Evaluating Quantum Support Vector Regression Methods for Price Forecasting Applications

Horst Stühler1, a, Daniel Pranjić2, b and Christian Tutschku2, c
1 Zeppelin GmbH, Graf-Zeppelin-Platz 1, 85766 Garching, Germany
2 Fraunhofer IAO, Nobelstraße 12, 70569 Stuttgart, Germany

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Abstract: Support vector machines are powerful and frequently used machine learning methods for classification and regression tasks, which rely on the construction of kernel matrices. While crucial for the performance of this machine learning approach, choosing the most suitable kernel is highly problem-dependent. The emergence of quantum computers and quantum machine learning techniques provides new possibilities for generating powerful quantum kernels. Within this work, we solve a real-world price forecasting problem using fidelity and projected quantum kernels, which are promising candidates for the utility of near-term quantum computing. In our analysis, we examine and validate the most auspicious quantum kernels from literature and compare their performance with an optimized classical kernel. Unlike previous work on quantum support vector machines, our dataset includes categorical features that need to be encoded as numerical features, which we realize by using the one-hot-encoding scheme. One-hot-encoding, however, increases the dimensionality of the dataset significantly, which collides with the current limitations of noisy intermediate scale quantum computers. To overcome these limitations, we use autoencoders to learn a low-dimensional representation of the feature space that still maintains the most important information of the original data. To examine the impact of autoencoding, we compare the results of the encoded data with the results of the original, unencoded dataset. We could demonstrate that quantum kernels are comparable to or even better than the classical support vector machine kernels regarding the mean absolute percentage error scores for both encoded and unencoded datasets.

1 INTRODUCTION

Machine learning (ML) methods of any kind are used to generate satisfying and reliable price forecasting applications for different use cases and industries. One example is the sector of heavy construction equipment dealers that rely heavily on accurate price predictions. Determining their fleet’s current and future residual value allows construction equipment dealers to identify the optimal time to resell individual pieces of machinery (Lucko et al., 2007; Chiteri, 2018). Using ML methods to calculate the residual value of construction equipment is of high interest and has already been tested in the past (Zong, 2017; Chiteri, 2018; Milošević et al., 2021; Shehadeh et al., 2021; Alshboul et al., 2021; Stühler et al., 2023). It has been shown, that the use of existing ML and automated machine learning (AutoML) methods generate good results for different applications and datasets (Zöller et al., 2021; Zoph and Le, 2016; Stühler et al., 2023).

Although generating desirable results, these methods have a strong demand for computational power needed to create accurate results within a reasonable runtime. Here is where quantum computers (QCs) with their promised quantum advantage (Shor, 1999; Harrow et al., 2009; Huang et al., 2021; Liu et al., 2021) come into play. The new field of quantum machine learning (QML) based on QCs provides new possibilities for generating powerful quantum-based ML applications with better accuracy and less time and power consumption.

A commonly employed approach in ML for both classification and regression tasks is the Support vector machine (SVM) (Steinwart and Christmann, 2008). SVMs depend on the creation of kernel matrices. Selecting the most appropriate kernel depends on the specific problem at hand, and QML methods pro-
vide new possibilities for generating potent quantum kernels (Huang et al., 2021; Thanasilp et al., 2022).

This study uses various fidelity and projected quantum kernel techniques to address an industrial price forecasting application (Stühler et al., 2023). Our analysis focuses on evaluating the most promising quantum kernels documented in the literature and assesses their performance against an optimized classical SVM kernel. Similar to the work presented in (Grossi et al., 2022), we use different feature set combinations of the dataset to examine the importance of the features and their impact on the results.

Our work extends previous studies regarding two novel aspects. (a) In contrast to previous works, our dataset contains categorical features that require conversion into numerical features, a task achieved through the implementation of the one-hot-encoding method. However, this process substantially augments the dataset’s dimensionality, which poses a challenge given the current constraints of noisy intermediate scale quantum (NISQ) computers. To address this issue, we employ autoencoders (Bank et al., 2020) to acquire a condensed representation of the feature space that retains the essential information from the initial data, as it was also done in the context of anomaly detection with QML in (Woźniak et al., 2023). (b) We extend the latter approach by not only using fidelity quantum kernels but also projected quantum kernels (Huang et al., 2021), which are promising candidates for the utility of near-term quantum computing schemes. We finally analyze the results of the different (Q)SVM methods and compare the results of the encoded data sets with those of the original data sets to investigate the impact of autoencoders on the entire pipeline.

