IBM Research

Quantum Theory and Application of Contextual Optimal Transport

aka **QontOT**

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International Conference on Machine Learning 2024

Find us:

- Wed 24 July 11:30 – 13:00
- Hall C 4-9 **#1211**

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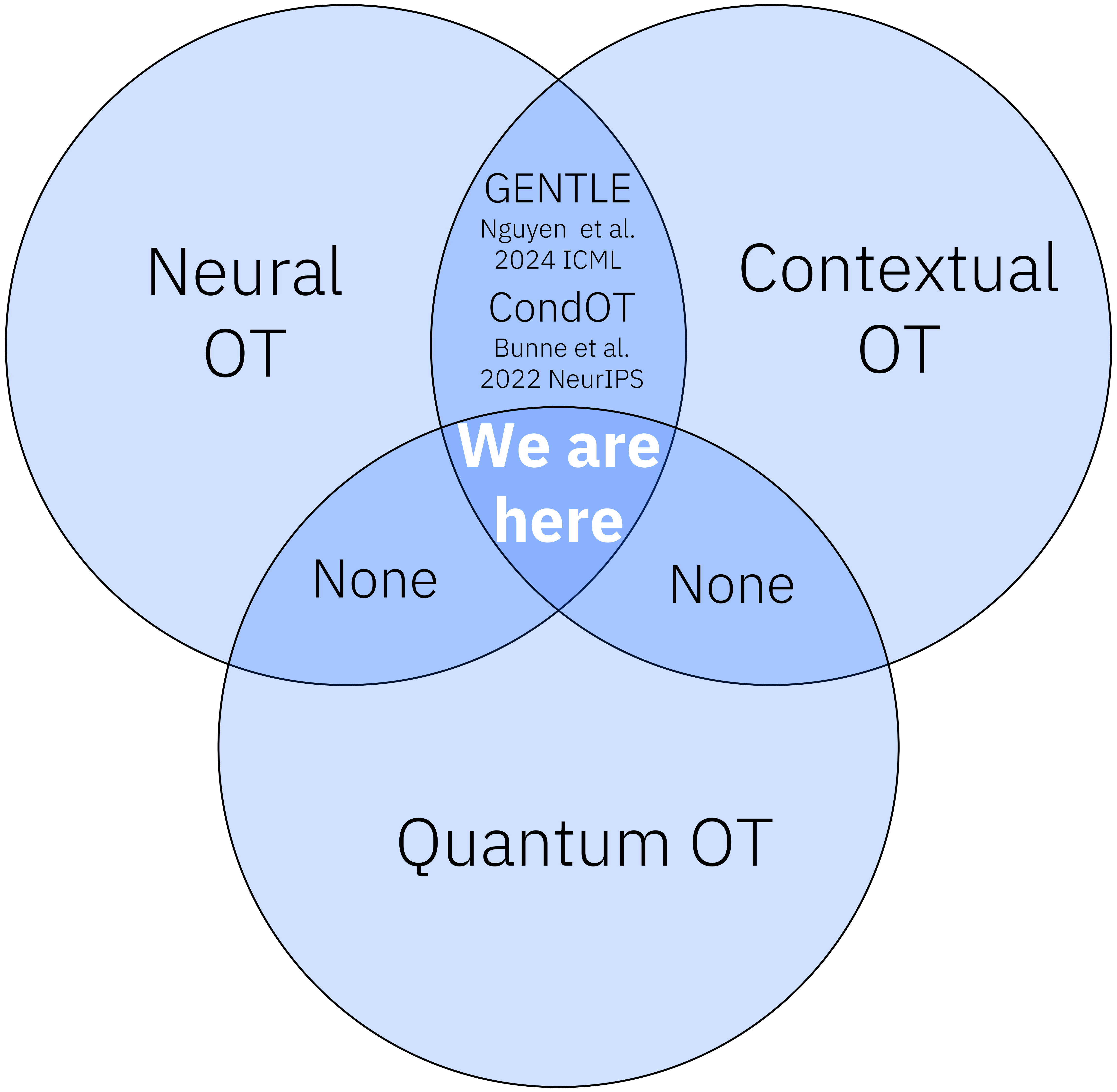
ICML
International Conference On Machine Learning

Quantum Contextual Optimal Transport = QontOT



Given contextual data

$$\big((\mu_i, \nu_i), c_i\big) \in \mathrm{X} \times \mathrm{K}_d^2$$

learn a global map T_θ

s.t. $T_\theta(c_i)\#\mu_i = \nu_i$

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Linking Optimal Transport and Quantum

If $\boldsymbol{U}$ is a unitary matrix

then $\boldsymbol{U} \odot \boldsymbol{U}$

is doubly stochastic

It is unknown whether a similarly natural classical

approach exists that can produce DSMs parametrically

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Problem setting and QontOT ansatz

