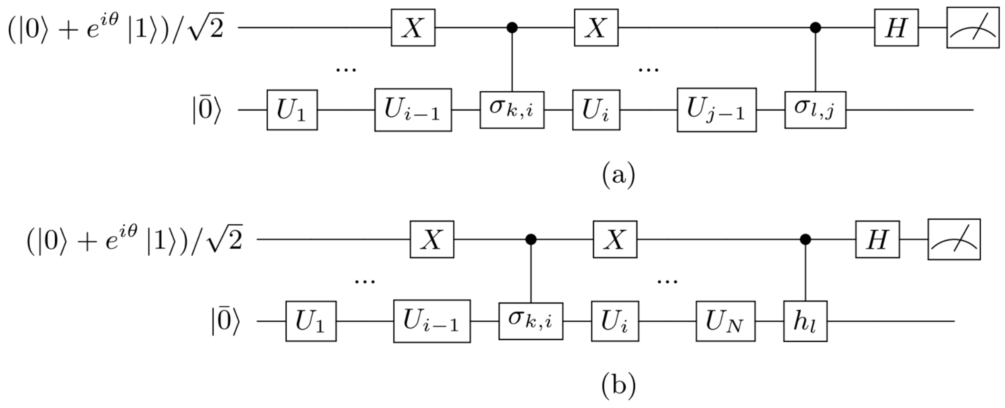
McLachlan's variational principle

$$\delta\|(\partial/\partial\tau + H - E_\tau)\,|\psi(\tau)\rangle\,\| = 0,\ \text{where}\ \|\rho\| = \mathrm{Tr}[\sqrt{\rho\rho^\dagger}]$$

$$\sum_j A_{ij}\dot{\theta}_j = C_i$$

$$A_{ij} = \Re\left(\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}\frac{\partial|\phi(\tau)\rangle}{\partial\theta_j}\right),$$

$$C_i = \Re\left(-\sum_\alpha \lambda_\alpha \frac{\partial\langle\phi(\tau)|}{\partial\theta_i} h_\alpha\,|\phi(\tau)\rangle\right)$$



$$\vec{\theta}(\tau+\delta\tau) \simeq \vec{\theta}(\tau) + \dot{\vec{\theta}}(\tau)\delta\tau = \vec{\theta}(\tau) + A^{-1}(\tau)\cdot C(\tau)\delta\tau.$$

McArdle, Sam, et al. "Variational quantum simulation of imaginary time evolution." *arXiv:1804.03023*(2018).

Fermionic marginals

$$\sum_i^M c_{k,i} \langle O_i \rangle = 0$$

1. RDMs are Hermitian;
2. the 2-RDM is antisymmetric;
3. the $(p-1)$-RDM can be obtained by contracting the p-RDM;
4. the trace of each RDM is fixed by the number of particles in the system e.g. the trace of the 1-RDM is equivalent to the number of particles;
5. RDMs correspond to positive semidefinite density operators.

$$\hat{H} = H + \sum_{k=1}^{K} \beta_k C_k = \sum_{i=1}^{M} \left(h_i + \sum_{k}^{K} \beta_k c_{k,i} \right) O_i$$

$$\langle H \rangle = \langle \hat{H} \rangle$$

$$\min_{\beta} \left(\sum_{i=1}^{M} \left| h_i + \sum_{k}^{K} \beta_k c_{k,i} \right| \right) \quad \text{or} \quad \min_{\beta} \left(\sum_{i=1}^{M} \left| h_i + \sum_{k}^{K} \beta_k c_{k,i} \right| \mathrm{Var}(O_i) \right)$$

Rubin et al. "Application of fermionic marginal constraints to hybrid quantum algorithms." *New Journal of Physics* 20.5 (2018): 053020.

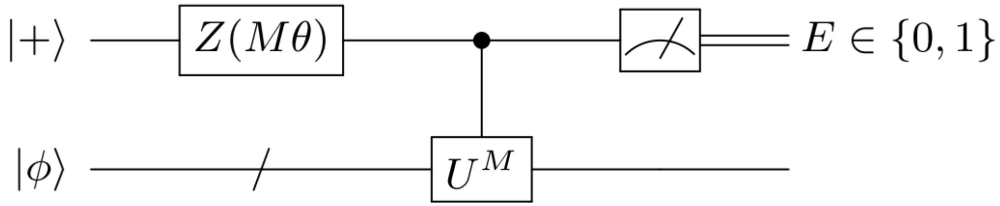
Accelerated VQE

U = $R(c\text{-}\Pi)R^\dagger P R(c\text{-}\Pi)R^\dagger P$

$$R : |0\rangle \mapsto |\psi(\lambda)\rangle$$

$$\Pi := I - 2\,|0\rangle\,\langle 0|$$

$$|\langle\psi|\,P\,|\psi\rangle| = \cos(\pm\phi/2)$$



$$P(E|\phi; M, \theta) = \frac{1 + (-1)^E \cos(M(\phi - \theta))}{2}$$

$$P(\phi|E; M, \theta) \propto P(E|\phi; M, \theta)P(\phi)$$

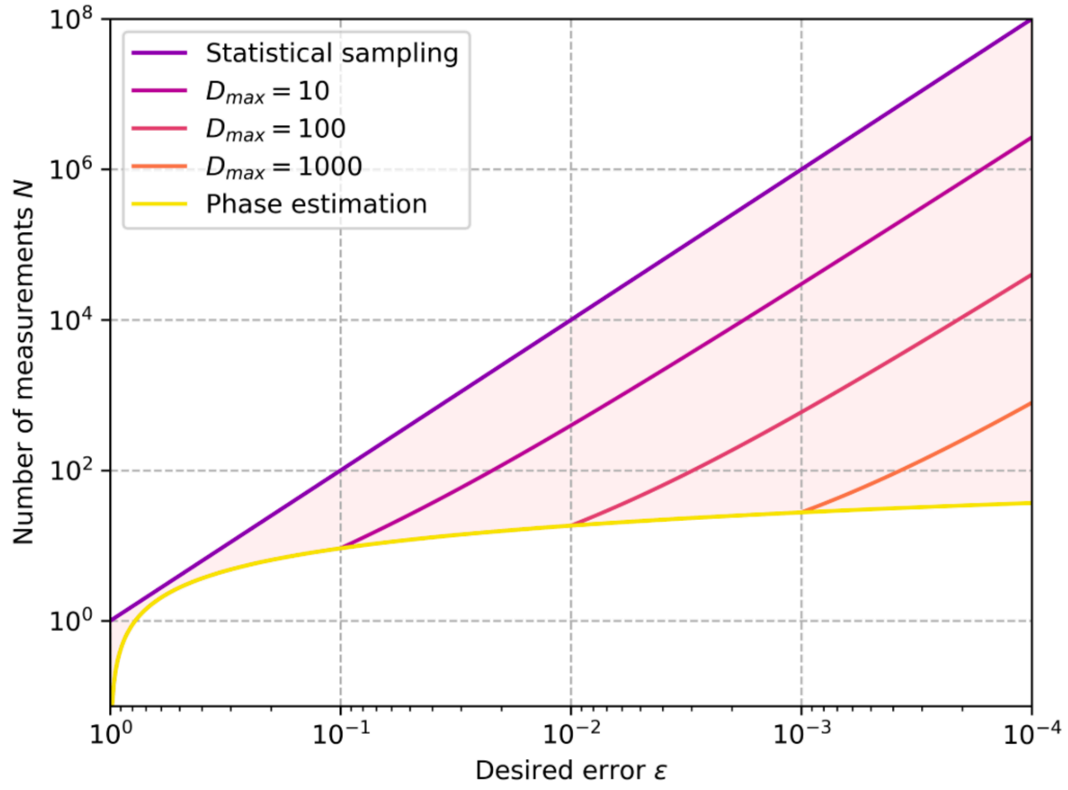
Measure (b_2, b_1)	Probability	Probability of $\|\phi\rangle$
$(0, 0)$	$\cos^2(\phi)\cos^2(\phi/2)$	$1/2$
$(0, 1)$	$\cos^2(\phi)\sin^2(\phi/2)$	$1/2$
$(1, 0)$	$\sin^2(\phi)/2$	$(1 + \sin\phi)/2$
$(1, 1)$	$\sin^2(\phi)/2$	$(1 - \sin\phi)/2$

Wang, Daochen, Oscar Higgott, and Stephen Brierley.
"Accelerated Variational Quantum Eigensolver." *Physical review letters* 122.14 (2019): 140504.

