Quantum Machine Learning using Gaussian Processes with Performant Quantum Kernels

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Quantum computers have the opportunity to be transformative for a variety of computational tasks. Recently, there have been proposals to use the un simulat ably of large quantum devices to perform regression, classification, and other machine learning tasks with quantum advantage by using kernel methods. While un simulat ably is a necessary condition for quantum advantage in machine learning, it is not sufficient, as not all kernels are equally effective. Here, we study the use of quantum computers to perform the machine learning tasks of one- and multi-dimensional regression, as well as reinforcement learning, using Gaussian Processes. By using approximations of performant classical kernels enhanced with extra quantum resources, we demonstrate that quantum devices, both in simulation and on hardware, can perform machine learning tasks at least as well as, and many times better than, the classical inspiration. Our informed kernel design demonstrates a path towards effectively utilizing quantum devices for machine learning tasks.

The growing size and quality of quantum computers, especially now that quantum supremacy has been demonstrated [1], has led to increased interest into practical applications. Quantum chemistry [2–5] and quantum dynamics [6–8] have shown small demonstrations and promising algorithms for the solution of scientific problems. Due to the exponential growth in the Hilbert space with the increasing size of quantum computers, machine learning has the potential to be a strong application of quantum computing, even in the near term [9]. The size of the Hilbert space, however, is not enough to guarantee an efficient machine learning algorithm. For instance, recent results on the optimization of quantum neural networks have shown the existence of barren plateaus in the training landscape [10, 11]. Nevertheless, demonstrations of quantum machine learning include using the quantum computer to encode data in a quantum state (often known as a feature map) and estimating the inner product, or kernel, of two data points. The value of the kernel can then be used in classical machine learning tasks, such as support vector machines for classification [12–14]. These demonstrations focused on the general framework of classification using quantum computers, but did not deeply discuss the important aspect of kernel design. Other methods have also been studied that directly use the output of the quantum computer for a regression task [15]. Though a quantum computer can generally prepare feature maps that are un simulatable on classical devices, not every feature map is capable of providing the same expressibility. In this manuscript, we demonstrate that a quantum computer can provide interesting, useful kernels for Gaussian Processes (GPs) for the tasks of regression and reinforcement learning. We show how classically proven kernels can inspire new quantum enhanced kernels while still maintaining the important features of the classical kernel. We start from coherent states, as they approximate the standard squared exponential kernel [e.g., 16], and show how such states can be prepared on both qudit and qubit hardware, demonstrating one-dimensional regression using a superconducting qubit architecture. Furthermore, we demonstrate that very small quantum devices with only a few operations can perform higher-dimensional regression better than the squared exponential kernel by utilizing entanglement and non-classicality. Finally, we demonstrate that small quantum devices can be used in a GP-based reinforcement learning scheme to solve the classical control problem of driving a one-dimensional car up a hill.

Gaussian Process Regression Gaussian Processes are flexible, nonparametric Bayesian models that are performant on a variety of statistical and machine learning tasks including regression and classification [16, 17], simulation surrogate modeling [18], robotics control [19], and reinforcement learning [20]. GP regression, which is summarized in the Methods section, predicts function values at un observed feature locations by calculation of the kernel between features, including both observed and unobserved. The choice of kernel thus directly influences regression quality. The kernel between points $x$ and $x'$ is implicitly calculated by a nonlinear feature map, $\phi(x)$, such that $k(x, x') = \langle \phi(x) | \phi(x') \rangle_F$, where the inner product is taken over a reproducing kernel Hilbert space $F$ with kernel $k(\cdot, \cdot)$. This mapping into higher-dimensional space where observation discrimination becomes linear is the celebrated “kernel trick” applied throughout machine learning. For quantum computing, we identify the fea-
A quantum computer can represent functions that classical computers cannot efficiently calculate [12], opening the door for interesting and powerful kernels exclusive to quantum computers. However, an unsimulatable feature map is not guaranteed to provide accurate machine learning results. Instead of starting with an unsimulatable feature map, we instead start with approximations of performant classical feature maps and show that quantum computers can enhance their performance by using additional quantum resources, such as entanglement. Figure 1 demonstrates the general method used in this paper. Classical data is encoded on the quantum computer using approximations of a feature map corresponding to a performant classical kernel. Extra quantum resources, such as entanglement, lead to a quantum enhanced feature map, which is mapped to quantum hardware. Through the quantum device, the kernel matrix is evaluated. Then, using GPs on classical computers, predictions are made using the calculated quantum kernel.

**Coherent State Quantum Kernel** A general kernel, prepared on a quantum computer, is simply the overlap of two quantum states, $k(x, x') = \langle \phi(x) | \phi(x') \rangle$, where $|\phi(x)\rangle$ is a quantum circuit or other state preparation procedure [12, 13]. There is freedom in the choice of feature map; different feature maps will have differing performance. Here, we construct quantum kernels inspired by coherent states because (i) the coherent state is easy to prepare on a variety of quantum devices and, (ii) the inner product of canonical coherent states produces the classically popular squared exponential kernel. A general (canonical) coherent state of complex parameter $\alpha$ is defined as

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle.$$  \hspace{1cm} (1)

The equation for the magnitude squared of the overlap between two canonical coherent states is $|\langle \alpha | \beta \rangle|^2 = e^{-|\alpha - \beta|^2}$, exactly the same form as the squared exponential kernel. The input data can be encoded in a variety of ways, but we choose to encode the data as $\alpha_i = x_i/(\sqrt{2}c_i)$, where $c_i$ are real hyperparameters, to maintain consistency with the standard definition of the squared exponential kernel. We also allow for an additional hyperparameter which scales the result by a constant, leading to the coherent state kernel

$$k(x, x') = s \prod_i \left| \frac{x_i}{\sqrt{2}c_i} - \frac{x_i'}{\sqrt{2}c_i} \right|^2,$$  \hspace{1cm} (2)

where the product is taken over data dimensions, $s$ is a scaling hyperparameter, and $|\frac{x_i'}{\sqrt{2}c_i}\rangle$ is a coherent state with parameter $\alpha = \frac{x_i'}{\sqrt{2}c_i}$.

Although true coherent states can naturally by prepared on a variety of systems, the ability to provide non-classicality on these systems can be difficult [21]. As such, we look at truncations of the coherent state that are amenable to preparation on near-term quantum devices such as weakly anharmonic superconducting resonator cavities or sequences of qubits, which can more easily prepare non-classical states due to their ability to perform universal quantum computation. To prepare these states, we note the full coherent state of eq. (1) can be prepared by applying the displacement operator to the vacuum state, i.e., $|\alpha\rangle = D(\alpha)|0\rangle = e^{\alpha(b^\dagger - b)}|0\rangle$, where $b^\dagger$ is a bosonic creation operator and we have now restricted
to real $\alpha$. Generally, $b^\dagger$ is an infinite dimensional object, but we can truncate the Hilbert space at some maximum number of levels $N$, giving a representation of the operator $b^\dagger$ in a finite Hilbert space, $b^\dagger_N$. A finite-dimensional coherent state can be prepared that approximates the full coherent state by using the finite-dimensional operators $b^\dagger_N$ in the displacement operator. This finite-dimensional displacement operator, $D_N(\alpha) = e^{\alpha(\hat{b}^\dagger_N - \hat{b}_N)}$, is also a natural operator on many quantum architectures, such as superconducting microwave cavities [22]. By using the finite-dimensional displacement operator on such systems, we can easily prepare approximations of the coherent state and follow with further manipulations using universal gates.

We will denote kernels using the finite-dimensional coherent state at some level $N$ as C-N. For qubit based systems, the finite-dimensional coherent state is not a natural operation. To prepare it, we first decompose the $N$ level operator into $\log_2(N)$ Pauli operators to get a qubit Hamiltonian. We then apply a Trotter decomposition [e.g., 23] to the exponential of the Hamiltonian to obtain a sequence of gates that are amenable to qubit based devices; details of this construction can be found in the Supplementary Information. The Trotter decomposition approximates the exponential of a sum of non-commuting terms as the product of exponentials of each term. Additional accuracy can be achieved by repeating the product of the exponentials with reduced coefficients. This becomes exact in the limit of infinite Trotter steps. We will denote kernels using the finite-dimensional coherent state of size $N$ prepared on qubits with a number of Trotter steps $m$ as CQ-N-tm. The use of the finite-dimensional Hilbert space, especially in the superconducting cavity and qubit regimes, allows for simple inclusion of non-Gaussian gates.