Comparison of conditional neural OT methods

Conditional neural OT	CondOT	GENTLE	QontOT
Cost-agnostic	❌	✅	✅
Explicit OT plan	❌	❌	✅
Gradient descent	✅	✅	❌
Quantum	❌	❌	✅

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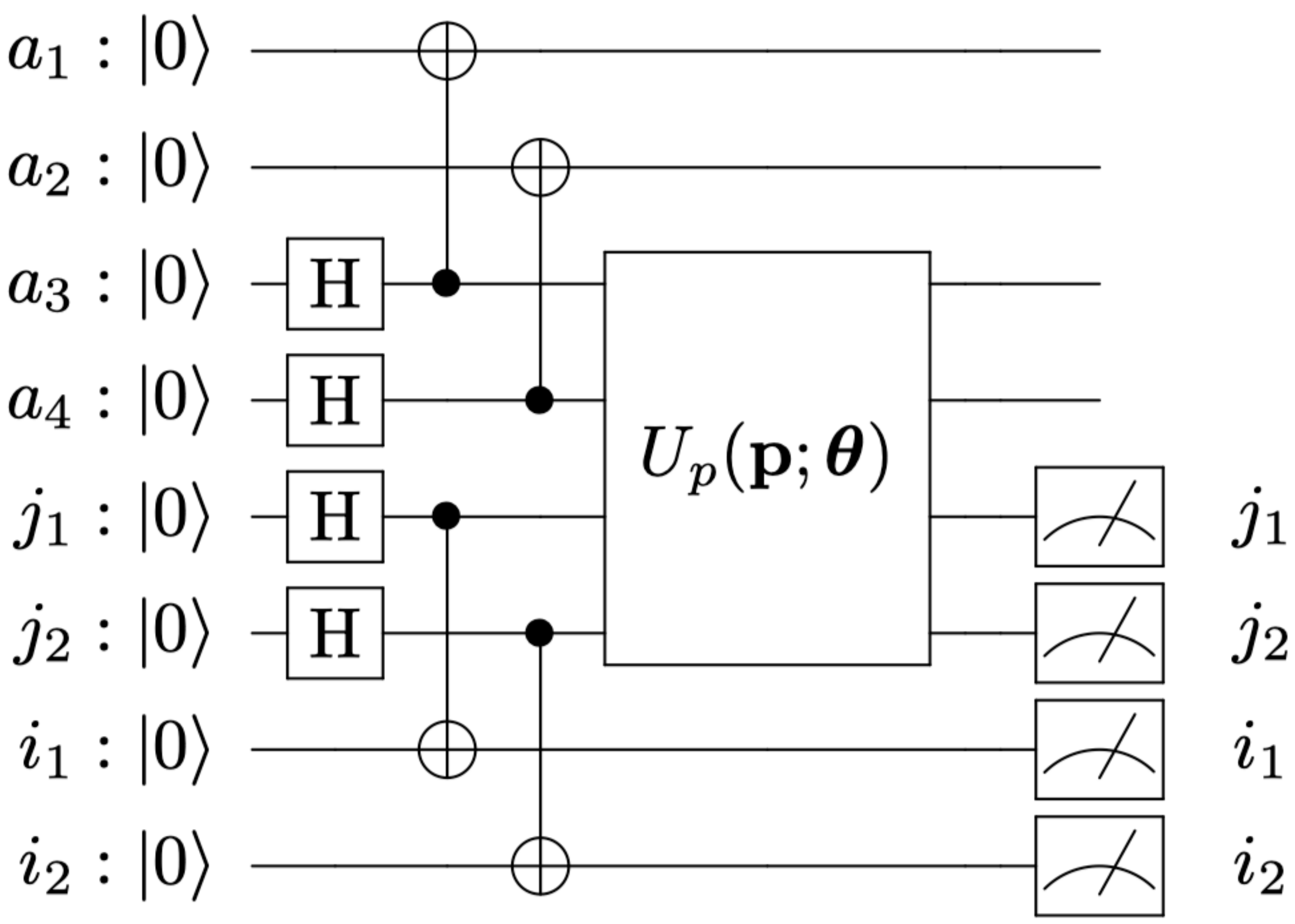
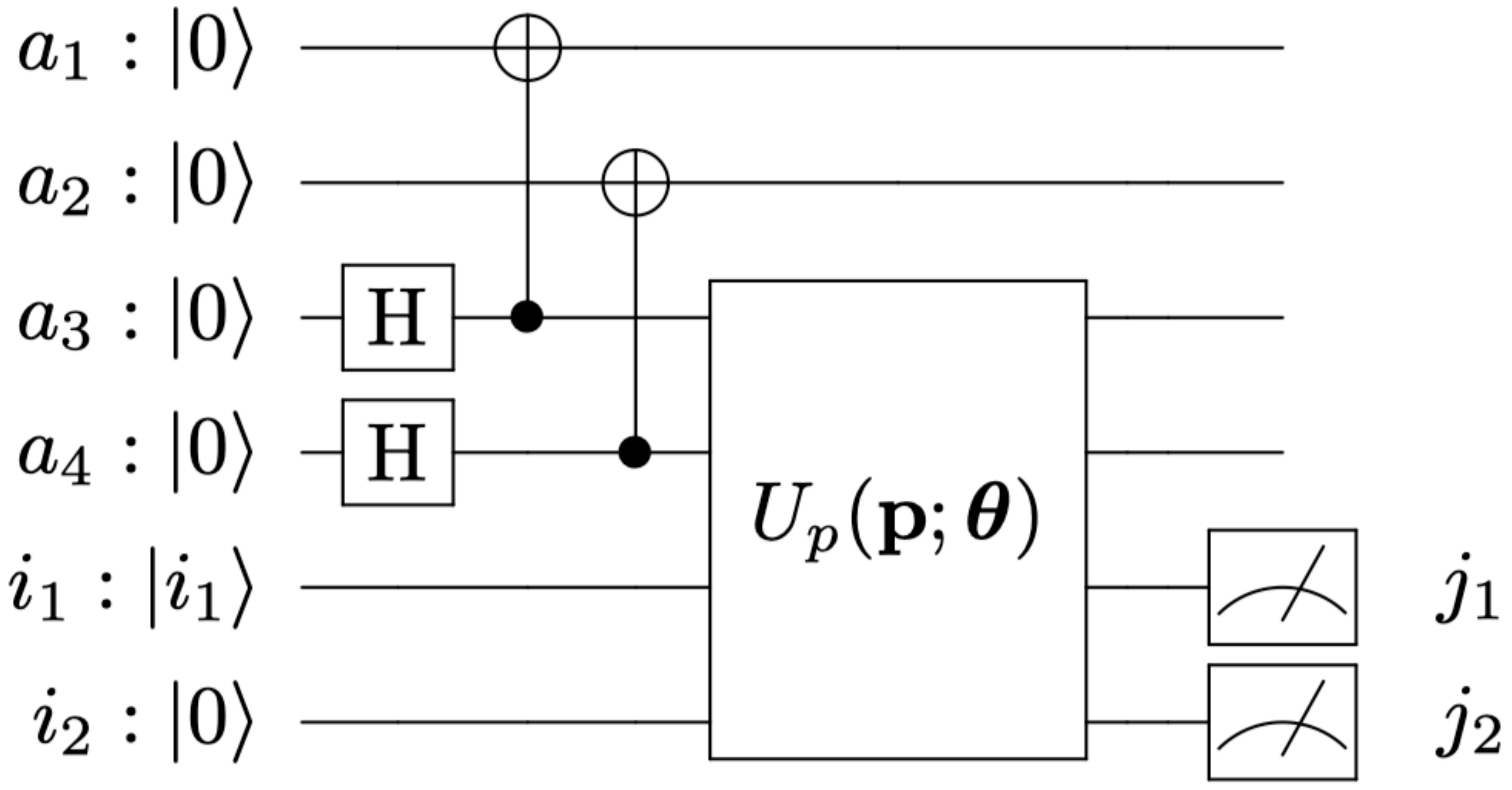
Circuit to produce DSMs