Accelerated VQE

$$f(\epsilon,\alpha)=\begin{cases}\frac{2}{1-\alpha}\left(\frac{1}{\epsilon^{2(1-\alpha)}}-1\right) & \text{if } \alpha\in[0,1)\\ 4\log\left(\frac{1}{\epsilon}\right) & \text{if } \alpha=1\end{cases}$$

Algorithm	Maximum coherent depth	Non-coherent repetitions	Total runtime
VQE	$O(C_R)$	$O(\frac{1}{\epsilon^2})$	$O(C_R\,\frac{1}{\epsilon^2})$
0-VQE	$O(C_R+\log n)$	$O(\frac{1}{\epsilon^2})$	$O((C_R+\log n)\,\frac{1}{\epsilon^2})$
1-VQE	$O((C_R+\log n)\,\frac{1}{\epsilon})$	$O(\log\frac{1}{\epsilon})$	$O((C_R+\log n)\frac{1}{\epsilon})$
α-VQE	$O((C_R+\log n)\,\frac{1}{\epsilon^\alpha})$	$O(f(\epsilon,\alpha))$	$O((C_R+\log n)\,\frac{1}{\epsilon^\alpha}f(\epsilon,\alpha))$

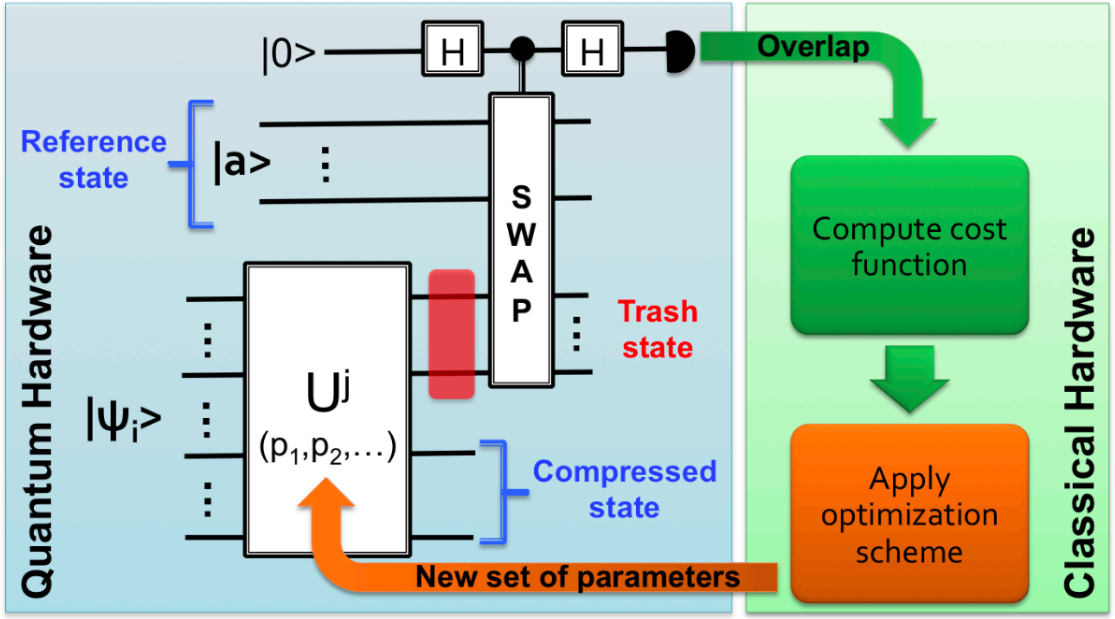


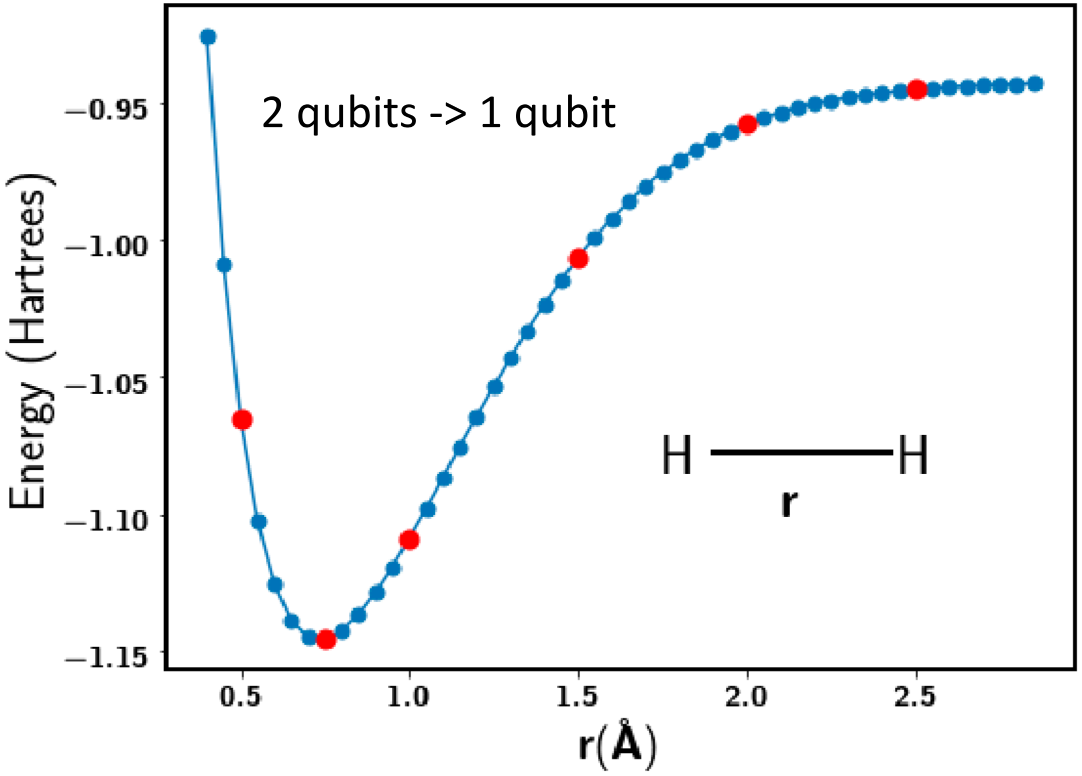
Wang, Daochen, Oscar Higgott, and Stephen Brierley.
"Accelerated Variational Quantum Eigensolver." *Physical review letters* 122.14 (2019): 140504.

