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),



Main question: after training a quantum model using a few known examples, can the model accurately classify even unseen data? L Banchi, J Pereira, S Pirandola

- 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**

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



PRX Quantum 2, 040321 (2021)



- Classify classical data (e.g. images)
- Embed images x onto a quantum state $x \mapsto \rho(x)$
- Decide the class from a quantum measurement $\{\Pi_{c}\}$
- M Schuld, N Killoran, Phys. rev. lett. 122 (4), 040504, (2019)
- V Havlicek, et al, Nature 567 (7747), 209, (2019)
- S Lloyd, et al, arXiv:2001.03622

QUANTUM EMBEDDINGS

(a) Data distribution





class/label c = "cat"



embedding circuit $x \mapsto \rho(x)$ decision via POVM Π_c

(c) Dilated measurements



optimization of POVM Π_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 Tr $\left[(\rho_{AB}^{T_B})^n\right]$

• J Gray, L Banchi, A Bayat, S Bose, Phys. Rev. Lett. 121, 150503 (2018)







QUANTUM CHANNEL DISCRIMINATION

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

- Images live in the physical world
- Optimise over the (entangled) input POVM

 \mathcal{X} $\rho(x)$ obstacle c = yes/no

• Optimise over the (entangled) input probe state of light and over the detection



QUANTUM BARCODES AND PATTERN RECOGNITION

a)

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

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

- 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)











OUAN^c SENS

Superoperators





-grad D ·grad G

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

5

• Favourable Scaling



FOR NOISE



HOW DO WE OPTIMISE? GRADIENTS!

- Parameter Shift Rule / Hadamard test for $e^{i\theta\hat{\sigma}}$ gates
- 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 distribu
- N Killoran, et al. Phys. Rev. Research (2019)
- L Banchi, N Quesada, J M Arrazola, Phys. Rev. A 102, 012417 (20

$$\Delta t = t(\theta) - t(\theta)$$

H.	
~2	

Ition

$$\begin{aligned}
\left| \frac{4}{6} \right\rangle - \left[\frac{i(1-s)(\hat{H}+\theta\hat{V})}{e^{i(1-s)(\hat{H}+\theta\hat{V})}} - \left[\frac{i}{e^{i(1-s)(\hat{H}+\theta\hat{V})}} - \left[\frac{i}{e^{i(1-s)(\hat{H}+\theta\hat{V})} - \left[\frac$$



MORE GRADIENTS!

- Gradient-based optimisation of "Quantum Programs" $\rho_{\text{output}} = \mathscr{E}[\rho_{\text{input}} \otimes \theta]$
- 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. 23 053024 (2021)

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







FOUNDATIONAL QUESTION: WHAT CAN WE EXPECT?

- We have a training set \mathcal{T} made of T correctly classified images
- We can empirically check generalisation using a testing set \mathcal{T}' with T' correctly classified images
- We choose a "good" quantum embedding $x \mapsto \rho(x)$ and optimal discrimination via POVM $\{\Pi_c\}$
- What training error / testing error can we expect?









"COMPLEXITY" OF QUANTUM EMBEDDINGS



Embedding complexity

 $\mathcal{G}_{\mathcal{T}}(\rho)$ $R(\Pi^*, \rho)$

L Banchi, J Pereira, S Pirandola PRX Quantum 2, 040321 (2021)

QUANTUM BIAS-VARIANCE TRADEOFF

Bound for the generalisation error

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

• Bound for the approximation error

X

$$\mathscr{A} = \sum_{x} \frac{|P(x|0) - P(x|1)|}{2} - \frac{\|\rho_0 - \rho_1\|_1}{2}$$

where $\rho_c = \sum P(x|c)\rho(x)$

Embedding complexity

Good embeddings should maximise I(C:Q) and minimise $I_2(X:Q)$

Spoiler: Information Bottleneck!

Two extreme cases:

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 $\mathscr{G}_{\mathscr{T}}(\rho) = 0$

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

In the numerical example we consider $x \mapsto |\psi(x)\rangle \langle \psi(x)|^{\otimes N}$ $|\psi(x)\rangle = \cos(x)|0\rangle + \sin(x)|1\rangle$

For large N

 $\begin{aligned} \mathscr{A}(\rho) \leq KF_{\max}^{N} \\ \mathscr{B} \approx \mathcal{O}(N) \\ \text{where } F_{\max} = \max_{\substack{x \neq y}} F(\rho(x), \rho(y)) \end{aligned}$

Proof from $\rho_{CXQ} = \sum P(c, x) |cx\rangle \langle cx| \otimes \rho(x)^{\otimes N}$

CX

QUANTUM KERNELS

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

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) L Banchi, J Pereira, S Pirandola PRX Quantum 2, 040321 (2021)

- $\mathscr{B} = \left[\mathrm{Tr}\sqrt{K} \right]^2$
- where $K_{xy} = \sqrt{p(x)p(y)} |\langle \psi(x) | \psi(y) \rangle|$ is a (normalised) **kernel** matrix. This makes the

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!

INFORMATION BOTTLENECK FOR QUANTUM CLASSIFIERS

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

IB principle (loss independent): minimise

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

Self-consistent solutions (similar for ρ)

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

L Banchi, J Pereira, S Pirandola PRX Quantum 2, 040321 (2021)

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

$$H = -\sum_{i=1}^{L} (\sigma_i^x \sigma_{i+1}^x + h \sigma_i^z), \qquad \Longrightarrow$$

Ordered (|h| < 1) / disordered (|h| > 1) phases

T : number of training samples per class S : number of measurement shots

VARIATIONAL QUANTUM INFORMATION BOTTLENECK (CQ)

Single-qubit "Data Re-uploading" Classifier

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

For two-qubit states the "re-upoading" embedding can be trained with an efficient variational minimisation of the IB Lagrangian

SUMMARY

Generalization error

L Banchi, J Pereira, S Pirandola PRX Quantum 2, 040321 (2021)

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 $R_{\mathcal{T}}(\Pi,\rho) = \frac{1}{T} \sum_{\substack{(c_k,x_k) \in \mathcal{T} \\ c \neq c_k}} \sum_{c \neq c_k} \operatorname{Tr}\left[\Pi_c \rho(x_k)\right] = 1 - \frac{1}{T} \sum_{\substack{(c_k,x_k) \in \mathcal{T} \\ (c_k,x_k) \in \mathcal{T}}} \operatorname{Tr}\left[\Pi_{c_k} \rho(x_k)\right]$

Abstract classification error

$$R(\Pi, \rho) = \mathbb{E}_{(c,x) \sim P(c,x)}$$

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

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