Circuit to embed transport maps

🚀 The circuit only emits DSMs

🚀 Every DSM can be produced





- Circuit scales logarithmically. Precisely we need at least $4(\log_2 n + 1)$ qubits to predict $n \times n$ matrices
- We need to collect at least $O(n \log n)$ circuit shots
- For satisfactory sampling error $\varepsilon = 0.01$ we even need $\geq O(n^2 / \varepsilon^2)$ shots

- Real data* would require $n \approx 10{,}000$, i.e., ≥ 56 qubits and with $\varepsilon = 0.01$ > 1T shots
- We use data with $n = 16$ $\rightarrow$ ≥ 20 qubits and 2.5M shots

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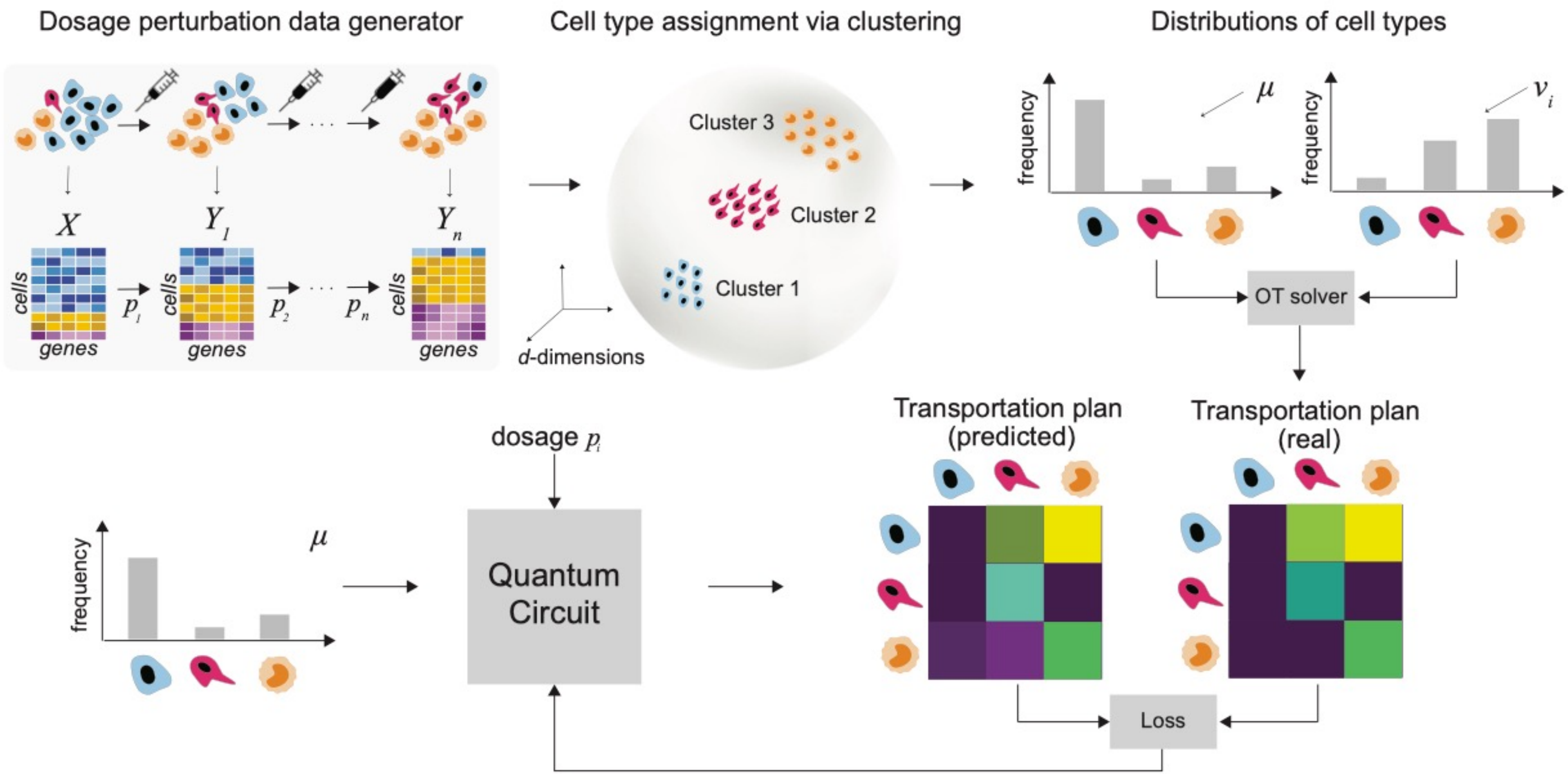
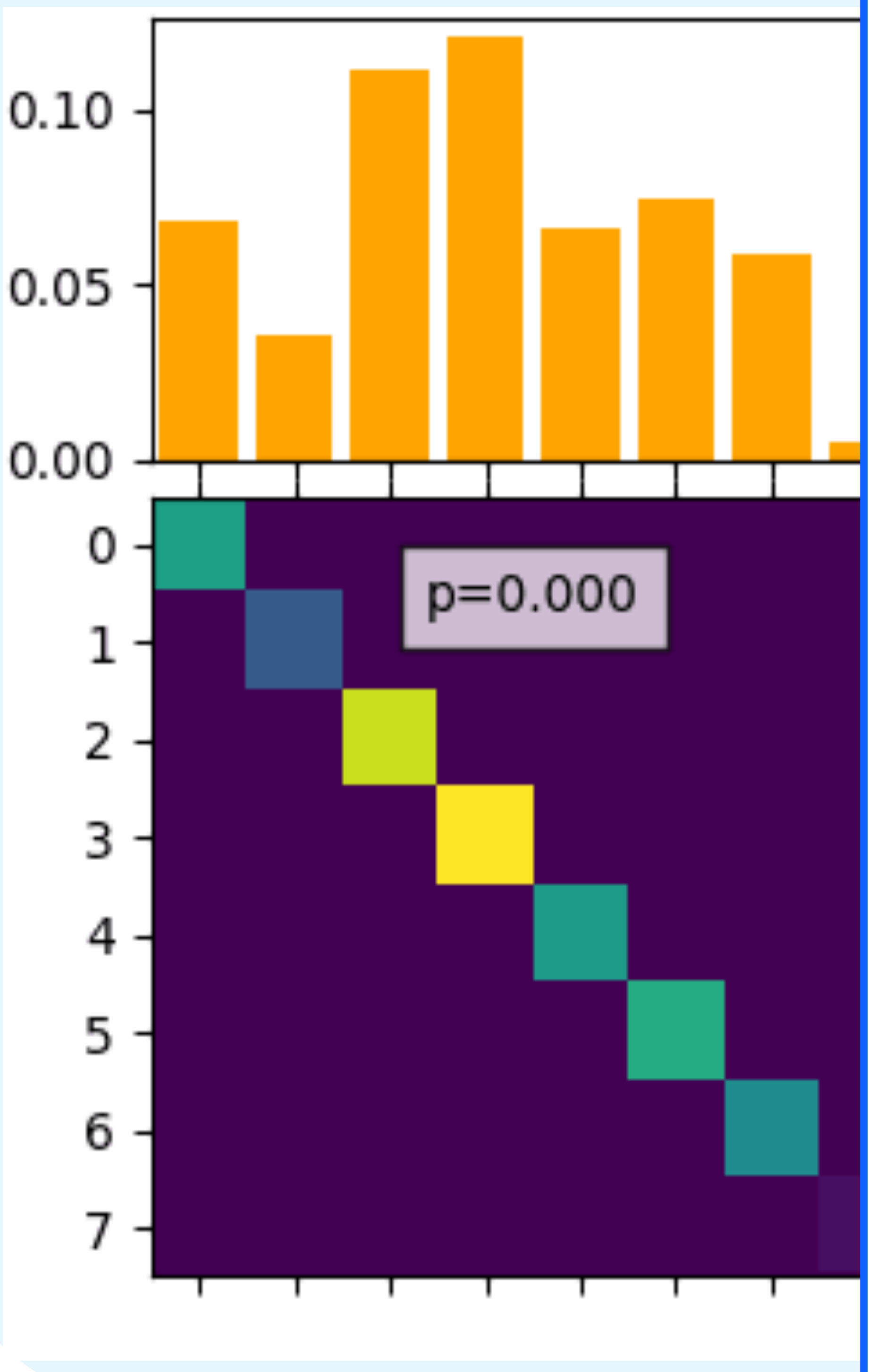
* Our application: single-cell perturbation response prediction

