## TRAINING AND TESTING: A QUANTUM-INFO PERSPECTIVE

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## QML @ FLORENCE

- Quantum Machine Learning in Florence
- Interest in Classical and Quantum data
- Foundational aspects: Generalisation
- Main focus: NISQ devices
- Quantum-Enhanced Classifiers (CQ)
- M Schuld, N Killoran, Phys. rev. lett. 122 (4), 040504, (2019),
- L Banchi, et al., Phys. Rev. Applied 14, 064026 (2020),

V Havlicek, et al, Nature 567 (7747), 209, (2019)
S Lloyd, et al, arXiv:2001.03622


Main question: after training a quantum model using a few known examples, can the model accurately classify even unseen data?

- Study generalisation using tools from quantum information theory
- Study how the Hilbert space dimension, noise, pooling etc. affect generalisation
- Bias-Variance tradeoff and Information Bottleneck principle


## QUANTUM EMBEDDINGS

(a) Data distribution

- Classify classical data (e.g. images)
- Embed images $x$ onto a quantum state $x \mapsto \rho(x)$
- Decide the class from a quantum measurement $\left\{\Pi_{c}\right\}$


> class/label $c=$ "cat"
(b) Quantum classifier

(c) Dilated measurements

optimization of POVM $\Pi_{c}$ $=$
optimization of unitary $U_{\mathcal{M}}$

## MANY-BODY PHYSICS (QQ/QC)

- Quantum Phase Recognition
- I Cong, S Choi, MD Lukin, Nature Physics 15, 1273 (2019)
- L Banchi, J Pereira, S Pirandola, PRX Quantum 2, 040321 (2021)
- Many-Body Entanglement Measurement from PPT-moments $\operatorname{Tr}\left[\left(\rho_{A B}^{T_{B}}\right)^{n}\right]$
- J Gray, L Banchi, A Bayat, S Bose, Phys. Rev. Lett. 121, 150503 (2018)

(b)



## QUANTUM CHANNEL DISCRIMINATION

detect objects $x$ from the scattered state of light $\rho(x)$


- Images live in the physical world
- Optimise over the (entangled) input probe state of light and over the detection POVM


## QUANTUM BARCODES AND PATTERN RECOGNITION

- Barcode classification must identify each pixel correctly
- Handwriting classification is easier as errors are tolerated!

$$
\mathrm{error} \simeq F\left(\rho_{\text {black }}, \rho_{\text {white }}\right)^{\text {Hamming }_{4 \leftrightarrow 9}}
$$

- L. Banchi, Q. Zhuang, S. Pirandola, Phys. Rev. Applied 14, 064026 (2020)
- C Harney, L Banchi, S Pirandola,

Phys. Rev. A 103, 052406 (2021)

- JL Pereira, L Banchi, Q Zhuang, S Pirandola, Phys. Rev. A 103, 042614 (2021)




## QUANTUM GANS FOR NOISE

 SENSING- SuperQGANs: Quantum Generative Adversarial Networks for learning Superoperators

P Braccia, L Banchi, F Caruso,
Phys. Rev. Applied 17, 024002 (2022)

- Favourable Scaling




## HOW DO WE OPTIMISE? GRADIENTS!

- Parameter Shift Rule / Hadamard test for $e^{i \theta \hat{o}}$ gates

$$
\nabla_{\theta} f=f\left(\theta_{1}\right)-f\left(\theta_{2}\right)
$$

- K Mitarai, M Negoro, M Kitagawa, K Fujii - Physical Review A, 2018
- M Schuld, V Bergholm, C Gogolin, J Izaac, N Killoran - Physical Review A, 2019

- Stochastic PSR for general Hamiltonian evolution $e^{i(\hat{H}+\theta \hat{V})}$
- L Banchi, G Crooks, Quantum 5, 386 (2021)
- Continuous variable systems / GBS distribution
- N Killoran, et al. Phys. Rev. Research (2019)
- L Banchi, N Quesada, J M Arrazola, Phys. Rev. A 102, 012417 (2020)


$$
\text { Gradient: } \nabla_{0}\langle\hat{A}\rangle=\mathbb{E}_{\text {smanas }}\left[\begin{array}{r}
1 \cdot\rangle\rangle-\langle\langle\cdot\rangle]]
\end{array}\right.
$$

## MORE GRADIENTS!

- Gradient-based optimisation of "Quantum Programs"

$$
\rho_{\text {output }}=\mathscr{E}\left[\rho_{\text {input }} \otimes \theta\right]
$$

