A Hybrid Quantum-Classical Workflow for Hyperparameter Optimization of Neural Networks

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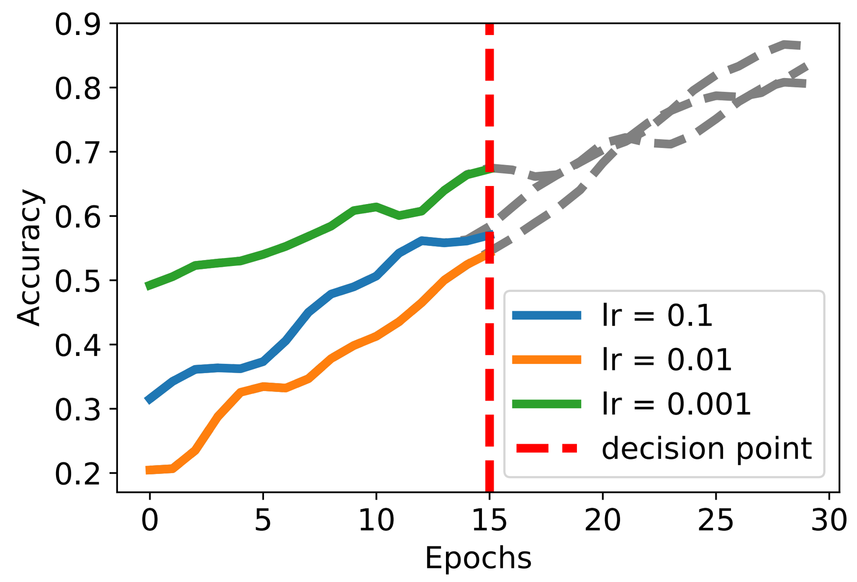
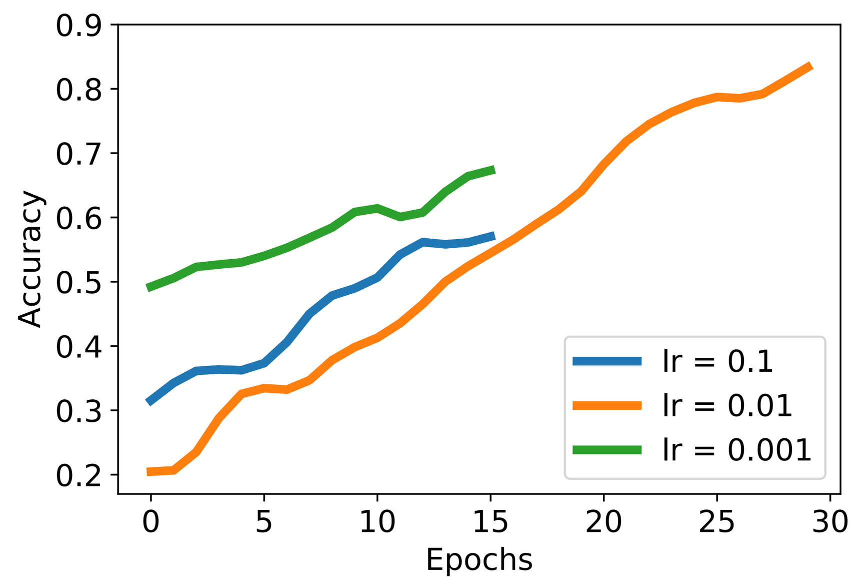
1. PROBLEM DEFINITION

- HPO requires significant computational resources
- Run trials on classical GPUs
- Early stopping of bad trials with Quantum Annealer (QA) by Quantum Support Vector Regression (Q-SVR) learning curve extrapolation



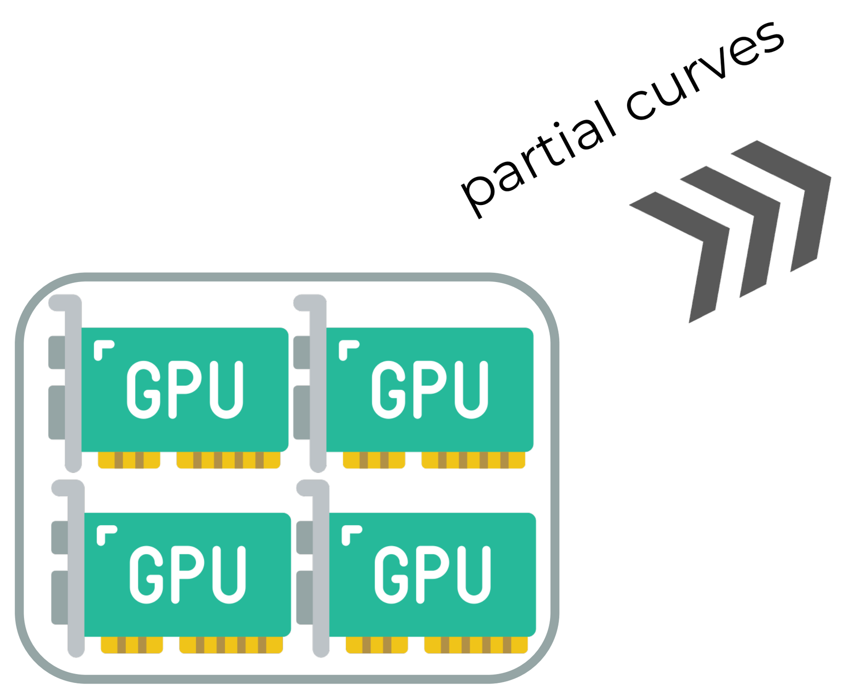
Good vs. bad trial?

