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Applying Genetic Algorithms to Optimize the Generalization Ability of Variational Quantum Circuits

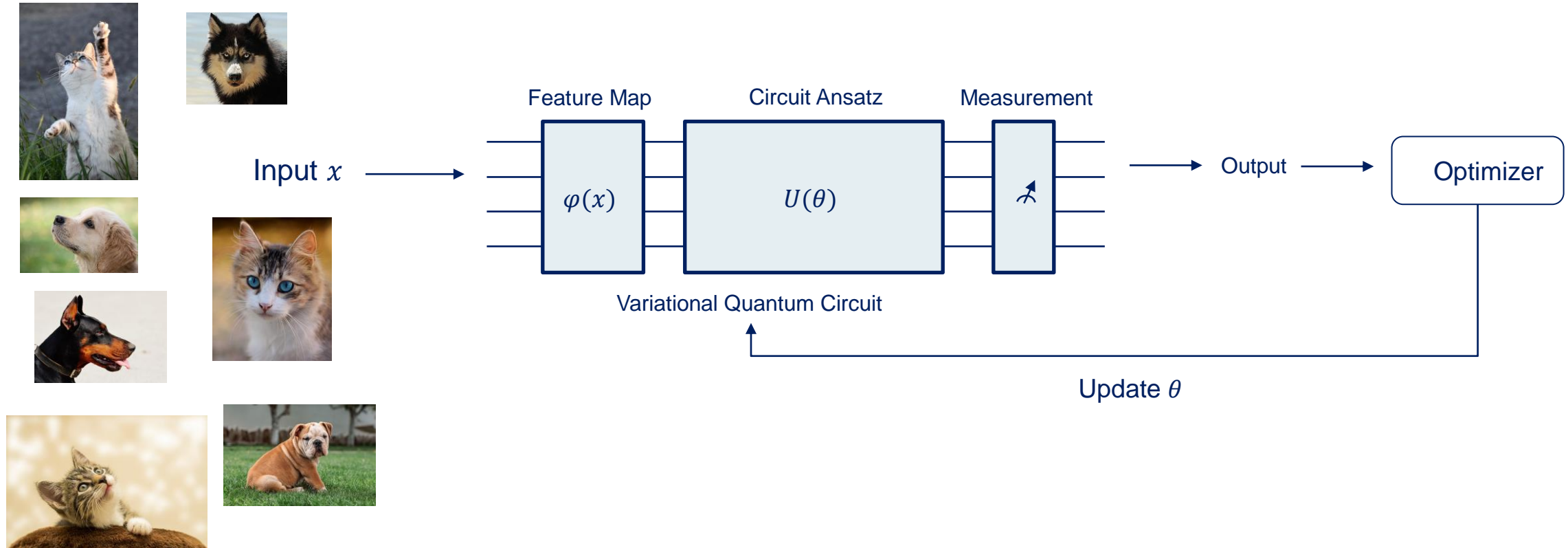
Leo Sünkel, Darya Martyniuk, Johannes Jung, and Adrian Paschke