The finite-dimensional displacement operator, and the qubit version thereof, define quantum feature maps that are approximations of the feature map of the classical squared exponential kernel. To measure the overlap between two points, we use the ‘echo’ technique [12, 15], where we measure the magnitude of the overlap between two points $x$ and $x'$ by measuring the population of the vacuum after application of the $D_N(\alpha)$ and $D_N^\dagger(\beta)$ to the vacuum, an example of which is shown in the circuit in Fig. 1. Since we are utilizing approximations of the coherent state, we can instead implement $D_N(\alpha - \beta)|0\rangle = D_N^\dagger(\beta)D_N(\alpha)|0\rangle$, reducing the total number of gates by a factor of two. The overlap between every pair of data points has to be calculated, resulting in the total number of quantum evaluations of the kernel scaling as the square of the number of data points.

We apply our classically inspired quantum feature maps to one-dimensional regression of the function $f(x) = x \sin(x)$. We simulate $M_{tr} = 40$ training points uniformly spaced in the region [0.1, 19.9] and perturb them with heteroscedastic Gaussian noise $\epsilon_i \sim \mathcal{N}(0, \sigma_i^2)$. We assume that the measurement variances $\sigma_i^2 \sim U[0, 1]$ are known. We then regress on $M_{te} = 100$ test points in the region [0,20], plotting the posterior mean as well as the 95% confidence interval. We use SciKit-Learn [24] to implement the GP regression and simulated the C-N and CQ-N-tm kernels using both the QuTiP [25] and QuaC [26, 27] simulation packages. The results and residuals of the regression are shown in Fig. 2. The C-4 kernel is able to regress at the same quality as the coherent state, while the two level case performs much worse (see Supplementary Information). This demonstrates that a very small quantum device with only a few operations, whether on a qudit or qubit platform, is able to regress $f(x) = x \sin(x)$ just as well as the coherent state. In the Supplementary Information, we apply the same regression technique to other functions, as well as with other levels of truncation and number of Trotter steps. The largest Hilbert space necessary was only sixteen states with, for the qubit kernel, only six Trotter steps.

We also implement the CQ-4-t3 kernel on the IBMQ quantum computer, Boeblingen, denoted by CQ-4-t3-HW. The use of NISQ hardware prompts us to apply an alternative GP prior model, given by

$$y = f + \epsilon + d. \quad (3)$$

Here, $y$, $f$, and $\epsilon$ are as in eq. (4) (see Methods), whereas $d_i \sim \mathcal{N}(0, \sigma_d^2)$ are i.i.d. Gaussian variates to capture the additional model discrepancy due to the hardware.
noise [28]. The noise inherent in the quantum computer results in much larger confidence intervals. However, note that the addition of model discrepancy term \( d \) allows the quantum computer to roughly capture the periodicity of the response function, all within the confidence intervals. Furthermore, the model discrepancy term allows the GP framework to include the effects of the sampling noise and decoherence from the quantum computer on the regression task. It could also potentially be used to understand the noise and provide application specific benchmarking.

Examining the results for various elements of the kernel directly can also lead to important insights. The diagonal of the kernel should be identically 1 multiplied by a prefactor; however, even when correcting measurement errors using Qiskit [29], the average of the diagonal elements is 0.98, without the prefactor. These errors are also present for points that are far apart in the feature space. Because we have the simulated kernel, we can compare small values of both the simulated and hardware kernels without the prefactor and model discrepancy terms. For the simulated kernel, training points 4 and 20 are considered very far away from each other and the kernel for these two points has a value of 1.7e-4. The corresponding point for the hardware kernel has a value of 0.02, significantly different. For the hardware kernel to have achieved the same value, it would need to have had only 1 shot out of the total 8192 shots not in the vacuum state. Various sources of noise, such as decoherence and remaining unmitigated readout noise, make the distinction between very similar and very distinct points difficult. Additional error mitigation techniques, such as noise extrapolation [30–34], could help alleviate these problems, but this still demonstrates an important restriction on near-term hardware for kernel-based quantum machine learning methods. Comparing very similar and very distant points is difficult in a noisy, shot-limited environment. Further details of the hardware implementation, including the full Gram matrix, as well as the optimal hyperparameters for all kernels, can be found in the Supplementary Information.

**Entanglement Enhanced Learning** Up until now, our quantum kernels have been simply approximations of classical kernels and offered no route to quantum advantage. Quantum advantage could be obtained by adding additional operations with additional universal gates after the preparation of finite-dimensional coherent states [12, 15]. Another route, which we explore here, is adding a hyperparameter that entangles the coherent states representing different data dimensions. Recall that the default coherent state (and standard classical squared exponential) kernel would simply take the product of the kernels of each data dimension (see eq. (2)). As an enhancement to this, we use the multimode squeezing operator to generate entanglement between the data dimensions for a multi-dimensional regression problem. Squeezing is a standard experimental technique for generating interesting quantum states, and finds use in quantum metrology, as it increases the sensing precision in one quadrature at the cost of others [35–37]. Two-mode squeezing has been demonstrated in a variety of architectures [38–40], including superconducting cavities [41]. Higher mode squeezing and other multimode interactions, while more difficult, have also been demonstrated [42, 43].

To generate the entanglement enhanced kernel, we first apply the two-mode squeezing operator to a pair of data dimensions, followed by the displacement operator, to generate two-mode squeezed coherent states. This is shown in the circuit in Fig. 1. The analytical form of such states and their overlap, in the infinite \( N \) limit, is derived in the Supplementary Information. We use a computationally tractable approximation of the analytic form to simulate these states. Squeezing represents a purely non-classical effect that goes beyond the approximations of the coherent state. Such squeezing operations can also be applied to finite-dimensional coherent states and can further be decomposed into a qubit form. The amount of squeezing is added as an additional hyperparameter in the kernel. It is important to note that certain Gaussian states with quadrature measurements can be simulated classically [44]; sources of non-Gaussianity can be added with further control, especially on systems capable of universal quantum computation.

We apply the two-mode squeezed kernel to the multidimensional regression problem of predicting the dynamics of a car on a hill, given its current position, \( x \); velocity, \( v \); and acceleration, \( a \). We entangle each pair of dimensions (\( x \) and \( v \), \( v \) and \( a \), and \( a \) and \( x \)) separately, take the product of each entangled kernel, and then take the square root of the total kernel to ensure that, in the limit of zero squeezing, the kernel is equivalent to the unentangled coherent state product kernel. Further details of the squeezed kernel can be found in the Supplementary Information.

| Kernel       | \( R^2 \) | \( \sigma_x \) | \( R^2 \) | \( \sigma_v \) |
|--------------|----------|---------------|----------|---------------|
| Coherent     | 0.9985   | 4.3e-4        | 0.9487   | 0.0277        |
| Squeezed     | 0.9983   | 5.4e-4        | 0.9549   | 0.0217        |
| C-8          | 0.9985   | 4.3e-4        | 0.9326   | 0.0496        |
| C-16         | 0.9985   | 4.3e-4        | 0.9508   | 0.0216        |
| C-32         | 0.9985   | 4.3e-4        | 0.9487   | 0.0276        |

**TABLE I.** Average \( R^2 \) values and standard deviations for dynamics regression using 10 training sets of \( M_{tr} = 128 \) random points each tested on \( M_{te} = 100 \) random test points.
and tabulate the results in Table I. The prediction of the next position ($x$) is very good for all of the kernels. The next velocity ($v$) is not regressed nearly as well, and it is here where the entanglement provides a quantifiable benefit. The average $R^2$ for the coherent kernel is 0.9487, whereas the squeezed has a significantly higher average score of 0.9549. Interestingly, the finite-dimensional coherent state of size sixteen also performs better than the full coherent state. $R^2$ scores for each training set can be found in the Supplementary Information.