Variational quantum machine learning

- Quantum autoencoder
- Quantum generative adversarial networks

Quantum autoencoder



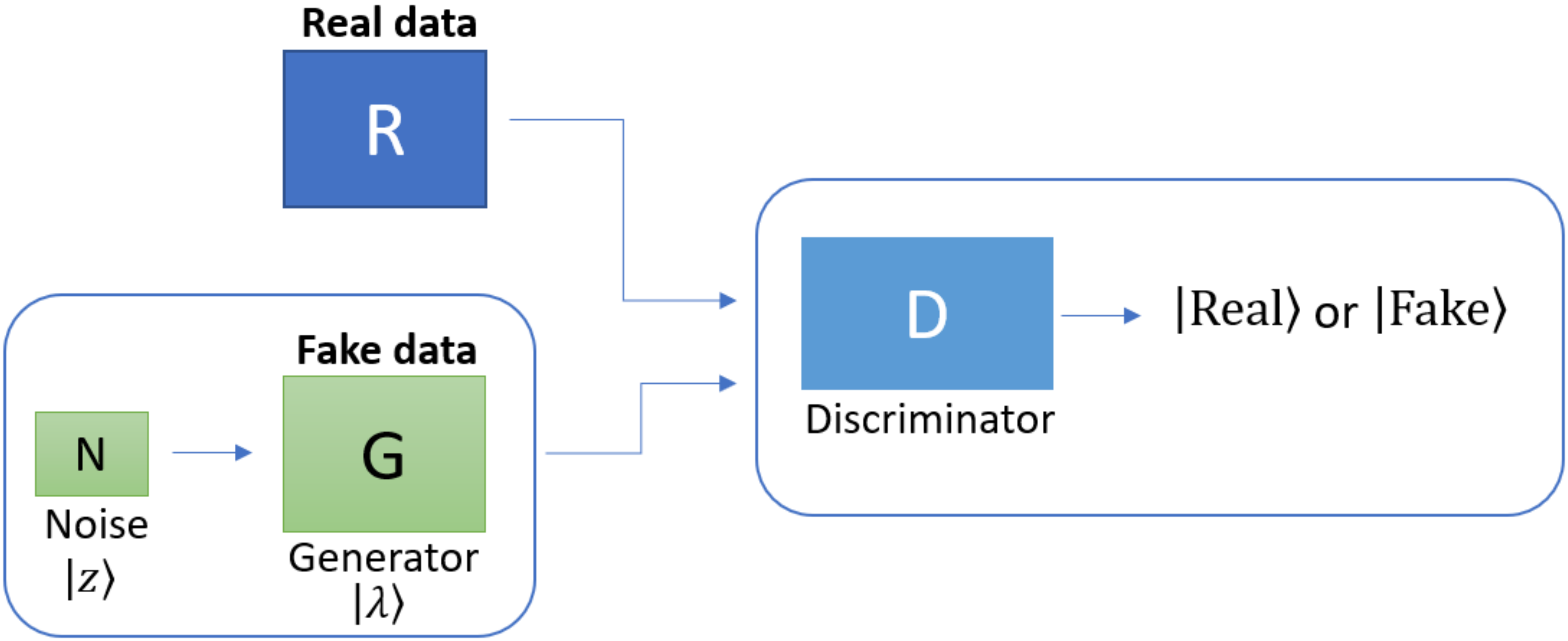


Romero et al. "Quantum autoencoders for efficient compression of quantum data." *Quantum Science and Technology* 2.4 (2017): 045001.

Quantum GANS

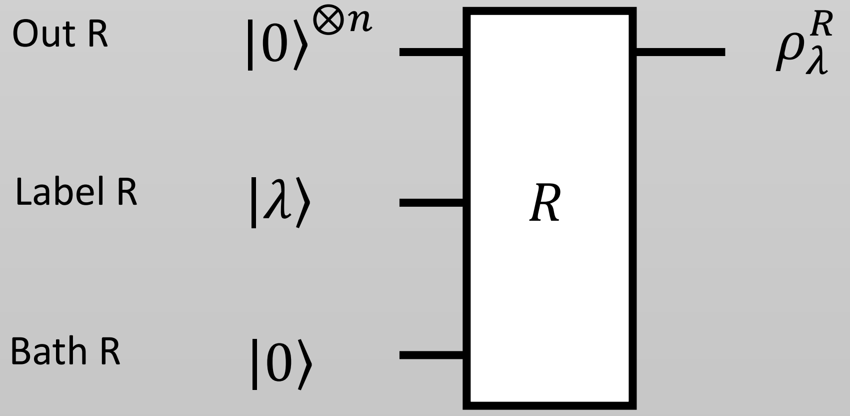
Dallaire-Demers, Pierre-Luc, and Nathan Killoran. "Quantum generative adversarial networks." *Physical Review A* 98.1 (2018): 012324.

Quantum GANs

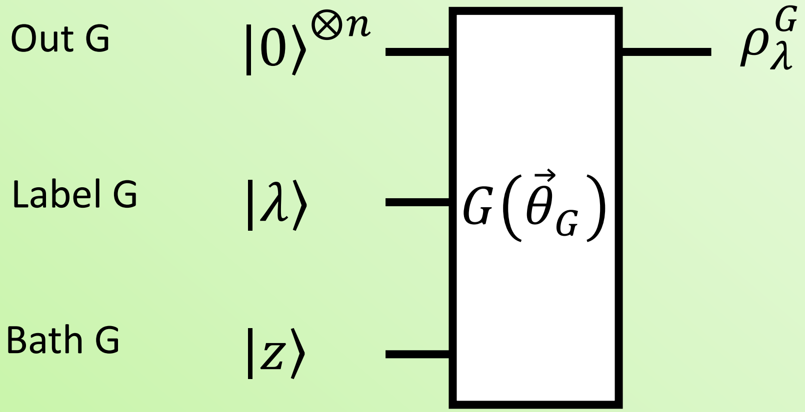


$$\rho = \{(p_1, |\psi_1\rangle); (p_2, |\psi_2\rangle); \ldots ; (p_d, |\psi_d\rangle)\}$$

Quantum sources of data



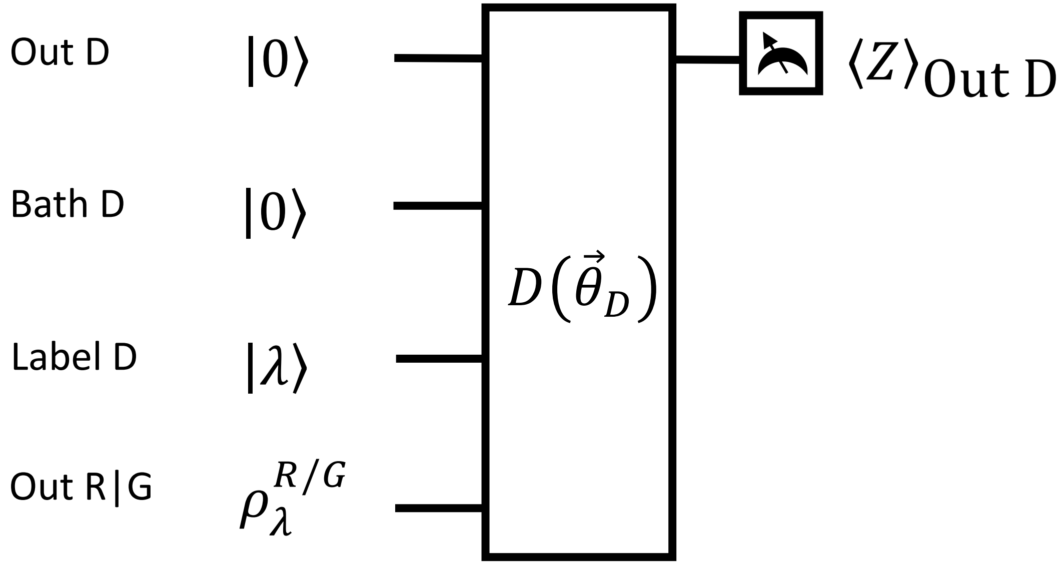
$$R(|\lambda\rangle) = \rho_\lambda^R$$



$$G\left(\vec{\theta}_G, |\lambda, z\rangle\right) = \rho_\lambda^G\left(\vec{\theta}_G, z\right)$$