The work is structured as follows: In section 2, we present related work. Section 3 describes the methodology. The main findings are presented in Section 4 followed by a conclusion.

2 RELATED WORK

2.1 Machine Learning for Price Prediction

In order to interpret the results within this paper and to embed these findings in the current literature, let us briefly recap the most related work and their special focus. (Zong, 2017) estimates the residual value of used articulated trucks using various regression models. Similarly, (Chiteri, 2018) analyses the residual value of $\frac{3}{4}$ ton trucks based on historical data from auctions and resale transactions. Furthermore, (Milošević et al., 2021) construct an ensemble model based on a diverse set of regression models to predict the residual value of 500 000 construction machines advertised in the USA. In addition, (Shehadeh et al., 2021) and (Alshboul et al., 2021) use various regression models to predict the residual value of six construction equipment types based on data from open-accessed auction databases. Finally, (Stühler et al., 2023) compared seven different state-of-the-art and well-established ML methods with three AutoML methods on a dataset generated from real online advertisements, consisting of 2910 datapoints from 10 different Caterpillar models.

All these research activities underline the advantages and necessity of ML methods when dealing with price forecasting applications.

2.2 Quantum Machine Learning

In the search for an advantage over classical methods with quantum computing, machine learning is expected to be one of the first fields to benefit from quantum computers (Biamonte et al., 2017). Quantum machine learning deals with incorporating quantum algorithms for learning problems. Proven quantum advantages in QML are based on algorithms that can only be executed on fault-tolerant QC (Shor, 1999; Harrow et al., 2009; Huang et al., 2021; Liu et al., 2021). As this field just started with the emergence of commercially available NISQ computers, the practical implementation of the already known algorithms is still in its infancy. There are three reasons why we decided to use quantum support vector machines (QSVMs): (a) The proven speed-up in a constructed theoretical problem based on the discrete logarithm (Liu et al., 2021). (b) From a mathematical point of view, classical SVMs are well understood within the statistical learning theory in terms of error bounds, convergence, robustness, and computational complexity (Steinwart and Christmann, 2008; Schölkopf et al., 2002; Vapnik, 1999; Cortes and Vapnik, 1995). Since for most QSVMs only the kernel estimation is done on a quantum computer, there are rigorous error bounds as well (Huang et al., 2021). (c) QSVMs are especially suitable for the NISQ era because of their shallow circuits. It should be noted that the SVM optimization can be formulated as a quadratic unconstrained binary optimization (QUBO) problem (Willsch et al., 2020; Cavallaro et al., 2020) and can hence be solved on a quantum annealer (Kadowaki and Nishimori, 1998; Das and Chakrabarti, 2005; Hauke et al., 2020). While this is its own research branch, we focus on kernel-based quantum regression in the scope of this paper.
3 METHODOLOGY

To examine the QML capabilities, we compare four quantum support vector regression (QSVR) methods, which will be introduced in chapter 3.4 and chapter 3.5 with a state-of-the-art classical support vector regression (SVR) implementation, introduced in chapter 3.3. The overall method and the case study pipeline are depicted in Figure 1 and explained in the subsequent sections. The developed source code is available on GitHub1.

3.1 Data Creation

The initial data was obtained by regularly collecting all advertisements from seven major construction equipment market portals2 over a time period of seven months. Table 1 shows the collected and selected features.