It is instructive to examine the optimal hyperparameters to understand how much entanglement is generated for each of the dimensions. A full list of the optimal hyperparameters, for all kernels, and for all training sets is given in the Supplementary Information. Notably, in the regression of the position, $x$, the optimal hyperparameters for every training set include a large amount of squeezing between the data dimensions representing the current position and current velocity and include very little squeezing otherwise. This implies that the current position and current velocity have strong correlation that can be used to predict the next position. In the regression of the velocity, $v$, there is, generally, much less squeezing in the optimal hyperparameters, and the most squeezing is between the current velocity and current acceleration. The amount of squeezing seen in the optimal hyperparameters represents the structure of the dynamical equations which generate the training points, and is supported by a simple linearization of the underlying equations.

In some training sets, the coherent and squeezed kernels perform the same for the regression of $v$. This is because the optimal hyperparameters create very little entanglement between the data dimensions, and essentially find the best unentangled kernel. This is one of the benefits of using entanglement enhanced but classically inspired kernels. We have a guarantee that the squeezed state kernel will perform at least as well as the coherent state (and, thus, the squared exponential) kernel in log marginal likelihood because the unentangled coherent states are a subset of the squeezed states. This gives a performance guarantee for the quantum kernels we have outlined in this manuscript; they will perform at least as well as their classical inspiration. It also allows for an efficient initial guess of the hyperparameters, which may be important due to the possibility of barren plateaus in quantum applications [10, 11].

Reinforcement Learning Given that a small quantum device, with and without entanglement, can accurately predict the dynamics of a car on a hill, we now explore using quantum kernels to perform reinforcement learning. In reinforcement learning, an agent observes its environment, decides a course of action, and gets a reward based on that action [45]. We use a GP framework to perform reinforcement learning on the classic control problem of driving a car up a hill [20, 46]; the agent is rewarded when the car reaches the goal. GP based reinforcement learning uses trained GPs to predict the dynamics, and an additional trained GP to predict the value function. In the GP reinforcement learning process, the car’s position ($x$), velocity ($v$), and acceleration ($a$) are all used in the regression. After converging the regression of the dynamics and of the value function, we use the trained GPs to control the car as it moves forward in time. The basic framework for reinforcement learning and the agent’s environment and goal are shown in Fig. 3(a).

Figure 3(b) shows the result of applying GP reinforcement learning to drive a car up a hill using the quantum kernels described earlier. The coherent state is able to rapidly reach the goal and stays there for the remainder of the simulation time. The finite-dimensional coherent state of eight levels (C-8), on the other hand, reaches the goal a few times but cannot keep the car there. With a Hilbert space size of sixteen levels (C-16), the car again
rapidly reaches the goal and stays there. Optimal hyperparameters for these kernels can be found in the Supplementary Information. This demonstrates that a small quantum computer can perform reinforcement learning. More demanding reinforcement learning tasks may necessitate the need for entanglement between the data dimensions.

Discussion We have demonstrated that small, noisy quantum devices with kernels inspired by and improving on well-studied classical kernels can be performant for a variety of GP-based machine learning tasks, including one- and multi-dimensional regression, as well as reinforcement learning. Utilizing a GP framework, the method allows for natural inclusion of the inevitable quantum noise as a model discrepancy term in the GP noise model [e.g., 28]. By using informed kernel design, inspired by performant classical kernels, we can provide guarantees that, in the absence of noise, the quantum computer will perform as well as its classical counterpart. The quantum computer, however, has additional quantum resources not available to the classical kernel, allowing for the possibility of more performant machine learning. This is demonstrated by using the resource of entanglement, through two-mode squeezing between data dimensions, in a form unavailable to classical kernels. We utilized this quantum enhancement to increase the performance of multi-dimensional regression of the dynamics of a controlled one-dimensional car.

The enhancement of a standard kernel represents an important element of this work to both quantum and classical machine learning. The squared exponential kernel, for example, can be described by an embedding into a quantum feature space through the canonical coherent state [16, 47]. Starting from this embedding, we can examine novel kernel design by examining the structure of the embedding. For instance, by using the squared exponential kernel as an inspiration for a quantum kernel, we start with a feature map that we can analyze, test, and understand using classical techniques. We can then design feature maps that have more structure or fill a larger volume of feature space than the canonical squared exponential feature maps by implementing operations that impose new structure on the embedding, potentially offering the ability to learn more complex functions, but without losing the well-studied features of the classical inspiration.

Though we have demonstrated that quantum devices can prepare interesting feature maps, the kernel-based GP method we used still has the draw back that the quantum computer needs calculate the kernel for every pair of data points. Given the capabilities of near-term hardware, this could make learning on large datasets infeasible, especially if hyperparameter optimization becomes costly. Solving the GP problem directly on the quantum hardware, without having to read off the whole kernel matrix, is a promising avenue for reducing this overhead. It has already been reported the HHL algorithm [48] could potentially perform the important matrix inversion step of the GP method [9], but further study is needed to understand the full solution of the GP on the quantum device. However, any future algorithm will still likely require interesting and performant feature maps, such as those studied here. Other quantum enhanced feature maps based on different classical kernels, such as the neural network kernel [49], should also be studied to understand the limits of expressibility on quantum devices. The use of improved quantum hardware for even more difficult machine learning tasks (such as Bayesian search problems [50] and other problems in filtering, prediction, and control) represents another promising direction.

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Author Contributions All author contributed to the research and writing of the paper. M. O. ran the GP learning tasks, simulated the quantum kernels, and designed the form of the squeezed kernel. I. R. G. provided the GP reinforcement learning code. B. W. P. provided descriptions and interpretations of GP learning. G. F. C. and M. D. S. proposed the idea of using coherent states for machine learning tasks.

Data/Code Availability The data and code that support the findings of this study are available from the corresponding author on reasonable request.

Competing Interests The authors declare no competing interests.

METHODS

Gaussian Process Regression

A GP specifies a prior distribution over functions, which combined with observations specifies a posterior distribution. A scalar GP is defined as a distribution \( GP(m(\cdot), k(\cdot, \cdot)) \), where \( m(\cdot) \) is a mean function (often set without a loss of generality to zero) and \( k(\cdot, \cdot) \) is...
a positive definite reproducing kernel on the input domain. A GP prior for \( n \) possibly multi-variate inputs \( X = \{x_1, \ldots, x_n\} \) and \( n \) scalar outputs \( y \) is

\[
y = f + \epsilon
f \sim \mathcal{N}(0, K_{X,X})
\epsilon_i \sim \mathcal{N}(0, \sigma_i^2).
\]

(4)

Here \( \mathcal{N} \) is the multivariate Normal (i.e., Gaussian) distribution, \( K_{X,X} \) is an \( n \times n \) matrix whose \((i,j)\)th element is \( k(x_i, x_j) \) and \( \epsilon \) is heteroscedastic measurement noise with prior variance vector \( \sigma^2 \) \( [\sigma_1^2, \ldots, \sigma_n^2] \). We assumed throughout that \( \sigma^2 \) is known a priori. The joint distribution of \( y \) and the response \( f_i \) of \( n \) unseen data \( X_i \) is

\[
\begin{bmatrix}
y \\
f_i \end{bmatrix} \sim \mathcal{N}
\begin{bmatrix}
0 \\
K_{X,X} + \Sigma
\end{bmatrix}
\begin{bmatrix}
K_{X,X} \\
K_{X,X}
\end{bmatrix}^{-1}
\begin{bmatrix}
f_i \\
X_i \end{bmatrix}.
\]

(5)

Here, \( \Sigma \) is a diagonal matrix whose \((i,i)\)th element is \( \sigma_i^2 \). This allows us to analytically derive the posterior of the response as

\[
f_i | X, X_i, \sigma^2, y \sim \mathcal{N}(\bar{f}_i, C)
\bar{f}_i \equiv K_{X_i,X} Q^{-1} K_{X,X} y
C \equiv K_{X_i,X} - K_{X_i,X} Q^{-1} K_{X,X}
Q_{X,X} \equiv K_{X,X} + \Sigma.
\]