Quantum discriminator

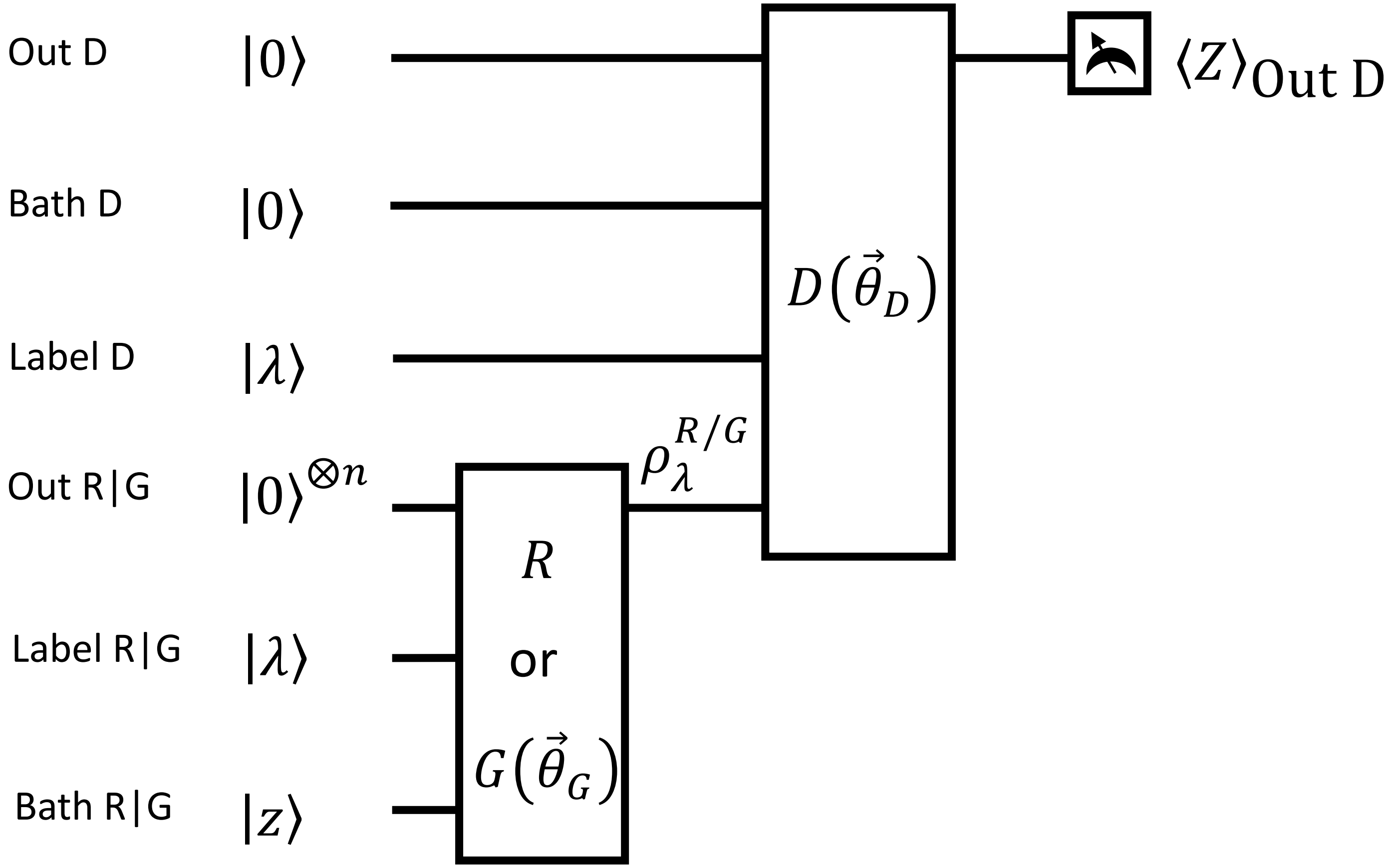
$$Z \equiv |\text{real}\rangle\langle\text{real}| - |\text{fake}\rangle\langle\text{fake}|$$



$$D\left(\vec{\theta}_D, |\lambda\rangle, \rho_\lambda^{R/G}\right)$$

The cost function

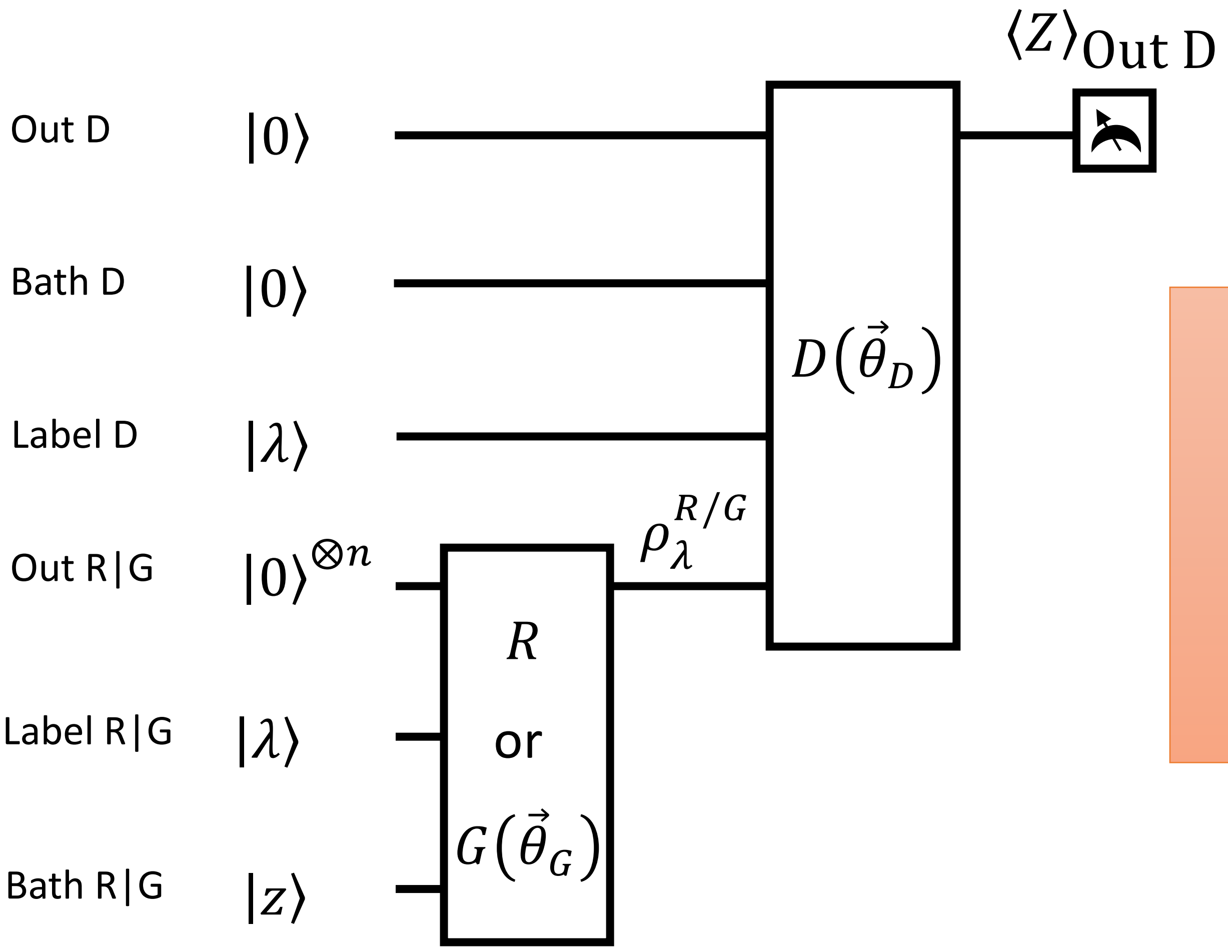
$$\min_{\vec{\theta}_G} \max_{\vec{\theta}_D} V\left(\vec{\theta}_D, \vec{\theta}_G\right)$$

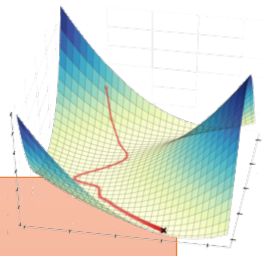


$$V\left(\vec{\theta}_D, \vec{\theta}_G\right) = \frac{1}{\Lambda}\sum_{\lambda=1}^{\Lambda} \Pr\left(\left(D\left(\vec{\theta}_D, |\lambda\rangle, R(|\lambda\rangle)\right) = |\text{real}\rangle\right) \cap \left(D\left(\vec{\theta}_D, |\lambda\rangle, G(\vec{\theta}_G, |\lambda, z\rangle)\right) = |\text{fake}\rangle\right)\right)$$

Can we formulate this in the language of quantum mechanics?