Table 1: Collected dataset features with types and examples.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brand</td>
<td>Categorical</td>
<td>Caterpillar</td>
</tr>
<tr>
<td>Model</td>
<td>Categorical</td>
<td>329</td>
</tr>
<tr>
<td>Extension</td>
<td>Categorical</td>
<td>E</td>
</tr>
<tr>
<td>Construction year</td>
<td>Numerical</td>
<td>2018</td>
</tr>
<tr>
<td>Working hours</td>
<td>Numerical</td>
<td>8536</td>
</tr>
<tr>
<td>Location</td>
<td>Categorical</td>
<td>Germany</td>
</tr>
<tr>
<td>Price</td>
<td>Numerical</td>
<td>59.000 €</td>
</tr>
</tbody>
</table>

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1 See https://tinyurl.com/ymmts5xc.
2 The market portals are Mascus, Catused, Mobile, MachineryLine, TradeMachines, Truck1, and Truckscout24.
Table 2: Excerpt of the Caterpillar 329 dataset.

<table>
<thead>
<tr>
<th>Extension</th>
<th>Construction year</th>
<th>Working hours [h]</th>
<th>Location</th>
<th>Price [€]</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>2012</td>
<td>10600</td>
<td>DE</td>
<td>77,000</td>
</tr>
<tr>
<td>D</td>
<td>2008</td>
<td>18180</td>
<td>CH</td>
<td>47,499</td>
</tr>
<tr>
<td>E</td>
<td>2012</td>
<td>11424</td>
<td>DE</td>
<td>72,900</td>
</tr>
<tr>
<td>E</td>
<td>2014</td>
<td>11500</td>
<td>DE</td>
<td>89,900</td>
</tr>
</tbody>
</table>

Table 3: Feature set combinations with the corresponding input and latent space dimensions. The features working hours & construction year form the basic subset and are the basis of all feature set combinations. The maximum size of the latent space is 10. All feature sets are encoded to guarantee comparability.

<table>
<thead>
<tr>
<th>Feature set</th>
<th>Input size</th>
<th>Latent size</th>
</tr>
</thead>
<tbody>
<tr>
<td>basic subset</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>basic subset + extension</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>basic subset + location</td>
<td>16</td>
<td>10</td>
</tr>
<tr>
<td>basic subset + extension + location</td>
<td>18</td>
<td>10</td>
</tr>
</tbody>
</table>

3.2 Autoencoding

The autoencoder (AE) (Tschannen et al., 2018; Ng et al., 2011) is an unsupervised learning algorithm that consists of two neural networks - the encoder and the decoder (see Figure 3). While the former is used to encode the input data in a reduced or dense representation, called latent representation, the latter is used to decode the original input from this reduced representation. One advantage of using an AE is its flexibility, i.e., the dimensionality of the latent space representation can be changed by adding or removing neurons, which is used to generate latent spaces depending on the size or dimensionality of the datasets.

As mentioned in section 3.1, we are dealing with four datasets with different, even feature set combinations, which are displayed in Table 3 together with their original and latent space dimensions. The features working hours & construction year form the basic subset. The maximum size of the latent space is 10. Therefore, if the input dimension is greater than 10, it will be reduced to 10 by the AE. Feature sets that are less than or equal to 10 are autoencoded with the latent space size equal to the input space dimension. This is done to guarantee consistency for all feature set combinations. We use the Adam optimizer, the Mean-Square-Error loss, the Relu activation for encoding, and the Sigmoid activation for decoding.

3.3 Support-Vector-Machines

Support vector machines (SVMs) are heavily used ML methods for linear or nonlinear classification and regression tasks mainly for small or medium-sized datasets (Géron, 2022). In contrast to a "simple" linear classifier, a support vector classifier (SVC) tries to find a separating hyperplane between two classes such that the distance between the closest training instances is maximized. This is called a large margin classifier. These closest instances are called support vectors. Hence the name support vector machine.

SVMs are designed to work in linearly separable feature spaces. If the data points are not linearly separable in the original feature space, the feature space can be transformed into a higher dimensional feature space, where the problem becomes linearly separable.

Figure 3: A typical autoencoder consists of two deep neural networks with multiple dense layers. The encoder transforms the input data into the latent space representation, which is reconstructed by the decoder. The autoencoder is trained to reduce the reconstruction error; hence, it trains a lower-dimensional representation of the input data in an abstract mathematical space.
ble. This computationally expensive transformation can be avoided using the kernel trick or kernel function. Commonly used kernel functions are the linear kernel, the polynomial kernel, and the radial basis function (RBF) kernel. Applying the kernel function to all data points results in the kernel matrix, a square matrix containing the similarity measures between all data points in the dataset. The kernel matrix is used to optimize the hyperplane that maximally separates the classes in the transformed, potentially high-dimensional feature space. This, in turn, avoids the computationally expensive transformation. We use GridSearch for the classical SVR algorithm to find the optimal kernel and hyperparameters.