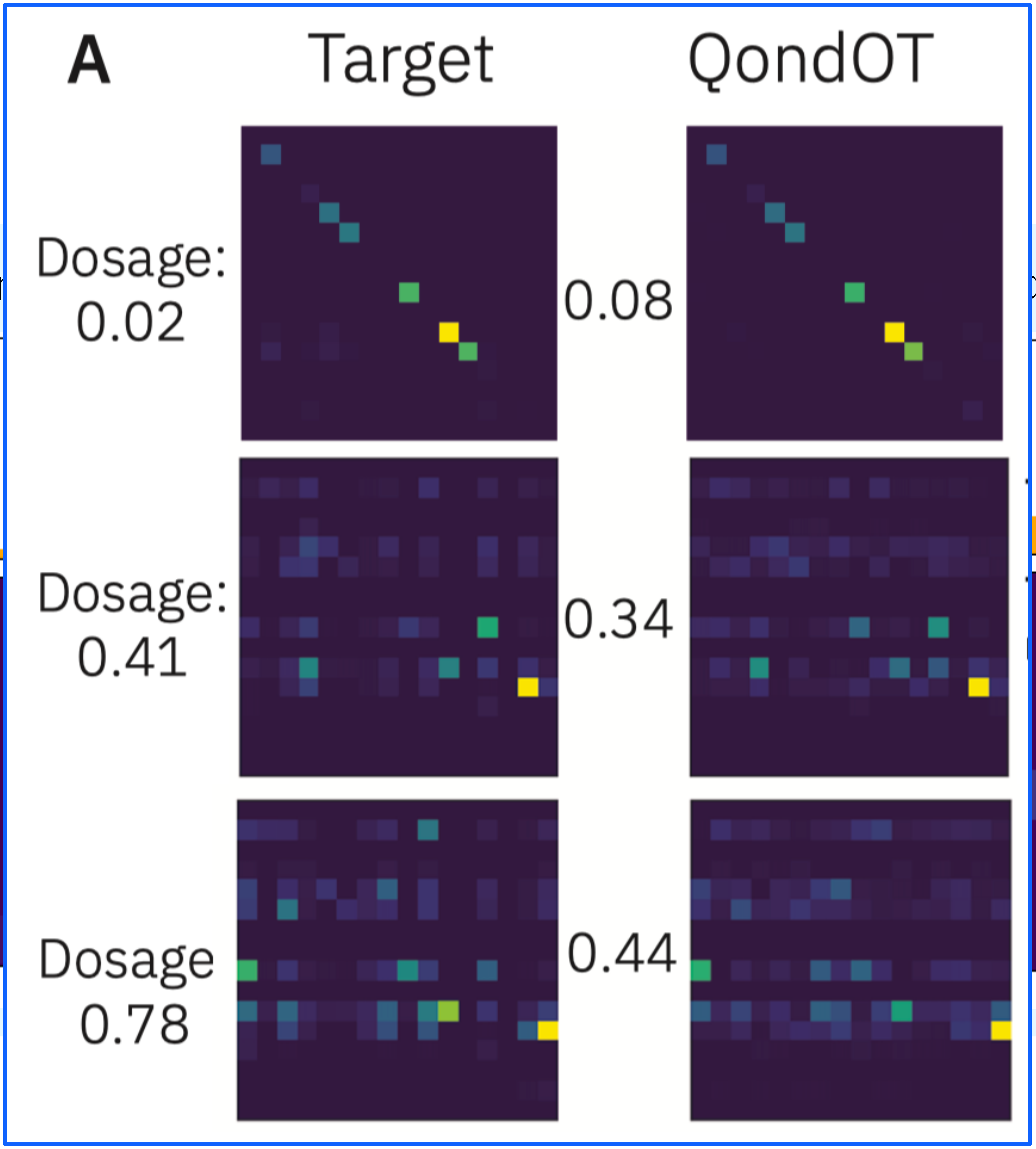
Application: Drug dosage response prediction