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Supplementary Information for Quantum Machine Learning using Gaussian Processes with Performant Quantum Kernels

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**QUBIT DECOMPOSITION OF TRUNCATED DISPLACEMENT OPERATOR**

In this section, we describe the Pauli decomposition of the finite-dimensional displacement operator, allowing for the preparation of finite-dimensional approximations of the coherent state on qubit devices. Recall that the definition of the finite-dimensional creation operator with \( N \) levels, \( \tilde{b}_N^\dagger \), is simply the full bosonic creation operator, \( \tilde{b}^\dagger \) truncated to a \( N \times N \) matrix. For example, given a truncation of \( N = 4 \) levels, we have

\[
\tilde{b}_4^\dagger = \begin{bmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & \sqrt{2} & 0 \\
0 & 0 & 0 & \sqrt{3} \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

(1)

The corresponding finite-dimensional displacement operator is simply \( \tilde{D}_N(\alpha) = e^{\alpha(\tilde{b}_N^\dagger - \tilde{b}_N)} \). To evaluate this on qubits, we numerically searched for decompositions of \( \tilde{b}_N^\dagger - \tilde{b}_N \) into Pauli strings, resulting in representations that used the smallest number of qubits possible. For \( N = 4 \), we have simply \( \tilde{b}_2^\dagger - \tilde{b}_2 = Y \). For \( N = 4 \), we have

\[
\tilde{b}_4^\dagger - \tilde{b}_4 = \frac{1}{2} \left( (1 + \sqrt{3})YI + (1 - \sqrt{3})YZ + \sqrt{2}(XY - YX) \right).
\]

(2)

For \( N = 8 \), we have

\[
\tilde{b}_8^\dagger - \tilde{b}_8 = \frac{1}{4} \left( (1 + \sqrt{3} + \sqrt{5} + \sqrt{7} + \sqrt{9} + \sqrt{11} + \sqrt{13} + \sqrt{15})YIII + (1 + \sqrt{3} + \sqrt{5} + \sqrt{7} - \sqrt{9} - \sqrt{11} - \sqrt{13} - \sqrt{15})YIZ \right. \\
+ (1 + \sqrt{3} - \sqrt{5} - \sqrt{7} + \sqrt{9} + \sqrt{11} - \sqrt{13} - \sqrt{15})YIZI + (1 + \sqrt{3} - \sqrt{5} - \sqrt{7} - \sqrt{9} - \sqrt{11} + \sqrt{13} + \sqrt{15})YIZZ \\
+ (1 - \sqrt{3} + \sqrt{5} - \sqrt{7} + \sqrt{9} - \sqrt{11} + \sqrt{13} - \sqrt{15})YZZI + (1 - \sqrt{3} + \sqrt{5} - \sqrt{7} - \sqrt{9} + \sqrt{11} - \sqrt{13} + \sqrt{15})YZZZ \\
\left. + (\sqrt{2} + \sqrt{6} + \sqrt{10} + \sqrt{14})(XY - YX)II + (\sqrt{2} + \sqrt{6} - \sqrt{10} - \sqrt{14})(XY - YX)IZ \right. \\
+ (\sqrt{2} - \sqrt{6} + \sqrt{10} - \sqrt{14})(XY - YX)ZI + (\sqrt{2} - \sqrt{6} - \sqrt{10} + \sqrt{14})(XY - YX)ZZ \\
\left. + (\sqrt{4} + \sqrt{12})(XXY - XYX - YXX + YYY)I + (\sqrt{4} - \sqrt{12})(XXY - XYX - YXX + YYY)Z \right) \\
+ \sqrt{8}(XXXY - XXYX - XYXX - YXXX + XYYY + XYYY + YXXX + YYYY).
\]

(3)

For \( N = 16 \), we have

\[
\tilde{b}_{16}^\dagger - \tilde{b}_{16} = \\
\frac{1}{8} \left( (1 + \sqrt{3} + \sqrt{5} + \sqrt{7} + \sqrt{9} + \sqrt{11} + \sqrt{13} + \sqrt{15} + \sqrt{17} + \sqrt{19} + \sqrt{21})YIII + (1 + \sqrt{3} + \sqrt{5} + \sqrt{7} - \sqrt{9} - \sqrt{11} - \sqrt{13} - \sqrt{15} - \sqrt{17} - \sqrt{19} - \sqrt{21})YIIIZ \right. \\
+ (1 + \sqrt{3} - \sqrt{5} - \sqrt{7} + \sqrt{9} + \sqrt{11} - \sqrt{13} - \sqrt{15} + \sqrt{17} - \sqrt{19} - \sqrt{21})YIZI + (1 + \sqrt{3} - \sqrt{5} - \sqrt{7} - \sqrt{9} - \sqrt{11} + \sqrt{13} + \sqrt{15} + \sqrt{17} - \sqrt{19} - \sqrt{21})YIZZ \\
+ (1 - \sqrt{3} + \sqrt{5} - \sqrt{7} + \sqrt{9} - \sqrt{11} + \sqrt{13} - \sqrt{15} + \sqrt{17} - \sqrt{19} + \sqrt{21})YZZI + (1 - \sqrt{3} + \sqrt{5} - \sqrt{7} - \sqrt{9} + \sqrt{11} - \sqrt{13} + \sqrt{15} + \sqrt{17} - \sqrt{19} + \sqrt{21})YZZZ \\
+ (\sqrt{2} + \sqrt{6} + \sqrt{10} + \sqrt{14} + \sqrt{18} + \sqrt{22})(XY - YX)II + (\sqrt{2} + \sqrt{6} - \sqrt{10} - \sqrt{14} - \sqrt{18} - \sqrt{22})(XY - YX)IZ \right. \\
+ (\sqrt{2} - \sqrt{6} + \sqrt{10} - \sqrt{14} - \sqrt{18} + \sqrt{22})(XY - YX)ZI + (\sqrt{2} - \sqrt{6} - \sqrt{10} + \sqrt{14} + \sqrt{18} + \sqrt{22})(XY - YX)ZZ \\
\left. + (\sqrt{4} + \sqrt{12} + \sqrt{16} + \sqrt{20})(XXY - XYX - YXX + YYY)I + (\sqrt{4} - \sqrt{12} - \sqrt{16} - \sqrt{20})(XXY - XYX - YXX + YYY)Z \right) \\
+ \sqrt{8}(XXXY - XXYX - XYXX - YXXX + XYYY + XYYY + YXXX + YYYY).
\]

(4)

This decomposition has obvious structure, but we have not developed a way to exploit that structure in a scalable manner. Even with a scalable algorithm to generate the qubit decomposition, it is clear that the resulting sum of Pauli strings will grow exponentially with the number of qubits, \( N_q \), as it includes all combinations of the identity and Pauli-Z matrices for \( N_q - 1 \) positions. For very large \( N \), this would be very inefficient, but, as shown in the main text, the small truncations show here are sufficient for many interesting machine learning tasks. Furthermore, since we only need \( \log_2(N) \) qubits, a brute force search may be sufficient. For larger \( N \), there are scalable methods of preparing coherent states on qubits using Dicke states [1, 2],

**ONE-DIMENSIONAL REGRESSION**

In this section, we provide additional results for the one-dimensional regression task, including different levels of truncation and number of Trotter steps for the function presented in the main text, \( f(x) = x \sin(x) \), as well as results for many kernels for two other functions,
FIG. 1: GP regression of $f(x) = x \sin(x)$. (a) Various levels of truncation for the finite-dimensional coherent kernel. Two levels is not sufficient to regress this function, but four, eight, and sixteen levels obtain accurate regressions. (b) Various numbers of Trotter steps for the finite-dimensional coherent kernel of four levels implemented on qubits. One or two Trotter steps is not sufficient to regress this function, but three and four Trotter steps regress well.