3.4 Feature Maps

Quantum feature maps are a way of mapping classical data into a quantum state, which is then used as an input to estimate a quantum kernel. There are several ways to encode the data, including amplitude encoding and the basis embedding method. The choice of which method to use depends on the problem being addressed. In (Schuld et al., 2017; Havlíček et al., 2019), it was shown that amplitude encoding outperformed the basis embedding method for certain datasets and vice versa for others. However, for NISQ applications, we encode the classical data with Pauli rotations as they comprise the most hardware-efficient method. We encode the k-th feature of the i-th data point $x^i \in [-1, 1]$ by using single-qubit rotations around the x-, y- or z-axis on the Bloch sphere denoted by $R_x, R_y, R_z$

$$R_x(x^i) = e^{-iXx^i/2},$$

$$R_y(x^i) = e^{-iYx^i/2},$$

$$R_z(x^i) = e^{-iZx^i/2},$$

where $X = |0\rangle \langle 1| + |1\rangle \langle 0|$, $Y = -i|0\rangle \langle 1| + i|1\rangle \langle 0|$ and $Z = |0\rangle \langle 0| - |1\rangle \langle 1|$ are Pauli matrices. A popular basis gate set used on NISQ computers is

$$\{\text{CNOT, Id, } R_z, \sqrt{X}, X\},$$

where CNOT is the only multi-qubit gate in that set that is able to introduce entanglement into the feature map. An example of such an encoding can be found in Figure 4 (note that this is the untranspiled circuit). In that feature map, we encode two features per qubit as a good tradeoff between resources and the expressivity of the model. The quantum feature map should be designed such that it cannot be simulated in polynomial time on a probabilistic classical computer, in accordance with the Gottesman-Knill theorem (Aaronson and Gottesman, 2004).

![Quantum Feature Map for 3 features without any entanglement.](image)

Figure 4: Quantum Feature Map for $n$ features without any entanglement (below: QSVR$_{re=0}$).

![Quantum Feature Map for 3 features with an entanglement between the encoding unitaries (as required by the inversion test, below: QSVR$_{re=lin}$.](image)

Entanglement, which is applied on QSVR$_{re=lin}$ in Figure 5, can enhance the expressive power of quantum feature maps, but it can also make the implementations of QSVMs more difficult due to the increased complexity of entangled quantum states. However, another way of increasing the expressivity of a quantum feature map is by the so-called data-reuploading scheme (Schuld et al., 2021; Jerbi et al., 2023), which is applied on QSVR$_{re=1}$ in Figure 6 to make a more expressive feature map. The entanglement layer, which is implemented by a ring of CNOTs, is in between the encoding rotations due to the way quantum kernel estimation is implemented (via the inversion test) in some of our experiments.

3.5 Quantum Kernels

We use two types of quantum kernels in our experiments: fidelity and projected quantum kernels. We use the inversion test for the quantum kernel estimation of the fidelity quantum kernels with the three feature maps introduced in section 3.4, whereas, for the projected quantum kernels, we use the DensityMatrix class from the Qiskit Quantum Information library.

Fidelity quantum kernels $k(x_i, x_j)$ via the inversion test are given by

$$k(x_i, x_j) = \left| \langle \psi(x_i) | \psi(x_j) \rangle \right|^2,$$

where $\psi(x_i) = U_\phi(x_i) |0\ldots0\rangle$ is the quantum state after passing through the quantum feature map $\phi(x_i)$ applied on the i-th classical datapoint. We
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Projected Quantum Kernels: $k(x_i,x_j)$ that we use are given by

$$k(x_i,x_j) = \exp\left(-\gamma \sum_{k=0}^{n_q} ||\rho_k(x_i) - \rho_k(x_j)||^2\right),$$

where $\gamma > 0$ and the reduced density matrix $\rho_k(x_i)$ denotes the density matrix $\rho(x_i)$ created by the quantum feature map applied on the datapoint $x_i$.