- L Banchi, J Pereira, S Lloyd, S Pirandola, npj Quantum Information 6 (1), 1-10, (2020)
- "Optimism" for training QGANS without limit cycles
- P Braccia, F Caruso, L Banchi, New J. Phys. 23053024 (2021)

$$
\begin{aligned}
& \boldsymbol{\theta}_{D}^{t+1}=\boldsymbol{\theta}_{D}^{t}+2 \eta_{D} \nabla_{\boldsymbol{\theta}_{D}} S\left(\boldsymbol{\theta}_{t}^{D}, \boldsymbol{\theta}_{t}^{G}\right)-\eta_{D} \nabla_{\boldsymbol{\theta}_{D}} S\left(\boldsymbol{\theta}_{t-1}^{D}, \boldsymbol{\theta}_{t-1}^{G}\right) \\
& \boldsymbol{\theta}_{G}^{t+1}=\boldsymbol{\theta}_{G}^{t}-2 \eta_{G} \nabla_{\boldsymbol{\theta}_{G}} S\left(\boldsymbol{\theta}_{t+1}^{D}, \boldsymbol{\theta}_{t}^{G}\right)+\eta_{G} \nabla_{\boldsymbol{\theta}_{G}} S\left(\boldsymbol{\theta}_{t}^{D}, \boldsymbol{\theta}_{t-1}^{G}\right)
\end{aligned}
$$

## Quantum

## FOUNDATIONAL QUESTION: WHAT CAN WE EXPECT?

- We have a training set $\mathscr{T}$ made of $T$ correctly classified images
- We can empirically check generalisation using a testing set $\mathscr{T}^{\prime}$ with $T^{\prime}$ correctly classified images
- We choose a "good" quantum embedding $x \mapsto \rho(x)$ and optimal discrimination via POVM $\left\{\Pi_{c}\right\}$
- What training error / testing error can we expect?

| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 |
| 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |
| 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 |



## "COMPLEXITY" OF QUANTUM EMBEDDINGS



Embedding complexity

## QUANTUM BIAS-VARIANCE TRADEOFF

- Bound for the generalisation error

$$
G_{\mathscr{T}} \leq 2 \sqrt{\frac{\mathscr{B}}{T}}+\sqrt{\frac{2 \log (1 / \delta)}{T}}
$$

- Bound for the approximation error

$$
\mathscr{A}=\sum_{x} \frac{|P(x \mid 0)-P(x \mid 1)|}{2}-\frac{\left\|\rho_{0}-\rho_{1}\right\|_{1}}{2}
$$

$$
\text { where } \rho_{c}=\sum P(x \mid c) \rho(x)
$$



Embedding complexity

$$
\begin{gathered}
\mathscr{B}=2^{I_{2}(X: Q)} \quad \mathscr{A} \leq K-\frac{2^{I(C: Q)}}{N_{C}} \\
\rho_{C X Q}=\sum_{c x} P(c, x)|c x\rangle\langle c x| \otimes \rho(x) .
\end{gathered}
$$

Good embeddings should maximise $I(C: Q)$ and minimise $I_{2}(X: Q)$

## Spoiler: Information Bottleneck!

Two extreme cases:
(
Embedding complexity

- Basis encoding: $x \mapsto \rho(x)=|x\rangle\langle x|$ minimum $\mathscr{A}(\rho)=0$, maximum $\mathscr{G}_{\mathscr{T}}(\rho)$
- Constant embedding : $x \mapsto \rho$ maximum $\mathscr{A}(\rho)$, minimum $\mathscr{G}_{\mathscr{T}}(\rho)=0$

$$
\begin{aligned}
& \mathscr{B}=2^{I_{2}(X: Q)} \\
& \mathscr{A} \leq K-\frac{2^{I(C: Q)}}{N_{C}}
\end{aligned}
$$

for MNIST with 8-bit colours

$$
28 \times 28 \times 8 \approx 6000 \text { qubits! }
$$

Bigger Hilbert spaces have lower approximation error, but larger generalisation error

In the numerical example we consider

$$
\begin{aligned}
x & \mapsto|\psi(x)\rangle\left\langle\left.\psi(x)\right|^{\otimes N}\right. \\
|\psi(x)\rangle & =\cos (x)|0\rangle+\sin (x)|1\rangle
\end{aligned}
$$

For large N

$$
\begin{aligned}
\mathscr{A}(\rho) & \leq K F_{\max }^{N} \\
\mathscr{B} & \approx \mathscr{O}(N)
\end{aligned}
$$

where $F_{\max }=\max _{x \neq y} F(\rho(x), \rho(y))$

Proof from $\rho_{C X Q}=\sum P(c, x)|c x\rangle\langle c x| \otimes \rho(x)^{\otimes N}$
(a)



## QUANTUM KERNELS

For pure state embeddings $\rho(x)=|\psi(x)\rangle\langle\psi(x)|$ we find

$$
\mathscr{B}=[\operatorname{Tr} \sqrt{K}]^{2}
$$

where $K_{x y}=\sqrt{p(x) p(y)}|\langle\psi(x) \mid \psi(y)\rangle|$ is a (normalised) kernel matrix. This makes the calculation $\mathscr{B}$ easier for large-dimensional embeddings.