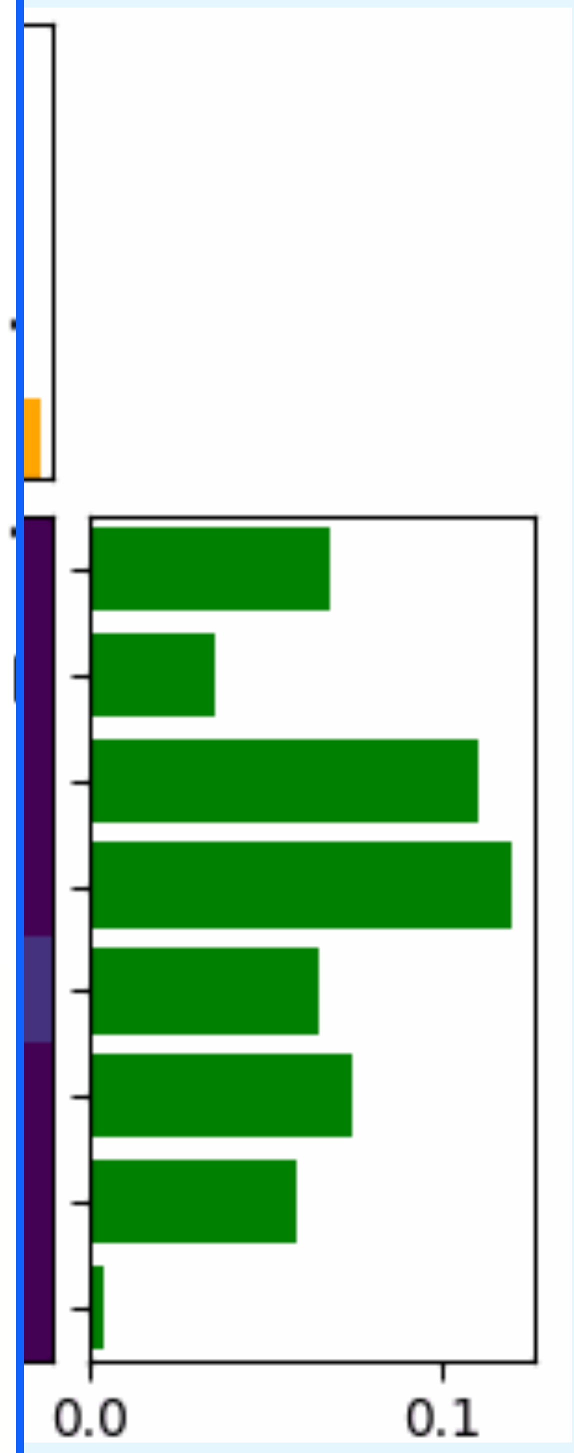


POC: Quantum can predict OT plans conditionally

Same cells, differen ... dosage







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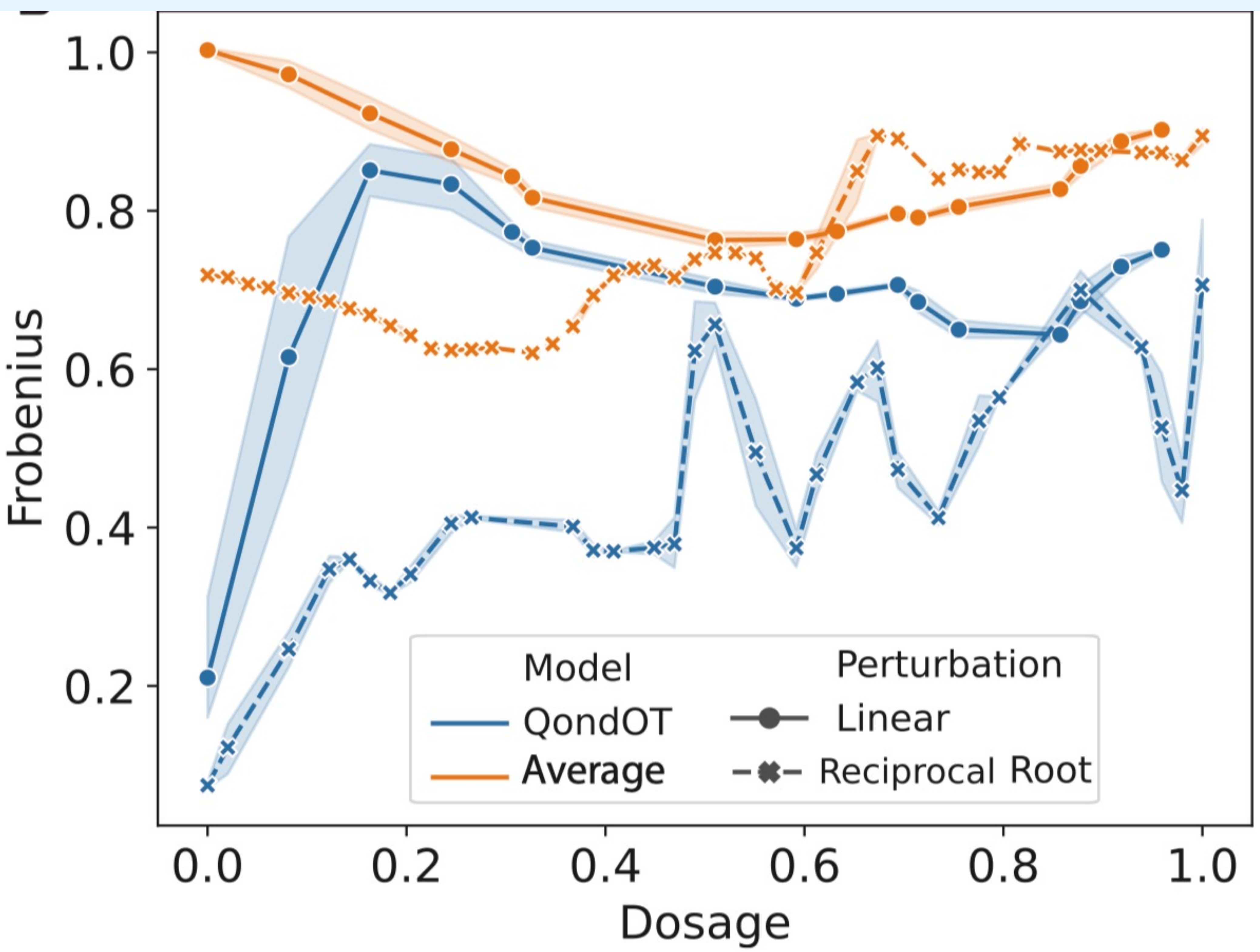
Qualitative results on cell type distribution prediction



	OT plan metrics		Marginal metrics	
Method	**SAE** (↓)	**Frob.** (↓)	L_2 (↓)	R^2 (↑)
Identity	1.10	1.04	0.18	0.47
QontOT-$\mathcal{L}_T$	0.78	0.61	0.17	0.49
QontOT-$\mathcal{L}_M$	0.92	0.68	0.16	0.57
CellOT	0.46	0.41	0.17	0.52
CellOT-homo	0.68	0.60	0.29	0.37
CondOT	0.45	0.40	0.18	0.56

- Learning distributions conditionally to dosage for different cost functions
- In out-of-distribution setting (not shown) still better than the two baselines (average & identity)
- Slightly inferior to SOTA classical neural OT when plans have arbitrary marginal distributions
- Next: Fix marginals to be uniform to better exploit inductive bias of QontOT

