Automatic Dimensionality Reduction for Quantum Classifiers

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Data sets that are specified by a large number of features are currently outside the area of applicability for algorithms that involve Quantum Machine Learning (QML). An immediate solution to this impasse is the application of dimensionality reduction methods to the high complexity data sets. Hence, we study the effects of different dimensionality reduction techniques by applying six conventional feature extraction algorithms and five autoencoder-based dimensionality reduction models to a particle physics data set with 67 features. The dimensionality reduction methods that are considered in this study are some of the most popular in the current literature and include Principal Component Analysis (PCA), Restricted Boltzmann Machine (RBM), a standard autoencoder (AE), a Sinkhorn AE [1], and an original variation on the latter which we call the Sinkclass AE.

In the context of quantum computing, dimensionality reduction is often needed for many real-world applications of QML and therefore plays a crucial role. In most practical scenarios, the data set's dimensionality tends to exceed the processing capabilities of commonly available quantum computers. Consequently, dimensionality reduction techniques are usually employed before loading the data into the QML algorithm. Previous studies have used various methods such as manual feature selection based on prior knowledge of the problem [2, 3], linear feature extraction techniques such as PCA [4–6], or more recent approaches involving dimensionality reduction through deep learning models, such as simple auto-encoders [3, 7, 8]. Additionally, a hybrid quantum-classical model has been proposed as well [9].

A Quantum Support Vector Machine (QSVM) is applied to the reduced representations obtained with our 11 methods to solve a binary classification problem: whether a Higgs boson is produced in proton collisions at the LHC. This data set is chosen because its features are quantum observables that can be computed from first principles within the framework of quantum field theory. Thus, it constitutes a good benchmark to test quantum machine learning algorithm performance, while also having a state of the art classical machine learning result [10] we can report to. Furthermore, there exists a quantum machine learning result on this data set that is obtained by using a rudimentary dimensionality reduction algorithm [3], which we reproduce, optimise, and use as a benchmark.

Method	Optimisation	MSE Loss $\times 10^{-4}$	BCE Loss	Classifier AUC	QSVM AUC
PCA	-	-	-	-	0.53 ± 0.01
RBM	-	-	-	-	0.65 ± 0.02
Vanilla AE	-	4.77	-	-	0.56 ± 0.01
Variational AE	MSE	4.49	-	-	0.56 ± 0.02
Sinkhorn AE	MSE	9.65	-	-	0.51 ± 0.01
Sinkclass AE	MSE	26.41	0.65	0.642 ± 0.003	0.50 ± 0.01
	BCE	24.69	0.61	0.734 ± 0.002	0.74 ± 0.01

TABLE I. The classification performance of the QSVM on the reduced representations of the data computed with a selection of our dimensionality reduction methods. The optimisation column refers to how the hyperparameters of that AE were optimised, whether to minimise the mean squared error or the binary cross entropy loss of the validation data . The losses are reported on the test data, along with the classifier AUC wherever the dimensionality reduction algorithm includes a classifier in its architecture. The Sinkclass AE, optimised for BCE minimisation leads to a QSVM pefrormance that is competitive with state of the art methods for this particular data set [10].

The results show that our autoencoder-based methods learn a better lower-dimensional representation of the data for the purposes of classification, leading to an increase of AUC by up to 40% AUC, as seen in Table I. Moreover, we observe that the AE based methods present, in general, better latent spaces for QSVM classification. For the AEs, we show that learning to perform the dimensionality reduction task at the same time as the classification task leads to more discriminative latent spaces. Hence, this study portrays a general heuristic of dimensionality reduction for QML applications: AE based dimensionality reduction is likely to give better results than conventional methods, especially when the dimensionality reduction task learned by the former is combined with the classification task.

[1] G. Patrini *et al.*, Sinkhorn autoencoders, in *Uncertainty in Artificial Intelligence* (PMLR, 2020) pp. 733–743.

[2] K. Terashi *et al.*, Event Classification with Quantum Machine Learning in High-Energy Physics, Comput. Softw. Big Sci. **5**, 2 (2021), arXiv:2002.09935 [physics.comp-ph].

[3] V. Belis *et al.*, Higgs analysis with quantum classifiers, EPJ Web Conf. **251**, 03070 (2021), arXiv:2104.07692 [quant-ph].

[4] S. Wu *et al.*, Application of quantum machine learning using the quantum kernel algorithm on high energy physics analysis at the lhc, Phys. Rev. Research **3**, 033221 (2021).

[5] S. L. Wu *et al.*, Application of quantum machine learning using the quantum variational classifier method to high energy physics analysis at the LHC on IBM quantum computer simulator and hardware with 10 qubits, J. Phys. G **48**, 125003 (2021), arXiv:2012.11560 [quant-ph].

[6] J. Schuhmacher, L. Boggia, V. Belis, *et al.*, Unravelling physics beyond the standard model with classical and quantum anomaly detection, Mach. Learn. Sci. Tech. **4**, 045031 (2023), arXiv:2301.10787 [hep-ex].

[7] K. A. Woźniak, V. Belis, E. Puljak, *et al.*, Quantum anomaly detection in the latent space of proton collision events at the LHC, " (2023), arXiv:2301.10780 [quant-ph].

[8] D. H. Ballard, Modular learning in neural networks, in *Proceedings of the sixth National Conference on artificial intelligence-volume 1* (1987) pp. 279–284.

[9] V. Belis, P. Odagiu, M. Grossi, F. Reiter, G. Dissertori, and S. Vallecorsa, Guided Quantum Compression for Higgs Identification, (2024), arXiv:2402.09524 [quant-ph].

[10] M. Donega, G. Kasieczka, T. Lösche, P. Musella, C. Reissel, and R. Wallny, Attention and dynamic graph convolution neural network in the context of classifying $t\bar{t}H(b\bar{b})$ vs. $t\bar{t}(b\bar{b})$ in the semi-leptonic top quark pair decay channel (2021), ML4Jets.