Motivation example

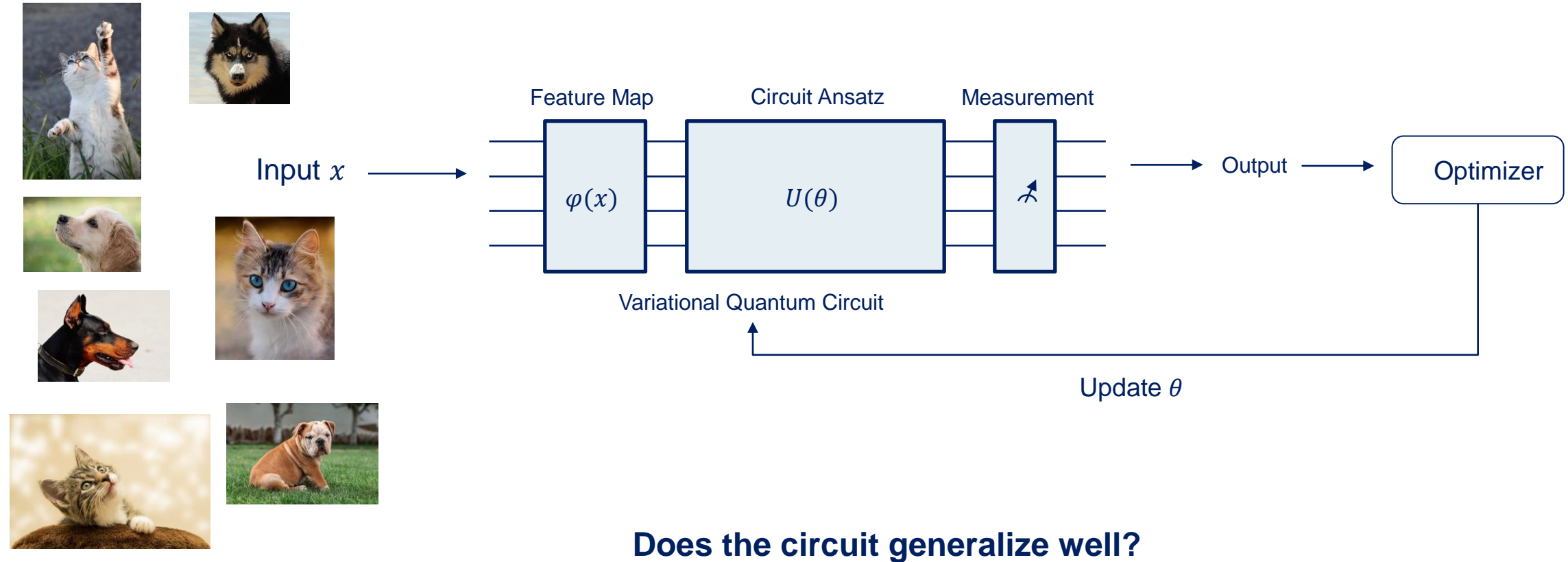
Variational Quantum Circuit





Motivation example

Variational Quantum Circuit



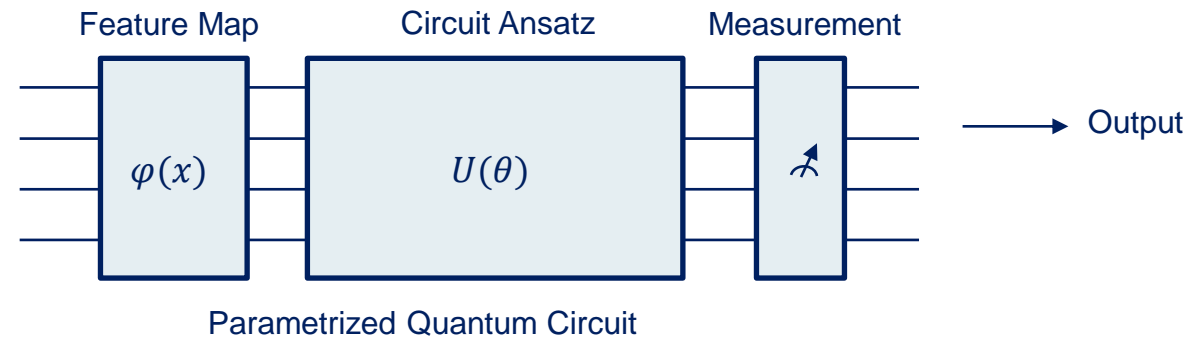


Motivation example

Parametrized Quantum Circuit



Input x

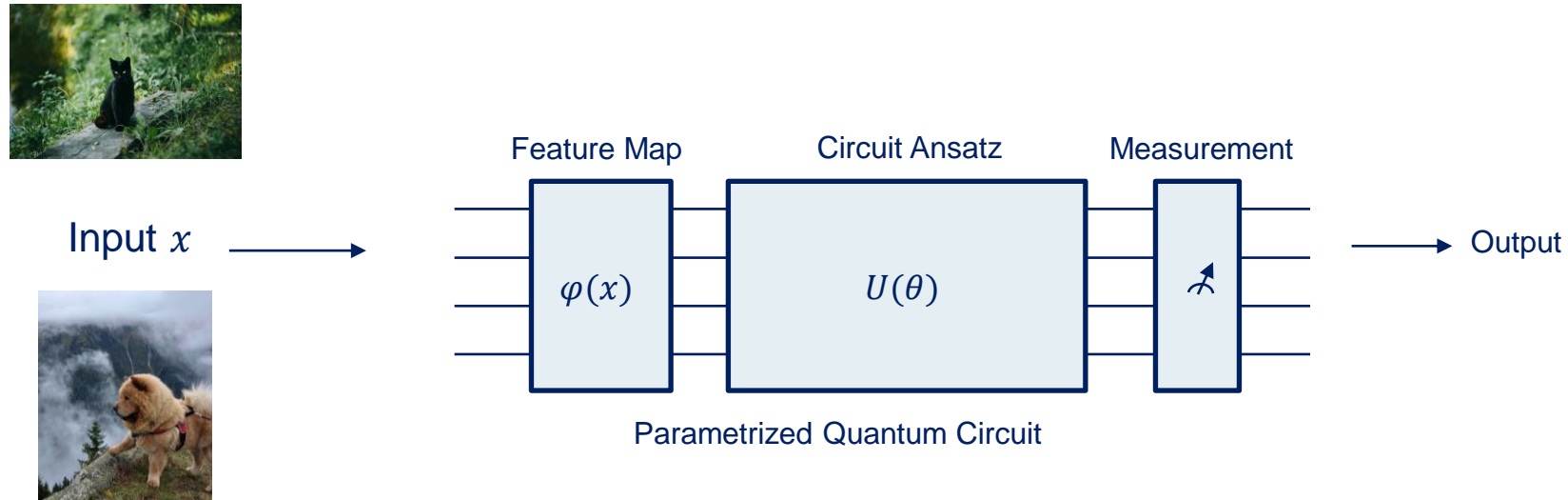


Does the circuit generalize well?