The quantum cost function





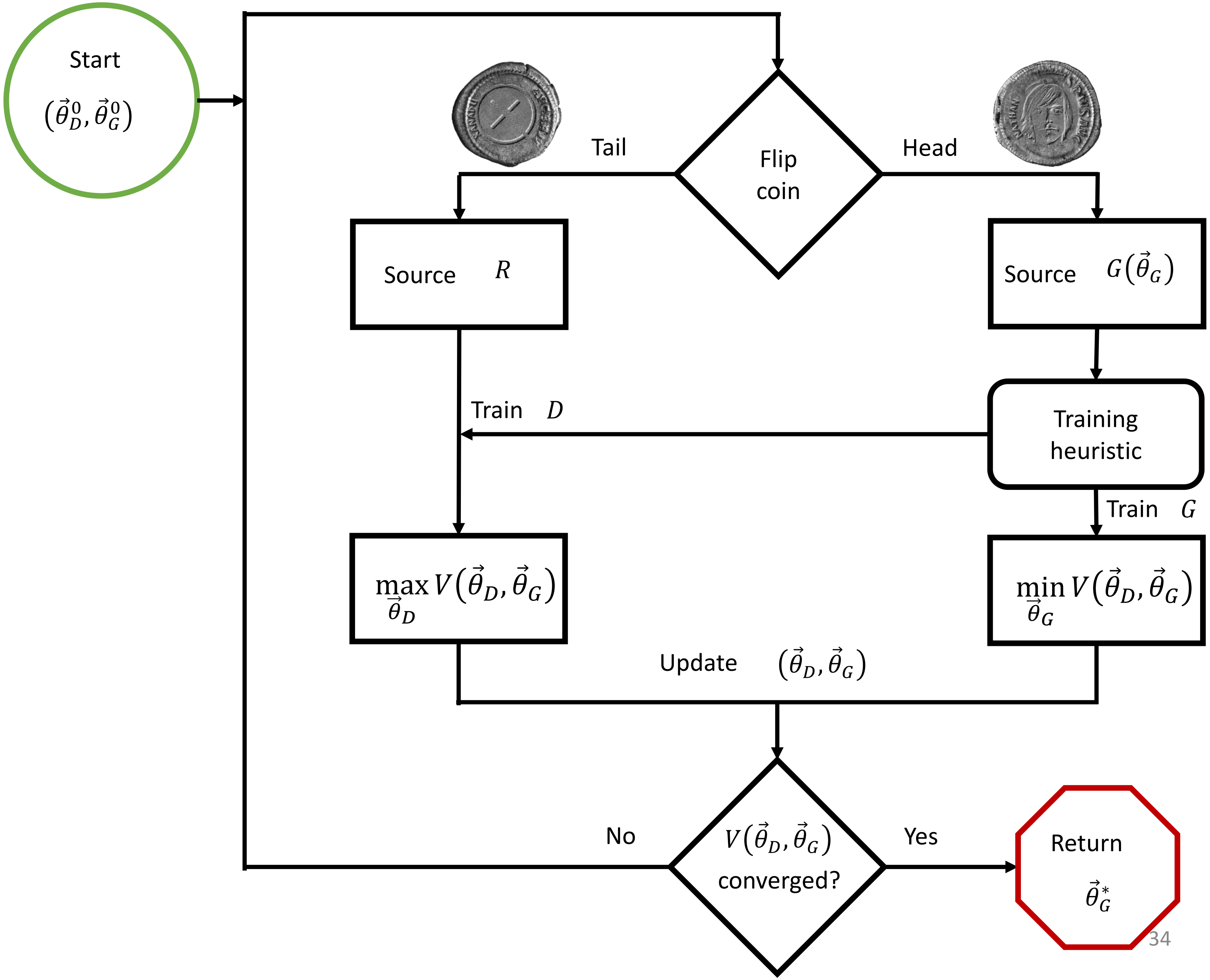
Gradient update rules:

$$\vec{\theta}_D^{k+1} = \vec{\theta}_D^k + \chi_D^k \nabla_{\vec{\theta}_D} V\left(\vec{\theta}_D^k, \vec{\theta}_G^k\right)$$

$$\vec{\theta}_G^{k+1} = \vec{\theta}_G^k - \chi_G^k \nabla_{\vec{\theta}_G} V\left(\vec{\theta}_D^k, \vec{\theta}_G^k\right)$$

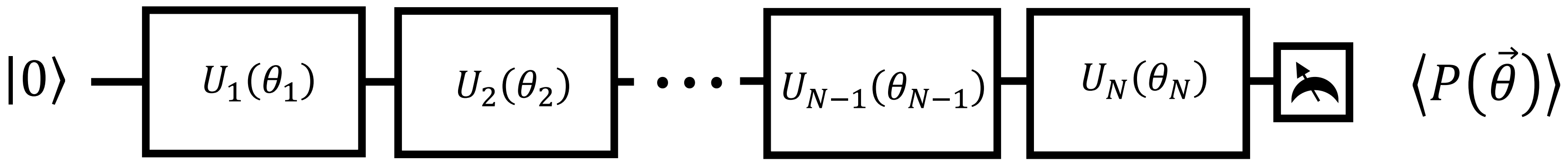
$$V\left(\vec{\theta}_D, \vec{\theta}_G\right) = \frac{1}{2} + \frac{1}{4\Lambda}\sum_{\lambda=1}^{\Lambda} \mathrm{tr}\left(\left(\rho_\lambda^{DR}\left(\vec{\theta}_D\right) - \rho_\lambda^{DG}\left(\vec{\theta}_D, \vec{\theta}_G, z\right)\right) Z\right)$$

Training

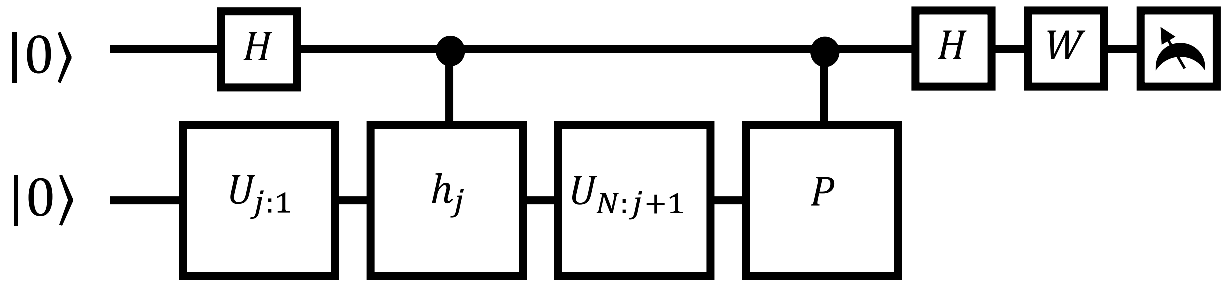

Start
$(\vec{\theta}_D^0, \vec{\theta}_G^0)$
Tail
Flip coin
Head
Source R
Source $G(\vec{\theta}_G)$
Train D
Training heuristic
Train G
$\max_{\vec{\theta}_D} V(\vec{\theta}_D, \vec{\theta}_G)$
$\min_{\vec{\theta}_G} V(\vec{\theta}_D, \vec{\theta}_G)$
Update $(\vec{\theta}_D, \vec{\theta}_G)$
No
$V(\vec{\theta}_D, \vec{\theta}_G)$ converged?
Yes
Return $\vec{\theta}_G^*$

A quantum circuit for gradients

$$\langle P(\vec{\theta})\rangle = \mathrm{tr}\left(\rho_0 U^\dagger(\vec{\theta}) P U(\vec{\theta})\right)$$



$$\frac{\partial}{\partial\theta_j}\langle P(\vec{\theta})\rangle = -\frac{i}{2}\mathrm{tr}\left(\rho_0 U^\dagger_{1:j}\left[U^\dagger_{j+1:N} P U_{N:j+1}, h_j\right] U_{j:1}\right)$$