FIG. 2: GP regression of $f_1(x)$ (top, eq. (5)) and $f_2(x)$ (bottom, eq. (6)) using the coherent kernel.

$$f_1(x) = x \sin\left(\frac{0.65x}{1 + 0.1x}\right) \cos(\sin(x))$$

$$f_2(x) = \frac{0.65x}{1 + 0.1x}.$$  

In summary, Fig. 1 demonstrates the convergence of the number of levels and number of Trotter steps for the regression problem studied in the main text. Figure 2 shows regression using coherent kernel for eqs. (5) and (6), providing the benchmark results for the other kernels. Figure 3 demonstrates that sixteen levels and five Trotter steps are necessary to regress the harder function of eq. (5), while Fig. 4 demonstrates that $f_2$ can be regressed with only a single qubit.
FIG. 3: GP regression of \( f_1(x) \) (eq. (5)). (a) Various levels of truncation for the finite-dimensional coherent kernel. Eight levels is not sufficient to regress this function, but sixteen and thirty-two levels obtain accurate regressions. (b) Various numbers of Trotter steps for the finite-dimensional coherent kernel of sixteen levels implemented on qubits. Four or five Trotter steps is not sufficient to regress this function, but six Trotter steps regresses well.

FIG. 4: GP regression of \( f_2(x) \) (eq. (6)). A truncation of only two levels is sufficient to regress this function; since the same implemented on qubits requires only one operation (Y), a single Trotter step is sufficient.
### Optimal Hyperparameters for One-Dimensional Regression

| Kernel     | $s$         | $c_1$         |
|------------|-------------|---------------|
| Coherent   | 1.000e+02  | 1.764e+00    |
| C-2        | 5.943e+01  | 1.379e+00    |
| C-4        | 1.000e+02  | 1.085e+00    |
| C-8        | 1.000e+02  | 2.921e+00    |
| C-16       | 1.000e+02  | 2.040e+00    |
| CQ-4-t1    | 5.873e+01  | 1.379e+00    |
| CQ-4-t2    | 1.885e+01  | 3.700e+00    |
| CQ-4-t3    | 9.570e+01  | 2.225e+00    |
| CQ-4-t4    | 6.982e+01  | 2.029e+00    |

**TABLE I:** Optimal hyperparameters for one-dimensional regression of $f(x) = x \sin(x)$. The bounds for $s$ were $[1e-2,1e2]$ and the bounds for $c_1$ were $[1e-3,1e3]$.

| Kernel     | $s$         | $c_1$         |
|------------|-------------|---------------|
| Coherent   | 3.074e+01  | 1.384e+00    |
| C-8        | 1.028e+01  | 1.621e+01    |
| C-16       | 1.094e+01  | 1.642e+01    |
| CQ-16-t4   | 1.000e+02  | 1.074e+01    |
| CQ-16-t5   | 1.000e+02  | 1.074e+01    |
| CQ-16-t6   | 9.289e+01  | 1.772e+00    |

**TABLE II:** Optimal hyperparameters for one-dimensional regression of $f_1(x)$, eq. (5). The bounds for $s$ were $[1e-2,1e2]$ and the bounds for $c_1$ were $[1e-3,1e3]$.

| Kernel     | $s$         | $c_1$         |
|------------|-------------|---------------|
| Coherent   | 1.189e+01  | 1.787e+01    |
| CQ-2-t1    | 1.028e+01  | 1.621e+01    |

**TABLE III:** Optimal hyperparameters for one-dimensional regression of $f_2(x)$, eq. (6). The bounds for $s$ were $[1e-2,1e2]$ and the bounds for $c_1$ were $[1e-3,1e3]$.

### ADDITIONAL HARDWARE KERNEL DETAILS

In this section we provide further details of the use of the IBM quantum computer, Boeblingen, for GP regression of the function $f(x) = x \sin(x)$. We use the qubit decomposition of eq. (2) and use a Trotter decomposition [3] of three steps to generate the finite-dimensional coherent kernel on qubits, labeled $\text{CQ-4-t3-HW}$. Because optimization on the hardware is time consuming, we instead use the optimal $c_i$ parameters from the C-4 kernel as fixed parameters for the $\text{CQ-4-t3-HW}$ kernel. We can still vary other hyperparameters, such as the scaling prefactor. We then compile the circuits, for all pairs of data points, using the Qiskit compiler [4], targeting the Boeblingen backend and using the highest optimization level. The form of the circuit, for any two points $x$ and $x'$, is shown in Fig. 5. We have omitted the parameters of each $u3$ gate; they depend on the specific values of $x$ and the fixed $c_i$. For the points $x = x'$, we know, a priori, that the resulting circuit should be identity. However, to keep the amount of noise between each pair of points the same, we force the evaluation of the kernel for $x = x'$ to have the same form as the $x \neq x'$ points. We use the full state measurement error mitigation available in Qiskit Ignis [4] to mitigate the effects of measurement error and use 8192 shots for each circuit. We also symmetrize the resulting kernel matrix, since, due to various noise sources, the evaluated values of $k(x,x')$ and $k(x',x)$ are not likely to be equal.

First, we show the results of evaluating the $\text{CQ-4-t3}$ kernel directly on the hardware. Note that this is different than the $\text{CQ-4-t3-HW}$ kernel, which includes an additional model discrepancy term (see main text). Figure 6(a) shows the Gram matrix (i.e., the kernel matrix) of the optimized $\text{CQ-4-t3}$ kernel evaluated in simulation for the training
FIG. 5: Form of the fully compiled two-qubit circuit used for the CQ-4-t3-HW kernel. Each $u3$ gate has different parameters, representing different single qubit rotations.

FIG. 6: Comparisons of the CQ-4-t3 kernel, evaluated in simulation and on the IBM Boeblingen quantum computer. (a) The CQ-4-t3 Gram matrix from simulation. (b) The CQ-4-t3 Gram matrix from hardware. (c) The relative error between the simulated and hardware Gram matrices.

points used in the main text for the regression of $f(x) = x \sin(x)$. Since we used a uniformly spaced grid of forty points, clear structure can be seen in the Gram matrix. Points that are close to each other (near the diagonal) are much more similar, represented by larger kernel values. There is a valley where points are considered very distant from each other, according to this kernel. Figure 6(b) shows the same kernel, with the same parameters and training points, evaluated on the IBM Boeblingen quantum computer. The structure is very evident, and, upon first glance, one might consider the two Gram matrices to approximately equal. However, as show in Fig. 6(c), the relative error between the two kernels can be very large. As explained in the main text, this is primarily due to the quantum computer not being able to accurately compute the kernel value for points that are very far away in the kernel space. This is represented by the large relative error, approaching differences up to a factor of 100. The simulated kernel has a minimum value of 0.016, while the kernel evaluated on the hardware has a minimum value of 1.92 for the same pair of points. This leads us to develop a new kernel, specifically for the hardware, which includes a model discrepancy term to account for the hardware errors.

Gaussian Process Prior Model for Quantum Hardware Experiments

In this subsection, we formally write down the GP prior model for our quantum hardware experiments, and provide some additional context for results given in the main body of the document. We restate our formulation of Eq. (4) of the main text, this time explicitly including the model discrepancy term. We utilize a $\mathcal{GP}(\mathbf{0}, k(\cdot, \cdot))$ prior for $n$ possibly multi-variate inputs $X = \{x_1, \ldots, x_n\}$ and $n$ scalar outputs $y$ given by

$$y = f + \epsilon + d$$

$$f \sim \mathcal{N}(\mathbf{0}, K_{X,X})$$

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2_i)$$

$$d_i \sim \mathcal{N}(0, \sigma^2_d).$$

Here $K_{X,X}$ is still an $n \times n$ matrix whose $(i,j)$th element is $k(x_i, x_j)$ and $\epsilon$ is heteroscedastic measurement noise with prior variance vector $\sigma^2 = [\sigma^2_1, \ldots, \sigma^2_n]$. $d$, however, is a homoscedastic model discrepancy term that incorporates unmodeled modeling error arising from measuring the quantum hardware. We assume that each $d_i$ is an unbiased
Gaussian with unknown prior variance \( \sigma_d^2 \). This model precipitates the following joint distribution of \( y \) and the response \( f^* \) of \( n^* \) unseen data \( X^* \):

\[
\begin{bmatrix} y \\ f^* \end{bmatrix} = \mathcal{N} \left( 0, \begin{bmatrix} K_{X,X} + \Sigma_d & K_{X,X^*} \\ K_{X^*X} & K_{X^*X^*} \end{bmatrix} \right),
\]