Motivation example

Parametrized Quantum Circuit

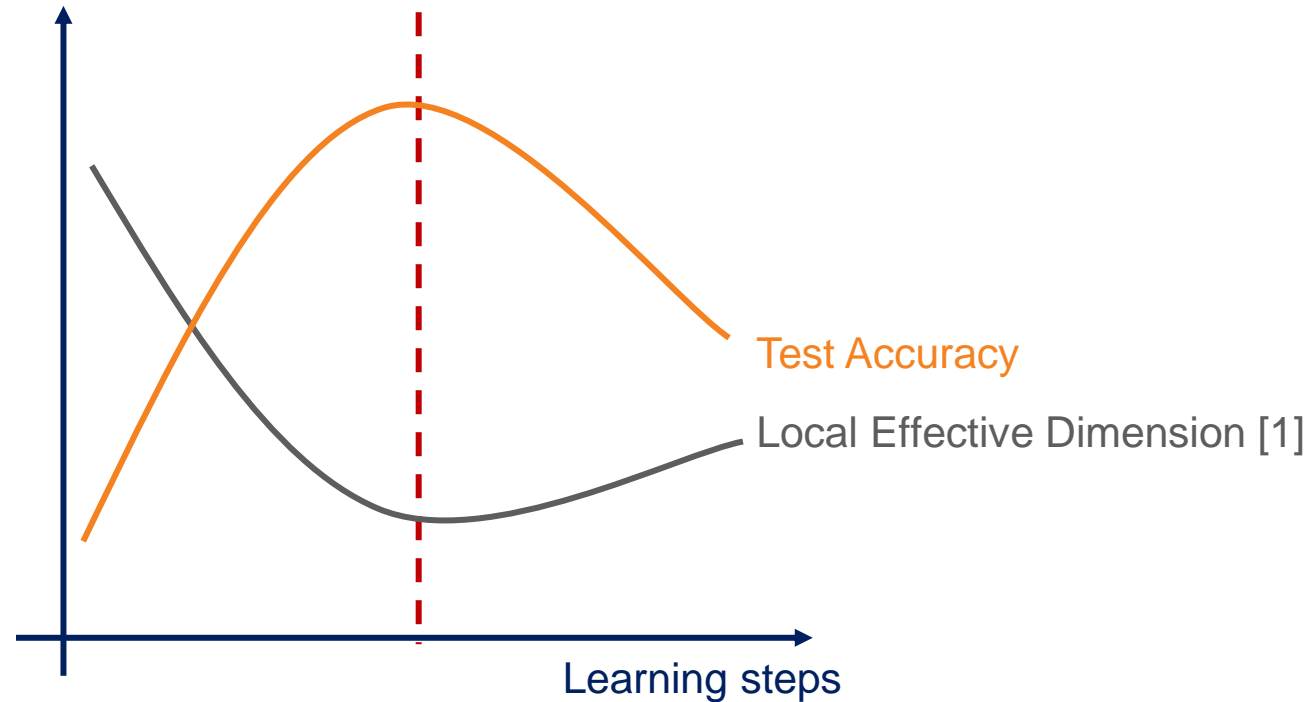


Does the circuit generalize well?

Manual search for a problem-specific quantum circuit is time-consuming!



Optimization Criteria



Optimization criteria:

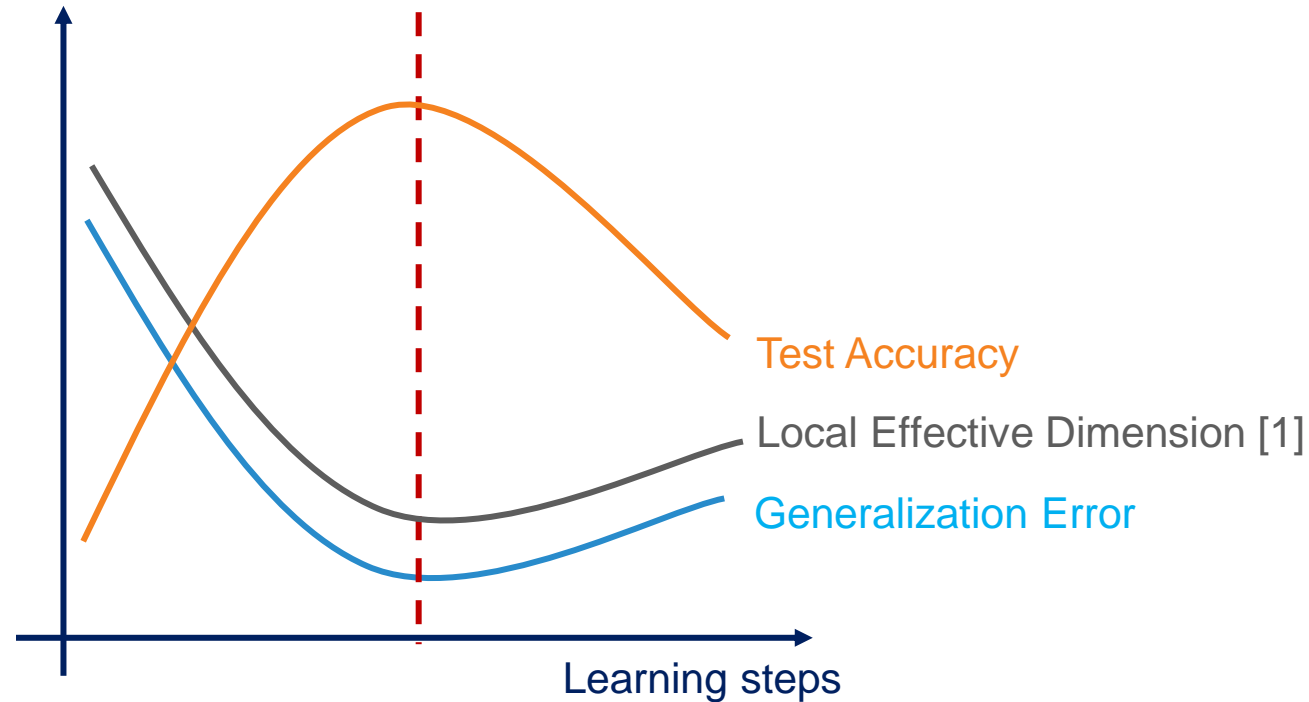
- $\operatorname{argmax}_{\theta} \text{test_accuracy}(f(x; \theta, M))$
- $\operatorname{argmin}_{\theta} \text{local_ED}(f(x; \theta, M))$

where $f(x; \theta, M)$ represents the ML model with parameters θ and structure M for given inputs x .

[1] Abbas, A., Sutter, D., Figalli, A., & Woerner, S. (2021). Effective dimension of machine learning models. *ArXiv, abs/2112.04807*.



Optimization Criteria



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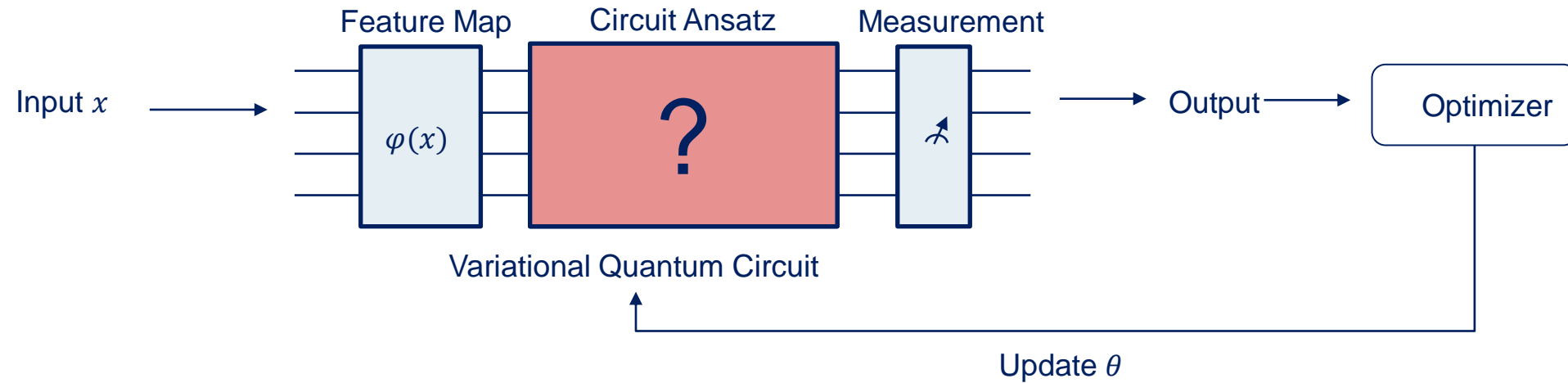
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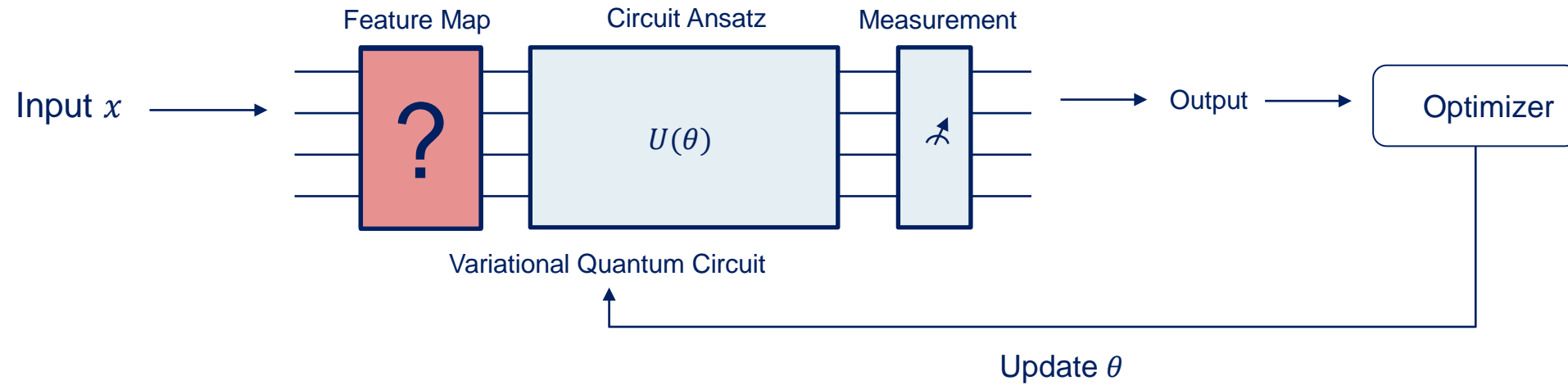