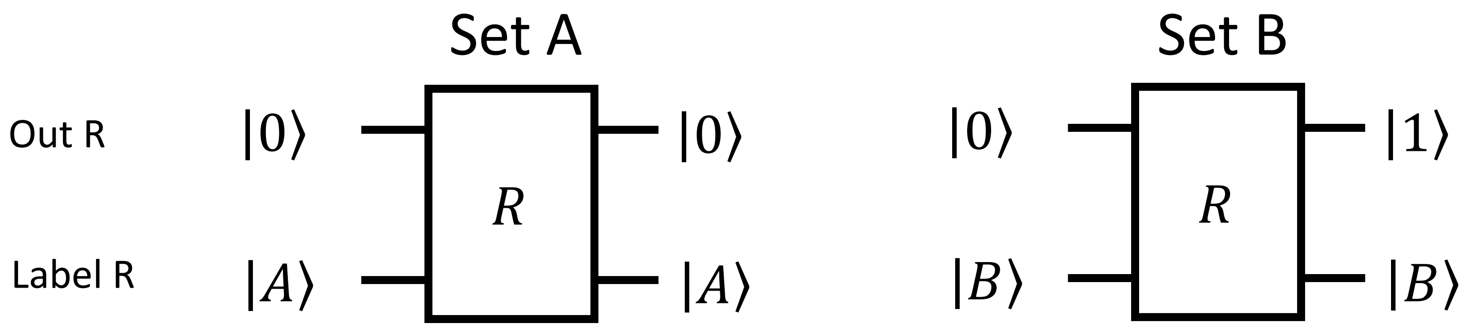
$$\langle Z\rangle_{\mathrm{Grad}} = \frac{\partial}{\partial\theta_j}\langle P(\vec{\theta})\rangle$$

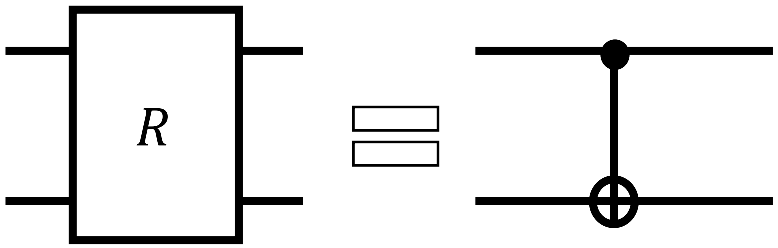
$$\langle Z\rangle_{\mathrm{Grad}} = \Pr\left(|x_{\mathrm{Grad}}\rangle = |0\rangle\right) - \Pr\left(|x_{\mathrm{Grad}}\rangle = |1\rangle\right)$$