Quantum kernels are used in

- Quantum support vector machines
- Quantum enhanced-feature space

Take home message: avoid $K \propto$ identity (bad generalisation)


To favour generalisation the final Hilbert space must be small, but the initial one can be big!

We may iteratively discard information via pooling layers (e.g. QCNN)

Pooling favours generalisation but harms the accuracy (via data processing)

Take home message: if low training error is achievable with pooling layers, then generalisation can only be better!

image from:
I Cong, et al. Nature Physics (2019)

## INFORMATION BOTTLENECK FOR QUANTUM CLASSIFIERS

$\rho(x)$ as "bottleneck" that squeezes the relevant information that $x$ provides about $c$

IB principle (loss independent): minimise

$$
\mathscr{L}_{I B}=I(X: Q)-\beta I(C: Q)
$$

Self-consistent solutions (similar for $\rho$ )

$$
\tilde{\lambda}_{z}|\psi(z)\rangle=e^{(1-\beta) \log \bar{\rho}+\beta \sum_{c} P(c \mid z) \log \rho_{c}}|\psi(z)\rangle
$$


$\beta=1.5$
(b)

$\beta=2.8$

(c)

## APPLICATIONS

## QUANTUM PHASE RECOGNITION (QQ)

Task: recognize the phases of matter of a quantum many-body system by taking measurements on the quantum system itself

$$
H=-\sum_{i=1}^{L}\left(\sigma_{i}^{x} \sigma_{i+1}^{x}+h \sigma_{i}^{z}\right), \quad \Longrightarrow \quad \mathscr{B} \simeq 5.9
$$




## VARIATIONAL QUANTUM INFORMATION BOTTLENECK (CQ)



$$
\left|\psi_{w}(x)\right\rangle=\prod_{\ell=1}^{L}\left[R^{z}\left(w^{z \ell} \cdot x+w_{0}^{z \ell}\right) R^{v}\left(w^{v \ell} \cdot x+w_{0}^{\nu \ell}\right)\right]|0\rangle,
$$

For two-qubit states the "re-upoading" embedding
can be trained with an efficient variational
For two-qubit states the "re-upoading" embedding
can be trained with an efficient variational minimisation of the IB Lagrangian
(a)
※ั
"Data Re-uploading" Classifier
Single-qubit

(b)


Testing error 4.5\%
Testing error $3.5 \%$

## SUMMARY



## CONCLUSIONS

- Quantum and Classical Algorithms to process either classical data (e.g. images) or quantum information encoded in quantum states
- Different applications:
- quantum pattern recognition with entanglement-enhanced quantum sensor
- Classification of quantum states and phases of matter
- Quantum embeddings of classical data
- Foundational aspects: generalisation \& sample complexity, information theoretic tools


## EXTRA SLIDES

- Empirical loss / training error

$$
R_{\mathscr{T}}(\Pi, \rho)=\frac{1}{T} \sum_{\left(c_{k}, x_{k}\right) \in \mathscr{T}} \sum_{c \neq c_{k}} \operatorname{Tr}\left[\Pi_{c} \rho\left(x_{k}\right)\right]=1-\frac{1}{T} \sum_{\left(c_{k} x_{k}\right) \in \mathscr{T}} \operatorname{Tr}\left[\Pi_{c_{k}} \rho\left(x_{k}\right)\right]
$$

- Abstract classification error

$$
R(\Pi, \rho)=\mathbb{E}_{(c, x) \sim P(c, x)}\left(\sum_{c \neq \tilde{c}} \operatorname{Tr}\left[\Pi_{\tilde{c}} \rho(x)\right]\right)=1-\mathbb{E}_{(c, x) \sim P(c, x)} \operatorname{Tr}\left[\Pi_{c} \rho(x)\right]
$$

- Optimal empirical measurement $\Pi^{\mathscr{T}}=\operatorname{argmin}_{\Pi} R_{\mathscr{T}}(\Pi, \rho)$
- Real optimal $\Pi^{*}=\operatorname{argmin}_{\Pi} R(\Pi, \rho)$
- Testing error

$$
R_{\mathscr{T}}\left(\Pi_{\mathscr{T}}, \rho\right)
$$