Optimizing Circuit Ansatz





Optimizing Feature Map

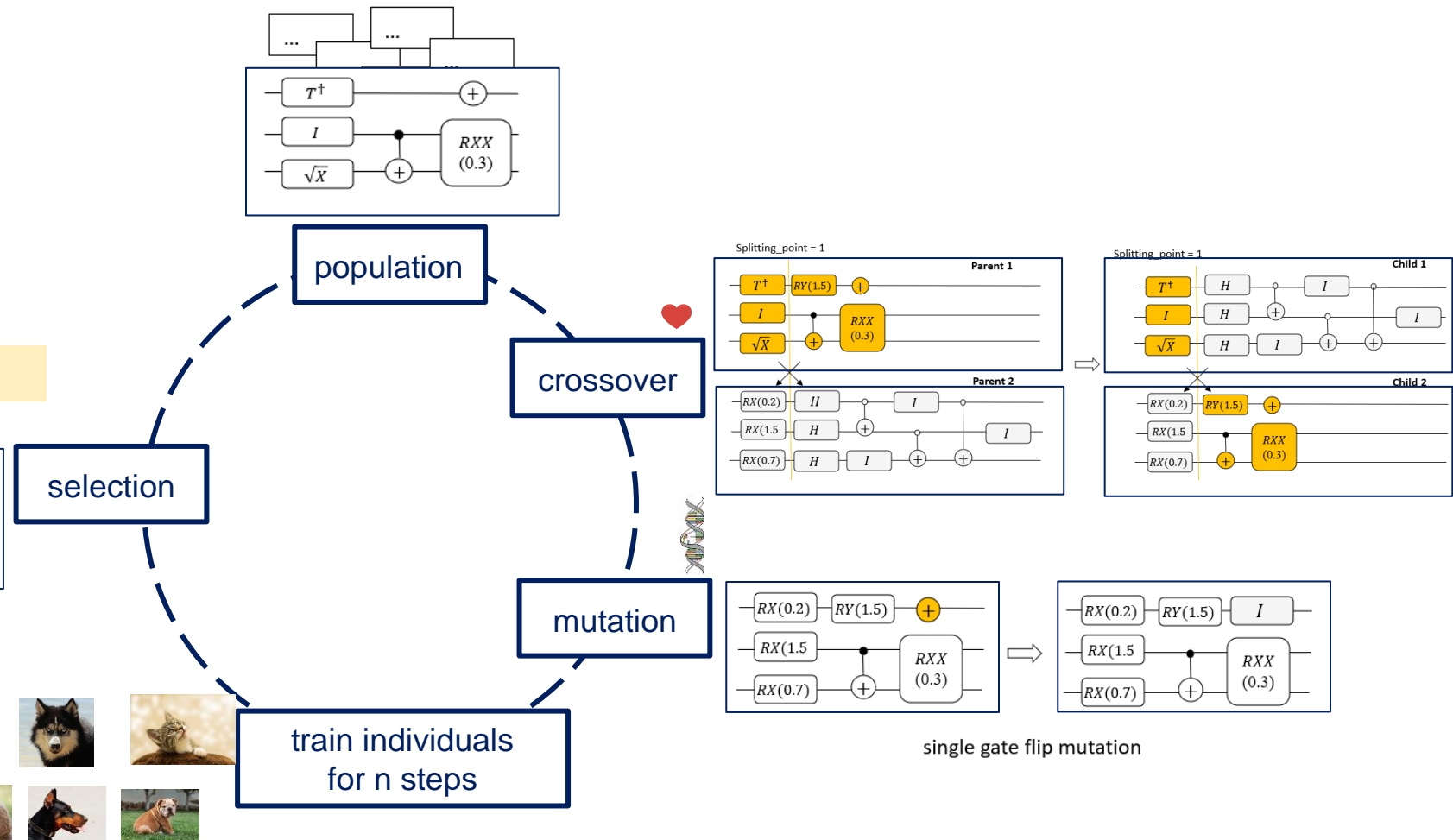
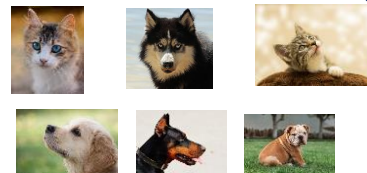
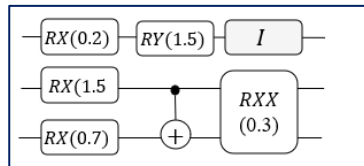
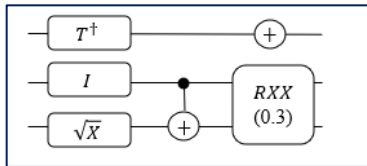