Self-adjoint & unitary

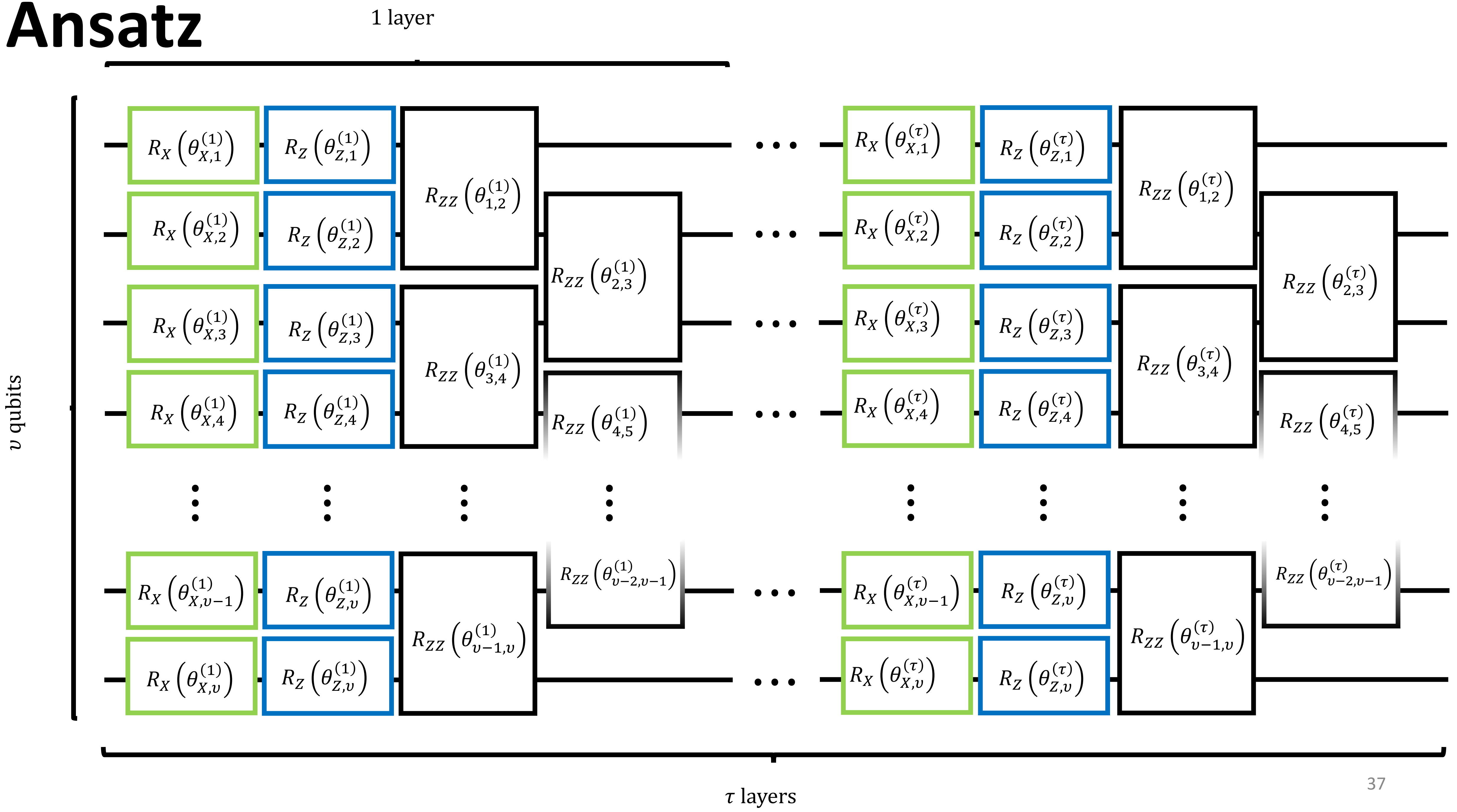
$$h_j = h_j^\dagger = h_j^{-1}$$

Simplest example

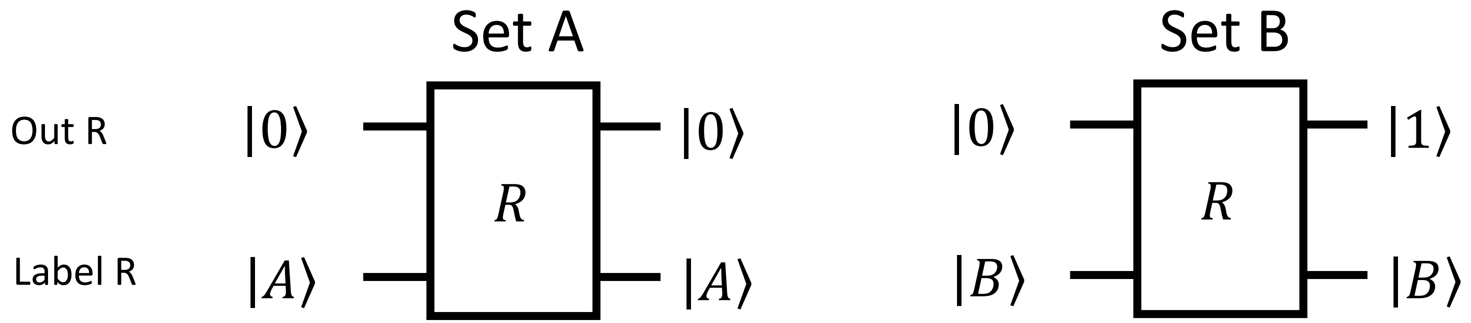


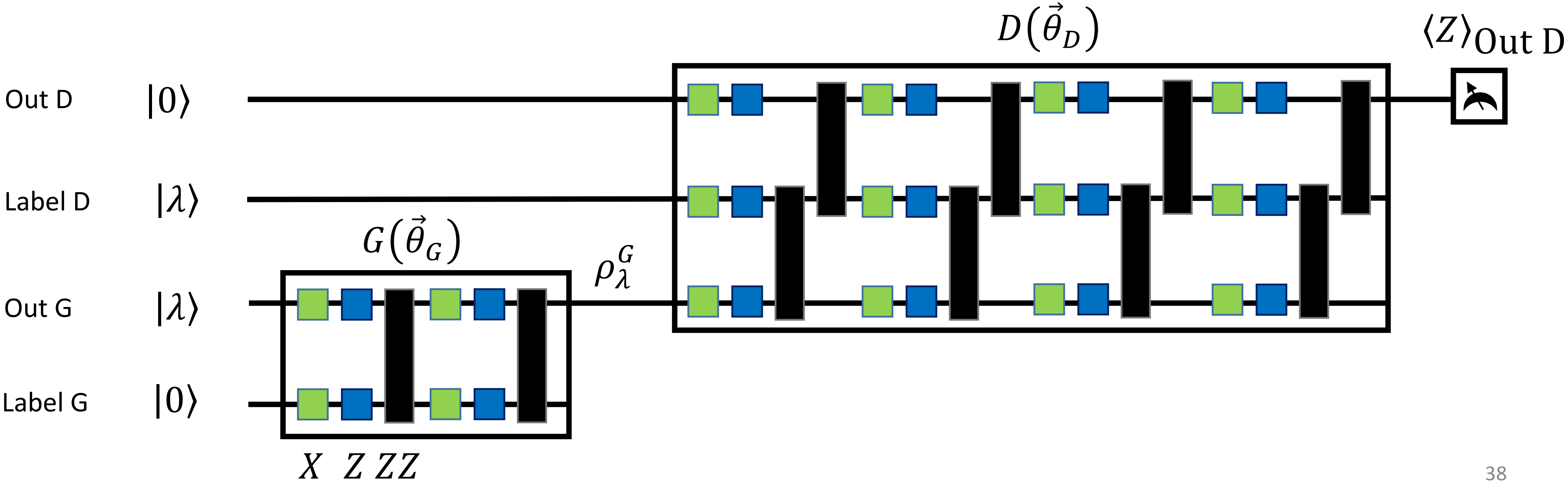


Ansatz


1 layer
$R_X\left(\theta_{X,1}^{(1)}\right)$
$R_Z\left(\theta_{Z,1}^{(1)}\right)$
$R_{ZZ}\left(\theta_{1,2}^{(1)}\right)$
$R_X\left(\theta_{X,2}^{(1)}\right)$
$R_Z\left(\theta_{Z,2}^{(1)}\right)$
$R_{ZZ}\left(\theta_{2,3}^{(1)}\right)$
$R_X\left(\theta_{X,3}^{(1)}\right)$
$R_Z\left(\theta_{Z,3}^{(1)}\right)$
$R_{ZZ}\left(\theta_{3,4}^{(1)}\right)$
$R_X\left(\theta_{X,4}^{(1)}\right)$
$R_Z\left(\theta_{Z,4}^{(1)}\right)$
$R_{ZZ}\left(\theta_{4,5}^{(1)}\right)$
$R_X\left(\theta_{X,\upsilon-1}^{(1)}\right)$
$R_Z\left(\theta_{Z,\upsilon}^{(1)}\right)$
$R_{ZZ}\left(\theta_{\upsilon-2,\upsilon-1}^{(1)}\right)$
$R_{ZZ}\left(\theta_{\upsilon-1,\upsilon}^{(1)}\right)$
$R_X\left(\theta_{X,\upsilon}^{(1)}\right)$
$R_Z\left(\theta_{Z,\upsilon}^{(1)}\right)$
$R_X\left(\theta_{X,1}^{(\tau)}\right)$
$R_Z\left(\theta_{Z,1}^{(\tau)}\right)$
$R_{ZZ}\left(\theta_{1,2}^{(\tau)}\right)$
$R_X\left(\theta_{X,2}^{(\tau)}\right)$
$R_Z\left(\theta_{Z,2}^{(\tau)}\right)$
$R_{ZZ}\left(\theta_{2,3}^{(\tau)}\right)$
$R_X\left(\theta_{X,3}^{(\tau)}\right)$
$R_Z\left(\theta_{Z,3}^{(\tau)}\right)$
$R_{ZZ}\left(\theta_{3,4}^{(\tau)}\right)$
$R_X\left(\theta_{X,4}^{(\tau)}\right)$
$R_Z\left(\theta_{Z,4}^{(\tau)}\right)$
$R_{ZZ}\left(\theta_{4,5}^{(\tau)}\right)$
$R_X\left(\theta_{X,\upsilon-1}^{(\tau)}\right)$
$R_Z\left(\theta_{Z,\upsilon}^{(\tau)}\right)$
$R_{ZZ}\left(\theta_{\upsilon-2,\upsilon-1}^{(\tau)}\right)$
$R_{ZZ}\left(\theta_{\upsilon-1,\upsilon}^{(\tau)}\right)$
$R_X\left(\theta_{X,\upsilon}^{(\tau)}\right)$
$R_Z\left(\theta_{Z,\upsilon}^{(\tau)}\right)$
υ qubits
τ layers