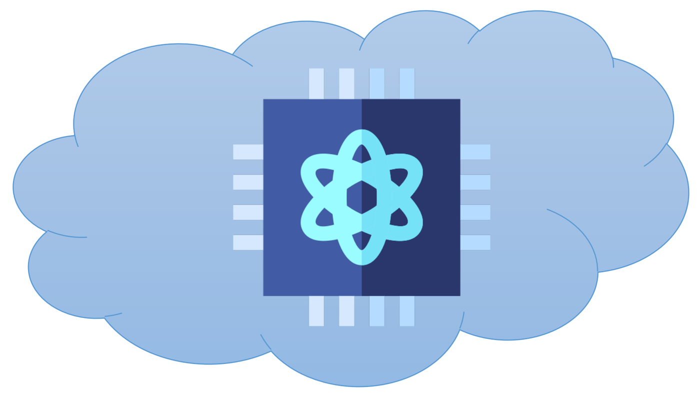


Only continue good trials!

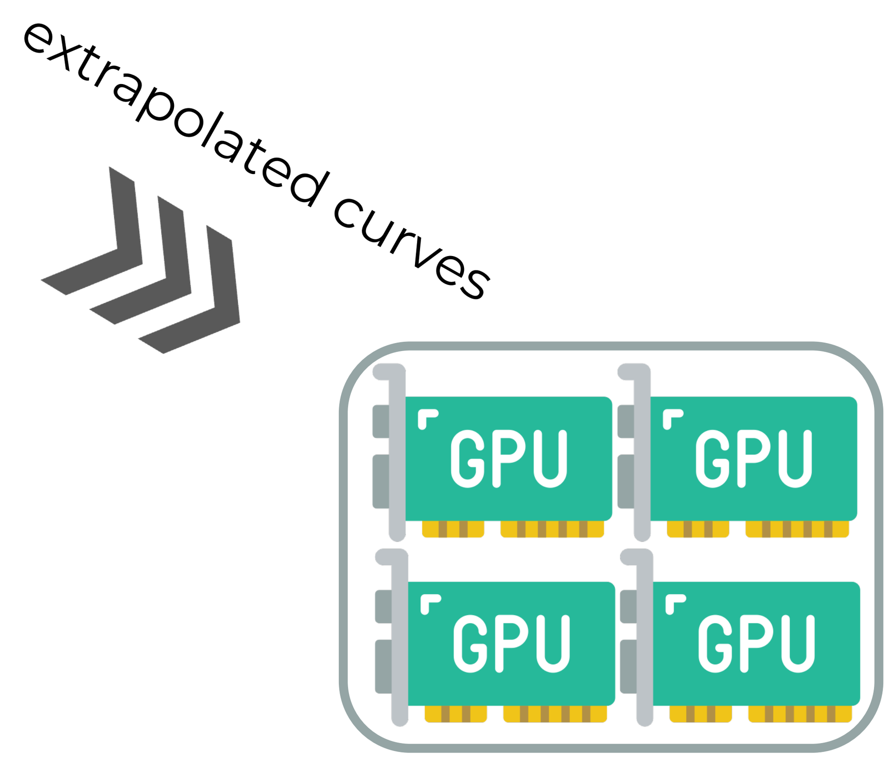
3. WORKFLOW

Three step workflow





Extrapolate learning curves with Q-SVR on the *Quantum Annealer* via D-Wave cloud



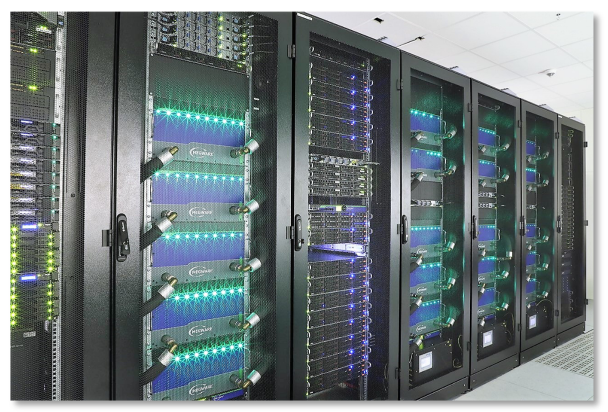
① Partial neural network training on *classical supercomputer*

② Extrapolate learning curves with Q-SVR on the *Quantum Annealer* via D-Wave cloud