Figure 6: Quantum Feature Map for $n$ features with entanglement and data re-uploading (below: QSVR$_{en=lim}$).

Figure 7: Quantum Feature Map for $n$ features with entanglement by CNOT gates (below: QSVR$_{proj}$).

3.6 Performance Metric

Within this work, we use the accuracy to benchmark the performance of the introduced methods.

Accuracy: measures the predictive power of an ML model. In the context of this work, the mean absolute percentage error (MAPE)

$$\text{MAPE} = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{y_i - \hat{y}_i}{|y_i|} \right|$$

is used to calculate the performance, with $y_i$ being the true value, $\hat{y}_i$ the predicted value and $n$ the number of data points.

4 RESULTS

This section presents the results of the experiments. All measurements were performed on a Ubuntu Linux 20.04.5 LTS system with 64 GB RAM and an AMD Ryzen Threadripper 192X 12-Core Processor. We used Qiskit (IBM-Qiskit, 2023; IBM, 2018) and...
Qiskit Aer (Wood, 2019) for all QC simulations and conducted five independent measurements with the identical 80% / 20% holdout training/test split.

### Accuracy

The accuracy, in terms of the MAPE, of the different methods is depicted in Figure 8 for the encoded datasets and in Figure 9 for the unencoded datasets. In particular, these figures visualize the following characteristics:

1. On the encoded datasets, all of the applied QSVR methods, with the exception of QSVR\(_{\text{proj}}\) for the complete dataset, perform better than the classical SVR implementation.
2. On the unencoded datasets, with the exception of the basic dataset, QSVR\(_{r\_e=0}^{m=0}\) or QSVR\(_{\text{proj}}\) perform better than the classical SVR method.
3. All results indicate good prediction qualities for the encoded and unencoded datasets as they are roughly within the interval \([0.13, 0.17]\).
4. QSVR\(_{r\_e=0}^{m=0}\) performs best in three out of four encoded feature sets. It shows the overall best performance for the encoded feature set but worst in three out of four unencoded feature sets. QSVR\(_{r\_e=0}^{m=ln}\) performs best for the unencoded feature sets. Examining these results in detail and the impact of AE on the different QSVR methods will be systematically analyzed in future work.
5. The encoded datasets exhibit much more variance than the unencoded datasets. This is due to the variance of the autoencoder. This exhibits the influence of the AE on the accuracy of the results. This fact needs to be taken into account for each calculation.
6. The impact of the features is obvious for both unencoded and encoded datasets. Adding the extension features to the basic subset downgrades the accuracy within the unencoded and encoded datasets. The best result is always achieved within
Figure 9: Accuracy for the unencoded feature sets, in form of MAPE. Diamonds depict the average results over 5 repetitions. Single measurements are displayed as dots. QSVR$_{proj}$ needs at least four features; therefore, there are no basic subset results for QSVR$_{proj}$.

the complete feature set.

The MAPE values of all five methods for the complete feature set of the encoded and unencoded data sets are depicted in Table 4.

5 CONCLUSION

This work analyzed the potential of QMLs methods as a substitution for linear, polynomial, or RBF kernels for the SVR algorithm. In our case study, predicting the residual value of used heavy construction equipment, all simulated QML methods were shown to be comparable or even better than the classical SVM kernels regarding the MAPE scores. Therefore, we showed that current state-of-the-art QSVR algorithms are able to substitute the classical SVR implementations.

It has to be mentioned that we only examined a limited number of QML methods on four variations of a single data set, so general statements are therefore limited by our choice of methods.

In order to strengthen the significance of our statistics, we will extend our survey to additional and in particular open-source data sets. This analysis will enable us to validate and substantially generalize the statements of our paper. Furthermore, we will examine the role of entanglement and the power of quantum kernels in more detail. We will analyze the impact of dimensionality reduction, which will be mandatory in the near future for datasets with larger feature sets, on the quantum model performance in future work. Finally, we will add more QML methods to our case study and integrate a real QC hardware backend into our framework to be able to run the QML algorithms on a real QC.

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REFERENCES