(11)

Here, \( \Sigma_d \) is a diagonal matrix whose \((i,i)\)th element is \((\sigma_i^2 + \sigma_d^2)\), incorporated the hardware-induced model discrepancy in the same form as the original GP prior presented in the main document. This formulation gives us the similar posterior of the response \( f^* \sim \mathcal{N}(\bar{f}^*, C) \), where

\[
\bar{f}^* \equiv K_{X^*,X} J^{-1} y
\]

(12)

\[
C \equiv K_{X^*,X} - K_{X^*,X} J^{-1} K_{X,X^*}
\]

(13)

\[
J \equiv K_{X,X} + \Sigma_d.
\]

(14)

**CQ-4-t3-HW Kernel**

To optimize the hyperparameters for the CQ-4-t3-HW kernel, we first take the values of the Gram matrix for the CQ-4-t3 with the scaling hyperparameter removed. This effectively fixes the \( c_i \) parameter (to the value 2.225), as defined above, but allows us to optimize the scaling hyperparameter (\( s \) in the main text) and the strength of the model discrepancy term (\( \sigma_d \) above) without making further calls to the quantum device. Figure 7 shows the resulting Gram matrix. Due to the inclusion of the model discrepancy term, the diagonal has a far greater value than the surrounding points. The general structure is still maintained. The optimal parameters were as follows: \( s = 7.469e+01 \), \( \sigma_d = 3.074e+01 \). The bounds for \( s \) were \([1e-2,1e2]\) and for \( \sigma_d \) were \([1e-3,1e3]\).

**ANALYTIC FORMULA OF SQUEEZED KERNEL**

In this section, we derive the analytic formula for the displaced, two-mode squeezed state that makes up the squeezed kernel used in the main text. The feature map for the squeezed kernel in three-dimensions is

\[
|\phi(x_1, x_2, x_3)\rangle = \prod_{\{i,j\}} D_i(\alpha_i) D_j(\alpha_j) S_{ij}(\gamma_{ij}) |0,0\rangle,
\]

(15)

where \( D_i \) is the displacement operator on system \( i \), \( \alpha_i = \frac{x_i}{\sqrt{2c_i}} \), \( S_{i,j} \) is the two-mode squeezing operator on systems \( i \) and \( j \) (see below), and the product is only taken over \( \{i,j\} \) pairs such the \( i > j \). The corresponding kernel is defined as

\[
K(x, x') = \prod_{\{i,j\}} k\left((x_i, x_j), (x'_i, x'_j)\right) = s \prod_{\{i,j\}} |0,0\rangle S_{ij}^\dagger(\gamma_{ij}') D_j^\dagger(\alpha_j') D_i(\alpha_i) D_j(\alpha_j) S_{ij}(\gamma_{ij}) |0,0\rangle.
\]

(16)
Note that this kernel does not include the square that the coherent kernel of the main text includes; this is because, as we will see, the squeezed kernel in the limit of zero squeezing double counts each data dimension.

We define the two-mode squeezed state with squeezing parameter $\gamma_{i,j}$ as [5]

$$\exp(\gamma_{ij}(b_i b_j - b_i^\dagger b_j^\dagger))[0,0] = \frac{1}{\cosh(\gamma_{ij})} \sum_{n=0}^{\infty} (-e^{i\Phi} \tanh(\gamma_{ij}))^n |n,n\rangle,$$

where $\Phi$ is a phase. For now, we will focus on just one pair of $i,j$ within the squeezed feature map, eq. (15). The displacement operators $D_i$ and $D_j$ can be brought into the infinite sum of the two-mode squeezed state, eq. (17)

$$\frac{1}{\cosh(\gamma_{ij})} \sum_{n=0}^{\infty} (-e^{i\Phi} \tanh(\gamma_{ij}))^n D_i(\alpha_i) D_j(\alpha_j) |n,n\rangle = \frac{1}{\cosh(\gamma_{ij})} \sum_{n=0}^{\infty} (-e^{i\Phi} \tanh(\gamma_{ij}))^n |(\alpha_i, n), (\alpha_j, n)\rangle,$$

where $|(\alpha_i, n), (\alpha_j, n)\rangle$ represent displaced number states in each dimension. We define the displaced number state as the displacement operator acting on a number state, $|\alpha, n\rangle = D(\alpha) |n\rangle$ and note that the overlap between two displaced number states has an analytic form [6]

$$\langle m, \alpha'| n, \alpha \rangle = \langle \alpha' | \alpha \rangle \sqrt{\frac{m!}{n!}} (\alpha' - \alpha)^n L_m^{n-m} ((\alpha' - \alpha)^2),$$

where $L_m^{n-m}$ is the associated Laguerre polynomial. With the overlap of displaced number states, we can now define the squeezed kernel for dimensions $i,j$ as

$$k\left((x_i, x_j), (x_i', x_j')\right) = \sum_{n=0, m=0}^{\infty} |\alpha_i| |\alpha'_i| |\alpha_j| |\alpha'_j| \tanh^m(\gamma_{i,j}) \tanh^m(\gamma_{i,j}') L_m^{n-m} ((\alpha_i' - \alpha_i)^2) L_m^{n-m} ((\alpha_j' - \alpha_j)^2).$$

Though the squeezed kernel has an analytic form, this infinite sum of associated Laguerre polynomials does not have a clear analytic form. Furthermore, in the $N$-mode squeezed case, or when squeezing is applied to multiple pairs of dimensions together, it is not clear that an analytic form can be derived. We approximate eq. (20) by truncating the sum to $n = 8, m = 8$, which we found to be converged for the parameter ranges we used in the paper.

It is instructive to look at the limit of the analytic form of the squeezed kernel, eq. (20), as it approaches 0 squeezing ($\gamma_{i,j} = 0$). Because $\tanh(0) = 0$, the only term in the infinite sum that survives is the $n = 0, m = 0$ term, since $\tanh(0)^0 = 1$. The associated Laguerre polynomials for $n = 0, m = 0$ are simply 1. As such, when there is zero squeezing, the squeezed kernel simply becomes the coherent kernel. However, with a non-zero amount of squeezing, the squeezed kernel is generating entanglement between data dimensions and accessing parts of the Hilbert space which the coherent kernel (and, therefore, the squared exponential kernel), cannot reach. Though there are ways of making correlated squared exponential kernels, they do not have the same form as squeezed kernel we have derived here. It uses the unique entanglement properties of the underlying quantum representation; as a larger number of modes are squeezed, the result accesses more and more of the underlying Hilbert space. Truncated squeezed kernels could also be defined, by using the truncated raising and lowering operators defined in the main text and above.

Though we have defined the analytic form of the squeezed kernel, we have not yet defined the form of the squeezing parameter, $\gamma_{i,j}$. The definition of the displacement parameters, $\alpha_i$, were defined to be consistent with the squared exponential kernel. Given that the squeezing parameter has no clear classical analog, we are free to define it as we choose. One choice, inspired by the definition of the displacement parameters, is to use the product of the data points multiplied by a hyperparameter $d_{ij}$; $\gamma_{i,j} = x_i x_j d_{ij}$.