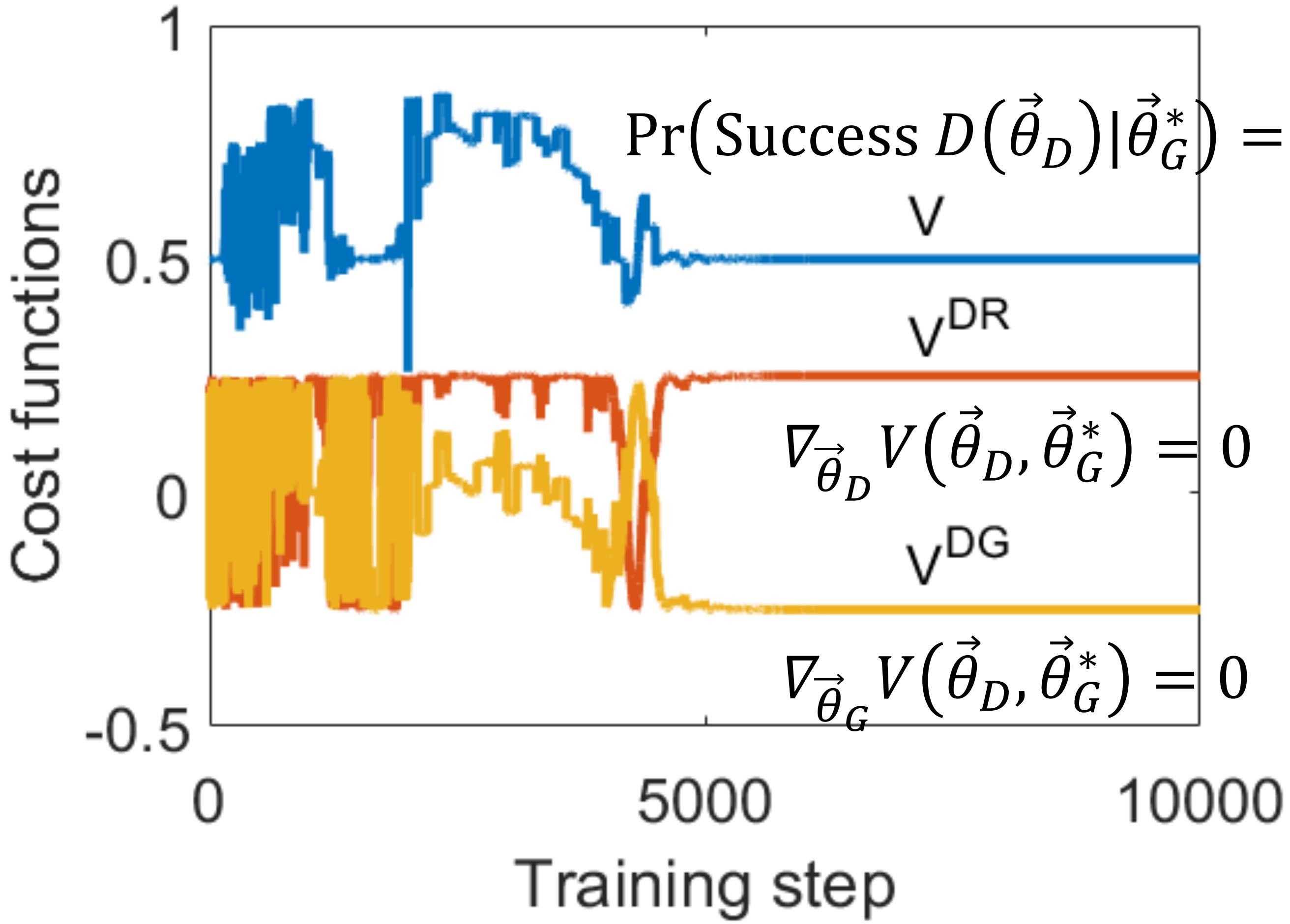
Solving the simple example





Numerical training

$$V^{DR}(\vec{\theta}_D) = \frac{1}{4\Lambda}\sum_{\lambda=1}^{\Lambda} \mathrm{tr}\left(\rho_\lambda^{DR}(\vec{\theta}_D)Z\right)$$



$$\Pr\left(\text{Success } D(\vec{\theta}_D)|\vec{\theta}_G^*\right) = \frac{1}{2}$$

$$\nabla_{\vec{\theta}_D} V(\vec{\theta}_D, \vec{\theta}_G^*) = 0$$

$$\nabla_{\vec{\theta}_G} V(\vec{\theta}_D, \vec{\theta}_G^*) = 0$$

$$V^{DG}(\vec{\theta}_D, \vec{\theta}_G) = -\frac{1}{4\Lambda}\sum_{\lambda=1}^{\Lambda} \mathrm{tr}\left(\rho_\lambda^{DG}(\vec{\theta}_D, \vec{\theta}_G, z)Z\right)$$

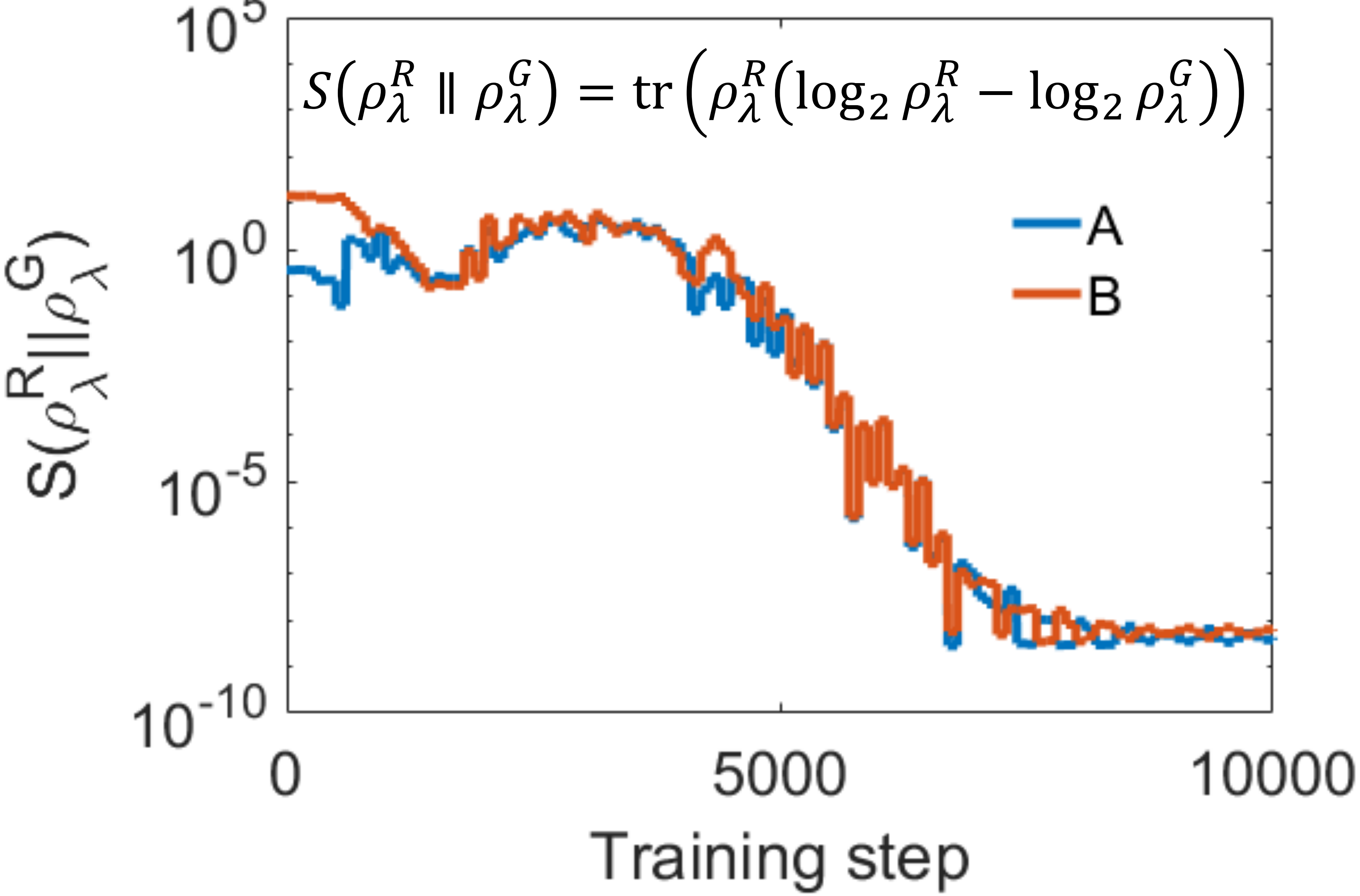
$$V(\vec{\theta}_D, \vec{\theta}_G) = \frac{1}{2} + V^{DR}(\vec{\theta}_D) + V^{DG}(\vec{\theta}_D, \vec{\theta}_G)$$

Performance analysis

$$\frac{1}{2}C(\vec{\theta}_G) \le \Pr\left(\text{Success } D(\vec{\theta}_D)|\vec{\theta}_G\right) \le 1 - \ldots$$

$$r_{\min} \le C(\vec{\theta}_G) \equiv \mathrm{tr}\left(\rho^R \rho^G(\vec{\theta}_G)\right) \le \mathrm{tr}((\rho \ldots$$

Quantum cross-entropy



Thank you!

Extra references

Kivlichan, Ian D., et al. "Quantum simulation of electronic structure with linear depth and connectivity." *Physical review letters* 120.11 (2018): 110501.

Temme, Kristan, Sergey Bravyi, and Jay M. Gambetta. "Error mitigation for short-depth quantum circuits." *Physical review letters* 119.18 (2017): 180509.

Santagati, Raffaele, et al. "Witnessing eigenstates for quantum simulation of Hamiltonian spectra." *Science advances* 4.1 (2018): eaap9646.

Lee, Joonho, et al. "Generalized Unitary Coupled Cluster Wave functions for Quantum Computation." *Journal of chemical theory and computation* 15.1 (2018): 311-324.

Motta, Mario, et al. "Low rank representations for quantum simulation of electronic structure." *arXiv:1808.02625* (2018).

Yung, Man-Hong, and Alán Aspuru-Guzik. "A quantum–quantum Metropolis algorithm." *Proceedings of the National Academy of Sciences* 109.3 (2012): 754-759.

Aspuru-Guzik, Alán, et al. "Simulated quantum computation of molecular energies." *Science* 309.5741 (2005): 1704-1707.