Kernels

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I. Part 1

In this section we implemented the kernelized ridge regression and support vector regression. In addition to the Linear kernel, we implemented the Polynomial kernel and the RBF kernel.

A. *Kernelized Ridge Regression Implementation*

This implementation is simple because the fitting algorithm has a closed-form solution:

$$\boldsymbol{\alpha} = (K_{\text{train}} + \lambda \mathbf{I})^{-1} \mathbf{y}$$

where K_{train} is the kernel matrix computed between training points, and λ is the regularization constant.

Then we can predict with:

$$\hat{\mathbf{y}} = K_{\text{test, train}} \boldsymbol{\alpha}$$

where $K_{\text{test, train}}$ is the kernel matrix computed between the test inputs and the training inputs.

B. *Support vector regression implementation*

Here we needed to adapt the Equation 10 from (Smola and Scholkopf, 2004) to a form which fits the requirements of the *cvxopt.solvers.qp*, that is:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^T P \mathbf{x} + \mathbf{q}^T \mathbf{x} \\ \text{subject to} \quad & G\mathbf{x} \leq \mathbf{h} \\ & A\mathbf{x} = \mathbf{b} \end{aligned}$$

where:

$$x = [\alpha_1, \alpha_1^*, \alpha_2, \alpha_2^*, \ldots]$$

The matrices were calculated as:

$$\begin{aligned} P_{2i,\,2j} &= k_{ij}, \\ P_{2i,\,2j+1} &= -k_{ij}, \\ P_{2i+1,\,2j} &= -k_{ij}, \\ P_{2i+1,\,2j+1} &= k_{ij}. \end{aligned} \qquad q = \begin{bmatrix} \varepsilon - y_1 \\ \varepsilon + y_1 \\ \vdots \\ \varepsilon - y_n \\ \varepsilon + y_n \end{bmatrix} \in \mathbb{R}^{2n}$$

$$G = \begin{bmatrix} -I_{2n} \\ I_{2n} \end{bmatrix} \in \mathbb{R}^{(4n)\times(2n)} \qquad h = \begin{bmatrix} \mathbf{0}_{2n} \\ C \cdot \mathbf{1}_{2n} \end{bmatrix} \in \mathbb{R}^{4n}$$

$$A = \begin{bmatrix} 1 & -1 & 1 & -1 & \ldots & 1 & -1 \end{bmatrix} \in \mathbb{R}^{1\times 2n} \qquad b = 0$$

where K is the kernel on the training data, n is the number of data points, ϵ is the margin of tolerance and C is the regularization constant defined as $1/\lambda$.

We can then predict as:

$$\hat{y} = K(X, X_{\text{train}}) \cdot (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) + b$$

where b is the bias.

C. *Fitting both methods to the 1-dimensional sine data*

We fit both methods, each with both kernels to the 1-D sine data, which we can see on Figure 1. Note that the support vectors are the data points where: $\alpha_i - \alpha_i^* > 1 \times 10^{-5}$. In Table I we can see the parameters we used for each model. Note that for the polynomial kernel to work, we needed to scale the data.

Model	Kernel	Parameters
SVR	RBF	$\sigma = 1$, $\varepsilon = 0.5$, $\lambda = 0.001$
Ridge Regression	RBF	$\sigma = 1$, $\lambda = 0.01$
SVR	Polynomial	$M = 10$, $\varepsilon = 0.7$, $\lambda = 0.0001$
Ridge Regression	Polynomial	$M = 10$, $\lambda = 0.001$

Table I
Parameters for SVR and Ridge Regression.