**ADDITIONAL RESULTS FOR DYNAMICS REGRESSION**

In this section, we provide additional results and tables of hyperparameters for the dynamics regression discussed in the main text. Figure 8(a) shows the $R^2$ values for each of the ten training sets. In the regression of the position, $x$, all truncations perform the same, while the squeezed kernel performs marginally better for some training sets, but marginally worse for many others. The regression of the velocity, $v$, is a harder regression task, as shown by the significantly smaller $R^2$ values. Here, the squeezed kernel performs better than the coherent kernel in many of the training sets, and significantly better in training set four. Figure 8(b) shows the absolute errors in the prediction of the velocity, $v$, in two training sets: four, where the squeezed kernel vastly out performs the coherent kernel and
FIG. 8: Example of applying quantum kernels to dynamics regression. (a) The position, $x$, is regressed very well by all kernels. The velocity, $v$, needs a truncated Hilbert space of size 32 before the finite-dimensional coherent state regresses as well as the full coherent state. The addition of non-classical resources, through two-mode squeezing, allows the squeezed kernel to regress better than the coherent kernel. (b) Comparison of velocity regression using the squeezed and coherent kernels on 100 random test points for two training sets.

seven, where the coherent kernel marginally outperforms the squeezed kernel. In training set four, it is clear that most of the points are regressed well by both the coherent and squeezed kernels, but there are few outliers which the coherent kernel predicts much worse than even the worst prediction of the squeezed kernel. In training set seven, both the coherent and squeezed states perform generally the same, with each having points that are better and worse.
Optimal Hyperparameters for Dynamics Regression

| Training Set | \( s \)          | \( c_x \)      | \( c_v \)      | \( c_a \)      |
|--------------|------------------|----------------|----------------|----------------|
| 0            | 3.709e-01        | 7.207e-01      | 3.432e+00      | 2.000e+01      |
| 1            | 3.738e-01        | 6.646e-01      | 3.360e+00      | 2.000e+01      |
| 2            | 3.714e-01        | 6.836e-01      | 2.919e+00      | 2.000e+01      |
| 3            | 4.380e-01        | 7.121e-01      | 3.122e+00      | 2.000e+01      |
| 4            | 3.716e-01        | 6.608e-01      | 2.984e+00      | 1.794e+01      |
| 5            | 3.994e-01        | 6.923e-01      | 3.061e+00      | 2.000e+01      |
| 6            | 3.269e-01        | 6.839e-01      | 3.143e+00      | 2.000e+01      |
| 7            | 4.277e-01        | 7.247e-01      | 3.092e+00      | 2.000e+01      |
| 8            | 3.680e-01        | 7.156e-01      | 3.106e+00      | 2.000e+01      |
| 9            | 4.027e-01        | 7.050e-01      | 2.988e+00      | 2.000e+01      |

**TABLE IV:** Optimal hyperparameters for \( x \) regression using the coherent kernel. The \( s \) bounds were [1e-3,1e3] and the \( c_i \) bounds were [1e-3,20].

| Training Set | \( s \)          | \( c_x \)      | \( c_v \)      | \( c_a \)      |
|--------------|------------------|----------------|----------------|----------------|
| 0            | 2.094e+00        | 3.893e-01      | 7.742e-01      | 8.488e+00      |
| 1            | 2.613e+00        | 1.405e-01      | 1.426e+00      | 3.040e+00      |
| 2            | 1.705e+00        | 2.305e-01      | 1.347e+00      | 6.378e+00      |
| 3            | 2.948e+00        | 3.137e-01      | 1.473e+00      | 9.742e+00      |
| 4            | 2.510e+00        | 5.187e-01      | 3.305e-01      | 9.321e+00      |
| 5            | 1.503e+00        | 3.096e-01      | 1.121e+00      | 2.102e+00      |
| 6            | 2.453e+00        | 3.814e-01      | 1.506e+00      | 2.528e+00      |
| 7            | 2.390e+00        | 4.250e-01      | 3.888e-01      | 9.811e+00      |
| 8            | 2.676e+00        | 3.908e-01      | 7.673e-01      | 9.559e+00      |
| 9            | 3.312e+00        | 4.367e-01      | 1.608e+00      | 7.734e+00      |

**TABLE V:** Optimal hyperparameters for \( v \) regression using the coherent kernel. The \( s \) bounds were [1e-3,1e3] and the \( c_i \) bounds were [1e-3,20].

| Training Set | \( s \)          | \( c_x \)      | \( c_v \)      | \( c_a \)      |
|--------------|------------------|----------------|----------------|----------------|
| 0            | 3.708e-01        | 7.208e-01      | 3.434e+00      | 2.000e+01      |
| 1            | 3.771e-01        | 6.650e-01      | 3.371e+00      | 2.000e+01      |
| 2            | 3.721e-01        | 6.834e-01      | 2.926e+00      | 2.000e+01      |
| 3            | 4.368e-01        | 7.114e-01      | 3.124e+00      | 2.000e+01      |
| 4            | 3.598e-01        | 6.520e-01      | 2.945e+00      | 1.742e+01      |
| 5            | 3.983e-01        | 6.929e-01      | 3.053e+00      | 2.000e+01      |
| 6            | 3.270e-01        | 6.838e-01      | 3.142e+00      | 2.000e+01      |
| 7            | 4.277e-01        | 7.246e-01      | 3.093e+00      | 2.000e+01      |
| 8            | 3.622e-01        | 7.121e-01      | 3.069e+00      | 2.000e+01      |
| 9            | 4.056e-01        | 7.059e-01      | 2.994e+00      | 2.000e+01      |

**TABLE VI:** Optimal hyperparameters for \( x \) regression using the C-8 kernel. The \( s \) bounds were [1e-3,1e3] and the \( c_i \) bounds were [1e-3,20].
TABLE VII: Optimal hyperparameters for \( v \) regression using the \( C-8 \) kernel. The \( s \) bounds were \([1e-3,1e3]\) and the \( c_i \) bounds were \([1e-3,20]\).

| Training Set | \( s \)       | \( c_s \)   | \( c_v \)   | \( c_a \)   |
|--------------|---------------|-------------|-------------|-------------|
| 0            | 2.012e+00     | 3.872e-01  | 7.620e-01  | 8.531e+00  |
| 1            | 8.837e+01     | 1.804e-01  | 2.131e+00  | 5.232e+00  |
| 2            | 1.883e+00     | 2.998e-01  | 1.270e+00  | 4.869e+00  |
| 3            | 3.474e+00     | 3.393e-01  | 1.434e+00  | 9.622e+00  |
| 4            | 1.712e+00     | 3.261e-01  | 9.069e-01  | 2.852e+00  |
| 5            | 1.427e+00     | 3.072e-01  | 1.114e+00  | 2.076e+00  |
| 6            | 2.433e+00     | 3.815e-01  | 1.498e+00  | 5.234e+00  |
| 7            | 1.883e+00     | 2.998e-01  | 1.270e+00  | 4.869e+00  |
| 8            | 3.474e+00     | 3.393e-01  | 1.434e+00  | 9.622e+00  |
| 9            | 1.712e+00     | 3.261e-01  | 9.069e-01  | 2.852e+00  |

TABLE VIII: Optimal hyperparameters for \( x \) regression using the \( C-16 \) kernel. The \( s \) bounds were \([1e-3,1e3]\) and the \( c_i \) bounds were \([1e-3,20]\).

| Training Set | \( s \)       | \( c_s \)   | \( c_v \)   | \( c_a \)   |
|--------------|---------------|-------------|-------------|-------------|
| 0            | 3.710e-01     | 7.206e-01  | 3.432e+00  | 2.000e+01  |
| 1            | 3.757e-01     | 6.643e-01  | 3.360e+00  | 2.000e+01  |
| 2            | 3.726e-01     | 6.836e-01  | 2.926e+00  | 2.000e+01  |
| 3            | 4.354e-01     | 7.114e-01  | 3.117e+00  | 2.000e+01  |
| 4            | 3.464e-01     | 6.534e-01  | 2.890e+00  | 1.700e+01  |
| 5            | 3.986e-01     | 6.921e-01  | 3.055e+00  | 2.000e+01  |
| 6            | 3.270e-01     | 6.839e-01  | 3.142e+00  | 2.000e+01  |
| 7            | 4.276e-01     | 7.245e-01  | 3.093e+00  | 2.000e+01  |
| 8            | 3.713e-01     | 7.149e-01  | 3.105e+00  | 2.000e+01  |
| 9            | 4.029e-01     | 7.051e-01  | 2.987e+00  | 2.000e+01  |

TABLE IX: Optimal hyperparameters for \( v \) regression using the \( C-16 \) kernel. The \( s \) bounds were \([1e-3,1e3]\) and the \( c_i \) bounds were \([1e-3,20]\).