③ Full training of best neural networks on *classical supercomputer*

Systems

DEEP-EST-ESB



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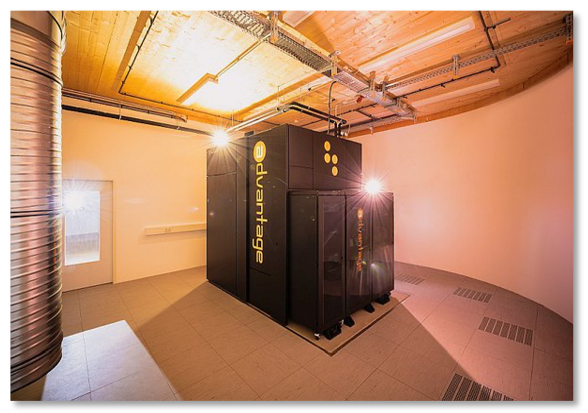
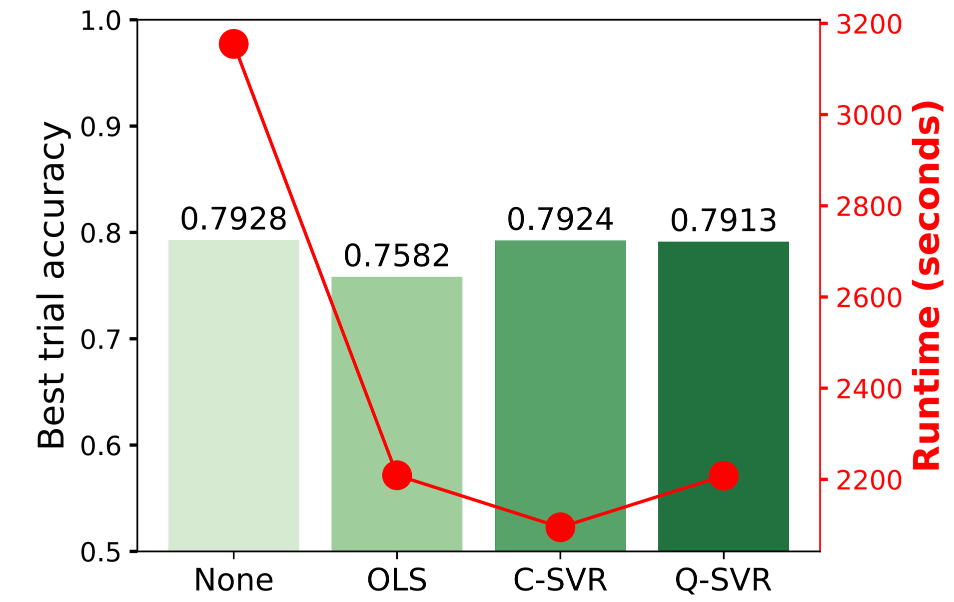


Hyperparameter Search Space

Convolutional neural network trained on cifar-10

Parameter	Range
Layers	[2, 3, 4]
Filters	[16, 32, 48, 64]
Batch size	[64, 128, 256, 512]
Learning rate	Log[1e-4, 1]
Momentum	Log[1e-4, 0.9]

4. RESULTS



- 100 trials with different early stopping methods
- No early stopping: longest runtime but highest accuracy
- Q-SVR: 30% shorter runtime while comparable accuracy

Why Quantum Support Vector Regression?

- C-SVR complexity $O(n^2)$ - $O(n^3)$
- Q-SVR complexity does not increase with problem size
- Quantum speedup possible in the future

2. THEORETICAL BACKGROUND

Performance Prediction:

- Regression on learning curve of a neural network can accurately predict final performance [Baker et al. 2018]

Quantum Support Vector Regression:

- QA solves quadratic unconstrained binary optimization (QUBO) problems: $E = \sum_{i \leq j} a_i Q_{ij} a_j, \quad a_{i,j} \in \{0,1\}$
- Reforumulate Classical Support Vector Regression (C-SVR) into QUBO form [Pasetto et al. 2022]:

Kernel function

$$L(\boldsymbol{\alpha}, \hat{\boldsymbol{\alpha}}) = \frac{1}{2}\sum_{n=0}^{N-1}\sum_{m=0}^{N-1}(\alpha_n - \hat{\alpha}_n)(\alpha_m - \hat{\alpha}_m)k(\boldsymbol{x}_n, \boldsymbol{x}_m) - \epsilon\sum_{n=0}^{N-1}(\alpha_n + \hat{\alpha}_n) + \sum_{n=0}^{N-1}(\alpha_n - \hat{\alpha}_n)y_n$$

Error margin

Number of qubits

$$\alpha_n = \sum_{k=0}^{K-1} B^{k-P} a_{Kn+k}$$

Encoding basis

$$\hat{\alpha}_n = \sum_{k=0}^{K-1} B^{k-P} a_{K(N+n)+k}$$

5. CONCLUSION

- Neural network training on classical machine
- Performance prediction on quantum machine
- Save 30% compute resources

REFERENCES

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