→ Contextual relaxed assignment problem

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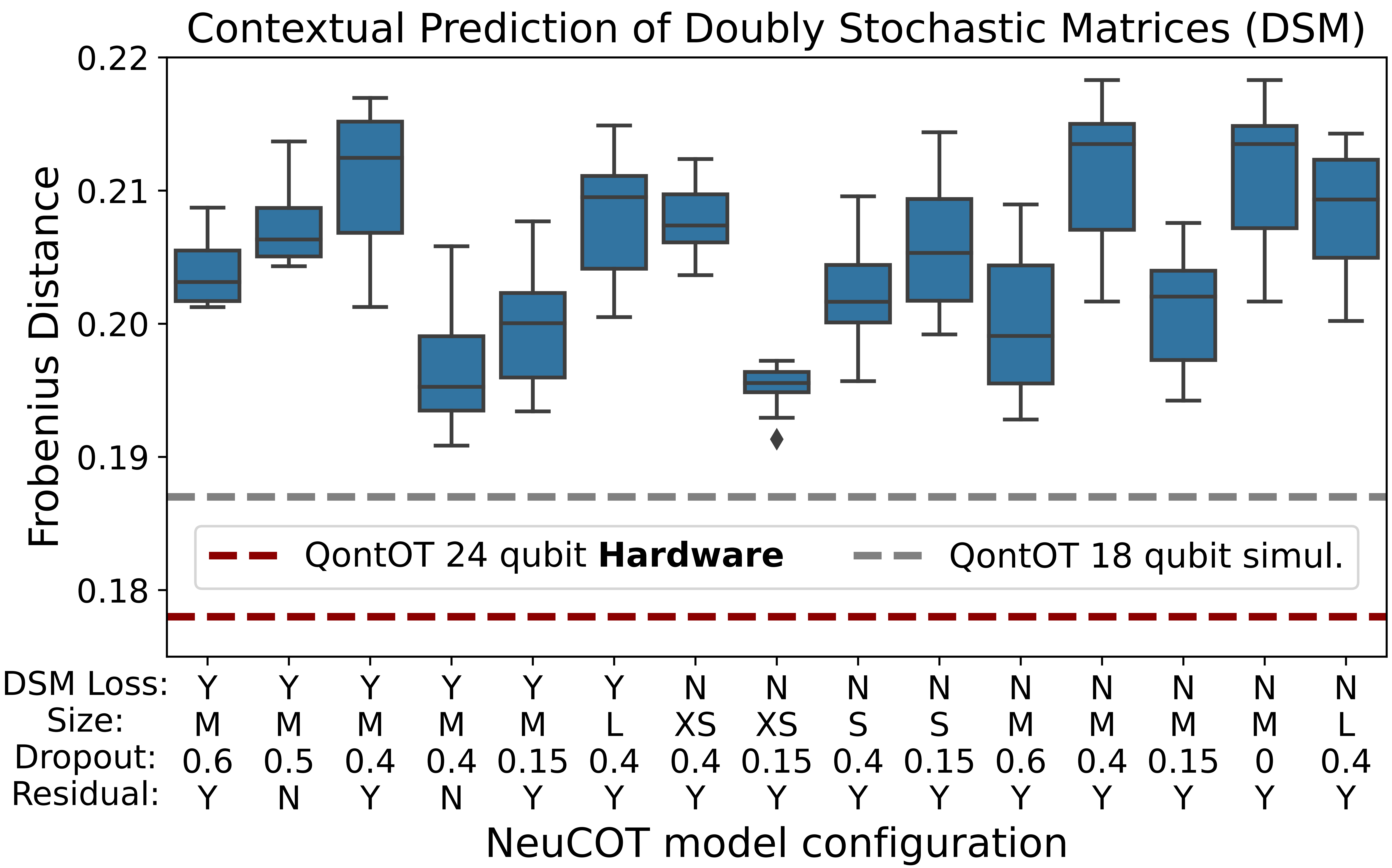
Hardware experiment on contextual relaxed assignment problem

Setup:

- 24 qubit experiment (IBM Sheerbroke)
- Depth 50, 70 ECR gates
- Dataset of 40 8x8 DSMs
- No error mitigation
- 235 optimization steps (gradient-free)

Result:

- Good convergence
- 24 qubit >> 18 qubit simulation
- Better performance than classical NNs (trained with Backprop)



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Thank you for your attention

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📖 Quantum Theory and Application of Contextual Optimal Transport
Mariella, N. et al. *International Conference on Machine Learning* (2024)

📖 Further details in the paper:

- Proofs on expressivity of circuit
- Generalization to multidimensional OT
- Comparison of optimizing marginals vs. transport plans
- Various circuit ablation studies (e.g., cost functions)
- ...

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