| Training Set | \( s \)       | \( c_s \)   | \( c_v \)   | \( c_a \)   |
|--------------|---------------|-------------|-------------|-------------|
| 0            | 2.064e+00     | 3.885e-01  | 7.730e-01  | 8.450e+00  |
| 1            | 3.670e+00     | 1.923e-01  | 1.323e+00  | 2.725e+00  |
| 2            | 1.701e+00     | 2.289e-01  | 1.396e+00  | 6.411e+00  |
| 3            | 3.035e+00     | 3.138e-01  | 1.473e+00  | 9.922e+00  |
| 4            | 4.134e+00     | 4.096e-01  | 1.507e+00  | 2.528e+00  |
| 5            | 2.451e+00     | 3.812e-01  | 1.507e+00  | 2.528e+00  |
| 6            | 3.002e+00     | 4.296e-01  | 1.606e-01  | 1.066e+01  |
| 7            | 2.691e+00     | 3.910e-01  | 7.689e-01  | 9.660e+00  |
| 8            | 3.415e+00     | 4.370e-01  | 1.615e+00  | 7.856e+00  |

TABLE X: Optimal hyperparameters for \( x \) regression using the \( C-32 \) kernel. The \( s \) bounds were \([1e-3,1e3]\) and the \( c_i \) bounds were \([1e-3,20]\).

| Training Set | \( s \)       | \( c_s \)   | \( c_v \)   | \( c_a \)   |
|--------------|---------------|-------------|-------------|-------------|
| 0            | 3.709e-01     | 7.207e-01  | 3.431e+00  | 2.000e+01  |
| 1            | 3.745e-01     | 6.642e-01  | 3.362e+00  | 2.000e+01  |
| 2            | 3.723e-01     | 6.840e-01  | 2.926e+00  | 2.000e+01  |
| 3            | 4.364e-01     | 7.116e-01  | 3.120e+00  | 2.000e+01  |
| 4            | 3.599e-01     | 6.519e-01  | 2.950e+00  | 1.747e+01  |
| 5            | 3.987e-01     | 6.925e-01  | 3.058e+00  | 2.000e+01  |
| 6            | 3.269e-01     | 6.840e-01  | 3.142e+00  | 2.000e+01  |
| 7            | 4.279e-01     | 7.244e-01  | 3.095e+00  | 2.000e+01  |
| 8            | 3.763e-01     | 7.099e-01  | 3.180e+00  | 2.000e+01  |
| 9            | 4.033e-01     | 7.051e-01  | 2.989e+00  | 2.000e+01  |
TABLE XI: Optimal hyperparameters for v regression using the C-32 kernel. The s bounds were [1e-3,1e3] and the c_i bounds were [1e-3,20].

| Training Set | s     | c_x  | c_v  | c_a  | \(\gamma_{xv}\) | \(\gamma_{va}\) | \(\gamma_{xa}\) |
|--------------|-------|------|------|------|----------------|----------------|----------------|
| 0            | 2.096e+00 | 3.893e-01 | 7.745e-01 | 8.491e+00 | 2.010e-00 | 2.357e-00 | 2.213e-01 |
| 1            | 2.598e+00 | 1.399e-01 | 1.426e+00 | 3.043e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 2            | 1.705e+00 | 2.305e-01 | 1.347e+00 | 6.373e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 3            | 3.040e+00 | 3.140e-01 | 1.426e+00 | 7.745e-01 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 4            | 2.505e+00 | 5.184e-01 | 1.347e+00 | 6.373e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 5            | 1.503e+00 | 3.094e-01 | 1.123e+00 | 2.103e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 6            | 2.455e+00 | 3.815e-01 | 1.507e+00 | 2.527e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 7            | 2.379e+00 | 4.247e-01 | 3.885e-01 | 9.789e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 8            | 2.691e+00 | 3.909e-01 | 7.690e-01 | 9.659e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |
| 9            | 3.398e+00 | 4.366e-01 | 1.615e+00 | 7.844e+00 | 2.020e-00 | 2.379e-00 | 2.213e-01 |

TABLE XII: Optimal hyperparameters for x regression using the squeezed kernel. The s bounds were [1e-3,1e3], the c_i bounds were [1e-3,20], and the \(\gamma_{ij}\) bounds were [0,19.999].

| Training Set | s     | c_x  | c_v  | c_a  | \(\gamma_{xv}\) | \(\gamma_{va}\) | \(\gamma_{xa}\) |
|--------------|-------|------|------|------|----------------|----------------|----------------|
| 0            | 5.048e-01 | 8.110e-01 | 5.663e+00 | 2.000e+01 | 2.213e-01 | 2.171e-05 | 1.622e-04 |
| 1            | 4.462e-01 | 7.857e-01 | 5.390e+00 | 2.000e+01 | 2.507e-01 | 3.996e-02 | 4.057e-03 |
| 2            | 4.827e-01 | 8.284e-01 | 5.771e+00 | 2.000e+01 | 2.468e-01 | 7.876e-05 | 6.075e-05 |
| 3            | 6.271e-01 | 8.332e-01 | 5.980e+00 | 2.000e+01 | 2.464e-01 | 2.159e-03 | 5.196e-03 |
| 4            | 4.374e-01 | 7.716e-01 | 5.806e+00 | 2.000e+01 | 2.685e-01 | 6.170e-02 | 2.121e-03 |
| 5            | 4.374e-01 | 7.716e-01 | 5.806e+00 | 2.000e+1 | 2.899e-01 | 2.476e-02 | 1.078e-05 |
| 6            | 4.374e-01 | 7.716e-01 | 5.806e+00 | 2.000e+01 | 2.899e-01 | 2.476e-02 | 1.078e-05 |
| 7            | 4.374e-01 | 7.716e-01 | 5.806e+00 | 2.000e+01 | 2.899e-01 | 2.476e-02 | 1.078e-05 |
| 8            | 4.374e-01 | 7.716e-01 | 5.806e+00 | 2.000e+01 | 2.899e-01 | 2.476e-02 | 1.078e-05 |
| 9            | 4.374e-01 | 7.716e-01 | 5.806e+00 | 2.000e+01 | 2.899e-01 | 2.476e-02 | 1.078e-05 |

TABLE XIII: Optimal hyperparameters for v regression using the squeezed kernel. The s bounds were [1e-3,1e3], the c_i bounds were [1e-3,20], and the \(\gamma_{ij}\) bounds were [0,19.999].
## Optimal Hyperparameters for Reinforcement Learning Results

| Kernel    | $s$   | $c_x$     | $c_v$  | $c_a$  |
|-----------|-------|-----------|--------|--------|
| Coherent  | 4.753e+01 | 1.469e-01 | 4.587e-01 |        |
| C-8       | 2.295e+01 | 2.427e-01 | 1.008e-01 |        |
| C-16      | 4.882e+01 | 1.865e-01 | 4.726e-01 |        |

### TABLE XIV: Optimal hyperparameters for value regression in the reinforcement learning task. The $s$ bounds were $[1e-3,1e2]$ and the $c_i$ bounds were $[0.05,10]$.

| Kernel    | $s$   | $c_x$     | $c_v$  | $c_a$  |
|-----------|-------|-----------|--------|--------|
| Coherent  | 3.827e-01 | 6.599e-01 | 3.292e+00 | 1.984e+01 |
| C-8       | 3.516e-01 | 8.144e-01 | 3.121e+00 | 2.000e+01 |
| C-16      | 4.405e-01 | 7.561e-01 | 3.981e+00 | 2.000e+01 |

### TABLE XV: Optimal hyperparameters for $x$ regression in the reinforcement learning task. The $s$ bounds were $[1e-3,1e3]$ and the $c_i$ bounds were $[1e-3,20]$.

| Kernel    | $s$   | $c_x$     | $c_v$  | $c_a$  |
|-----------|-------|-----------|--------|--------|
| Coherent  | 6.111e+00 | 3.710e-01 | 2.334e+00 | 1.656e+01 |
| C-8       | 1.969e+00 | 5.406e-01 | 1.675e+00 | 4.988e+00 |
| C-16      | 3.304e+00 | 4.852e-01 | 1.842e+00 | 7.301e+00 |

### TABLE XVI: Optimal hyperparameters for $v$ regression in the reinforcement learning task. The $s$ bounds were $[1e-3,1e3]$ and the $c_i$ bounds were $[1e-3,20]$.
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