Optimizing generalization ability of variational circuits with GAs

Fitness value:

$$\text{test_accuracy}(f(x; \theta, M)) - \text{local_ED}(f(x; \theta, M))$$

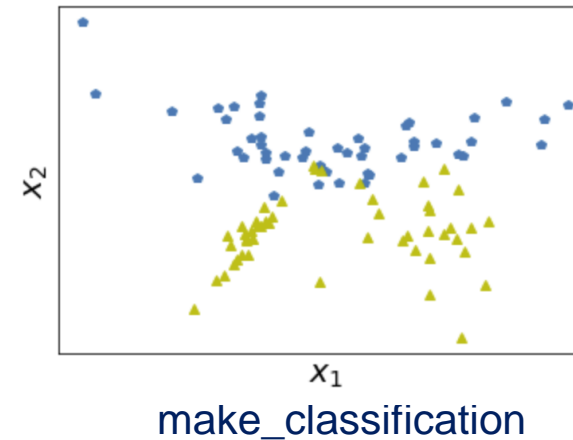
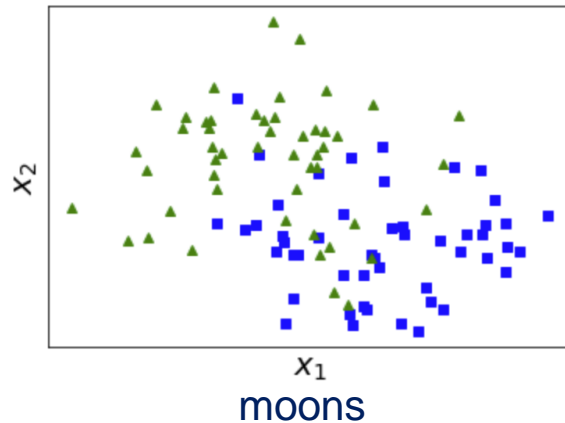


[2] Leo Sünkel et al. (2023): GA4QCO: genetic algorithm for quantum circuit optimization, arXiv:2302.01303



Experimental Setup

Datasets [3]



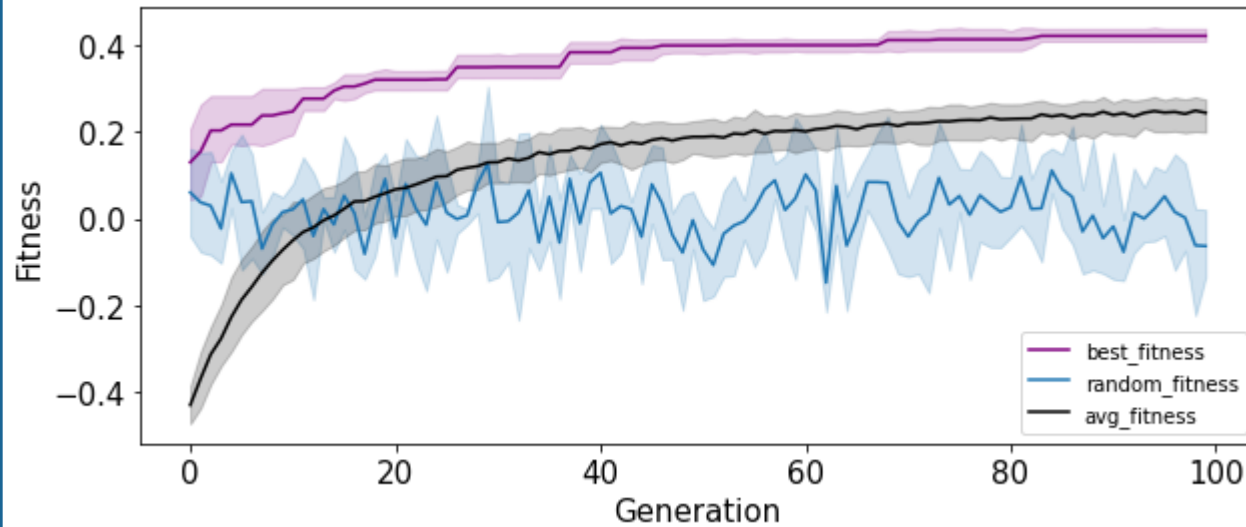
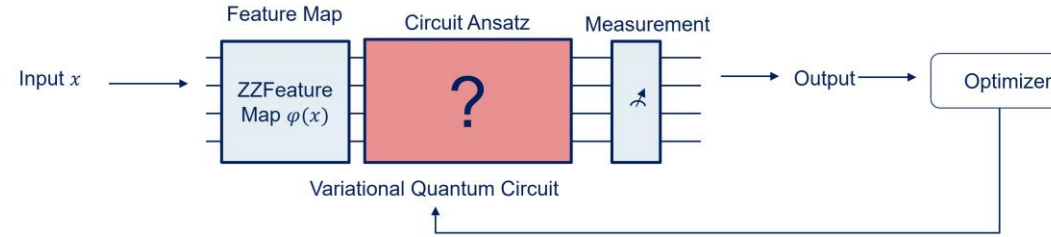
Configuration:

- `n_generations = 100`
- `population_size = 100`
- `n_learning_iterations = 30`

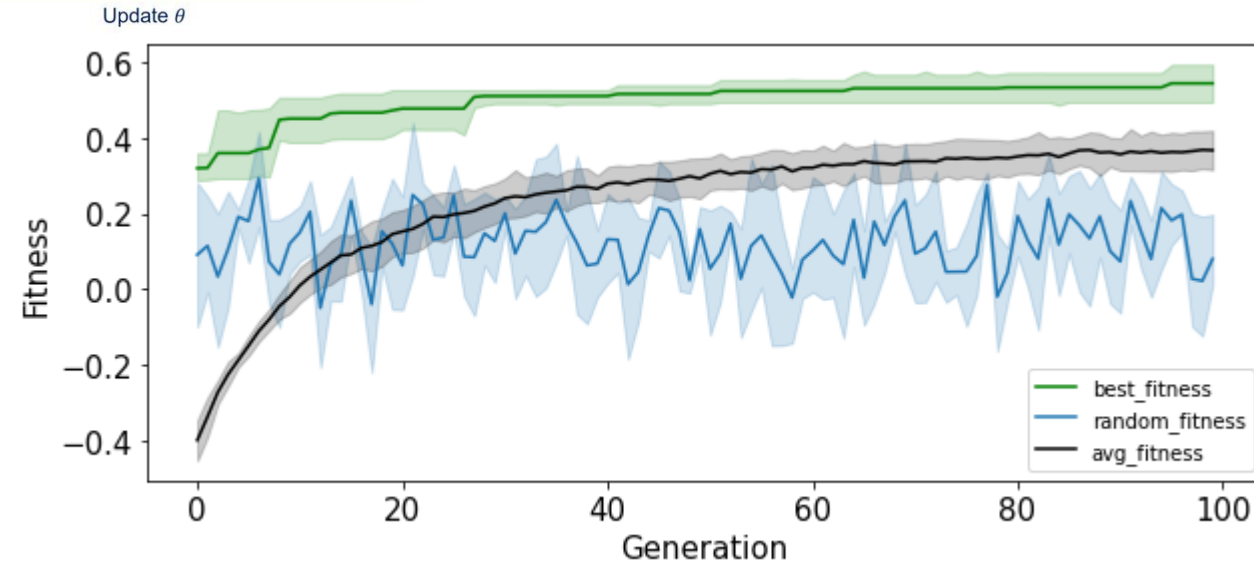
Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Louppe, G., Prettenhofer, P., Weiss, R., Weiss, R.J., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., & Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. *ArXiv, abs/1201.0490*.



Optimizing Circuit Ansatz



Results on the „moons“ dataset



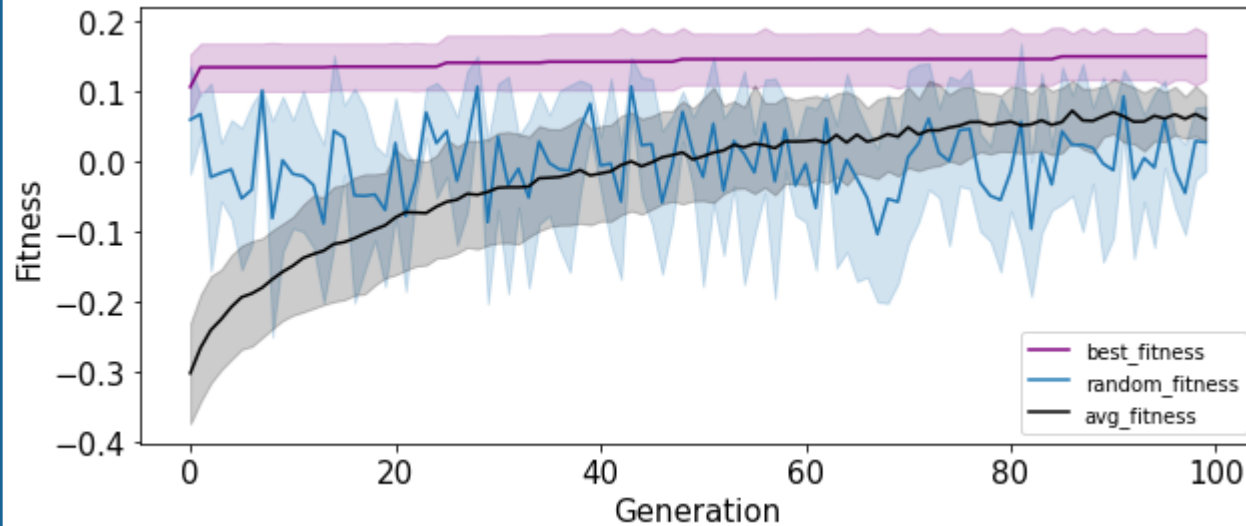
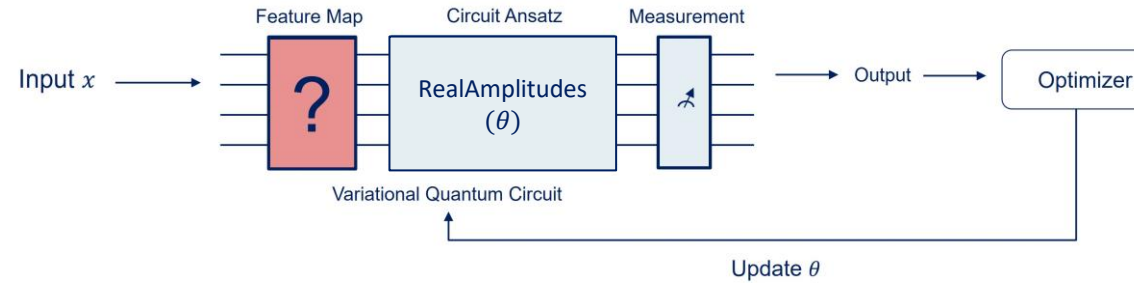
Results on the „make_classification“ dataset

Figure 1: Best, average and random fitness value per generation during the ansatz optimization

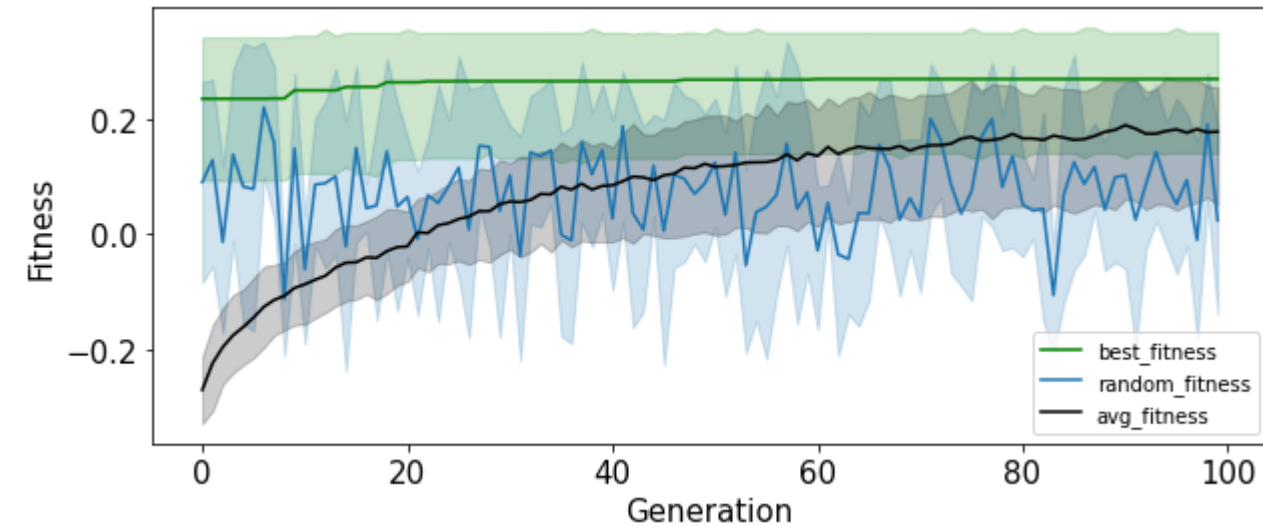
* Over 4 seeds



Optimizing Feature Map



Results on the „moons“ dataset



Results on the „make_classification“ dataset

Figure 2: Best, average and random fitness value per generation during the feature map optimization

* Over 4 seeds



Conclusion

- We applied genetic algorithms to optimize VQCs with respect to the generalization ability.
- While the preliminary results show that approach works in principle, further investigation is needed for deeper understanding the effect of the VQC structure on the generalization ability.

Next steps

- Extend experiments by using more qubits and features
- Deeper analysis of optimized circuits (performance, further trainability and patterns)
- Improve the search



Thank you!

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References

- [1] Abbas, A., Sutter, D., Figalli, A., & Woerner, S. (2021). Effective dimension of machine learning models. *ArXiv, abs/2112.04807*.
- [2] Leo Sünkel et al. (2023): GA4QCO: genetic algorithm for quantum circuit optimization, arXiv:2302.01303
- [3] Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Louppe, G., Prettenhofer, P., Weiss, R., Weiss, R.J., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., & Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. *ArXiv, abs/1201.0490*.