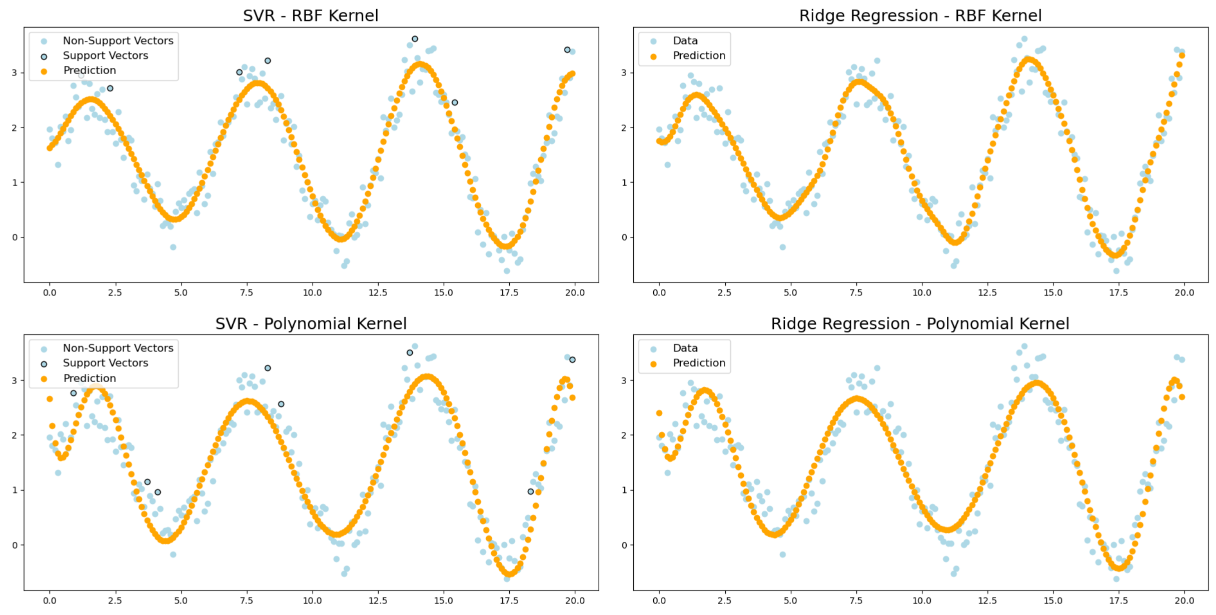

Figure 1. Comparison of SVR and Ridge Regression

II. Part 2

A. Results

For this part, we applied both methods and kernels to the *housing2r* dataset. For the polynomial kernel, we evaluated different degrees: $M \in [1, 10]$. For the RBF kernel, we tested a wide range of standard deviations: $\sigma \in \{0.001, 0.01, 0.1, 1, 2, 3, 4, 5, 8, 10, 100\}$. This range includes values that produce smoother decision boundaries (larger σ) as well as more complex ones (smaller σ).

To assess predictive performance, we used 10-fold cross-validation. We considered two strategies for selecting the regularization parameter λ: a fixed value $\lambda = 1$, and a data-driven approach using nested cross-validation (with 6 folds in the inner loop) to tune λ for each split.

Uncertainty estimates were computed assuming asymptotic normality of the cross-validation results. Specifically, we calculated the standard deviation across folds and divided by $\sqrt{n}$, where n is the number of folds.

To get a somewhat sparse SVR solution, we set $\epsilon = 5$. Figure 2 shows the results. Note that with an even larger ϵ the solution could get even more sparse however then the performance started degrading. Note that the numbers above and below the curves indicate the number of support vectors (Since we use cross validation, we calculated the average number of support vectors across the splits and rounded it) for each configuration.

B. Disscussion

The first comparison we can draw from Figure 2 concerns the choice of kernel. The polynomial kernel tends to overfit quickly at higher degrees. For both Ridge Regression and SVR, a degree of 2 gives the best performance.

The RBF kernel is also quite sensitive to the σ parameter, especially for Ridge Regression. Very small σ values lead to overfitting and high loss, while values in the range of 1 to 10 yield the best results. Larger σ values result in underfitting and worse performance.

Overall, all the models with best chosen parameters achieve MSE between 26 and 28, so other factors should influence model choice. Ridge Regression benefits from a closed-form solution and faster training, making it suitable when training time is critical. SVR, on the other hand, requires more training time due to the optimization solver, but inference can be faster and more memory-efficient since it relies only on support vectors. For this particular dataset, we pick the Kernelized Ridge regression as the better option.

Both kernels achieve similar performance (at the best parameters) and yield a comparable number of support vectors at their optimal configurations, so either could be a suitable choice.

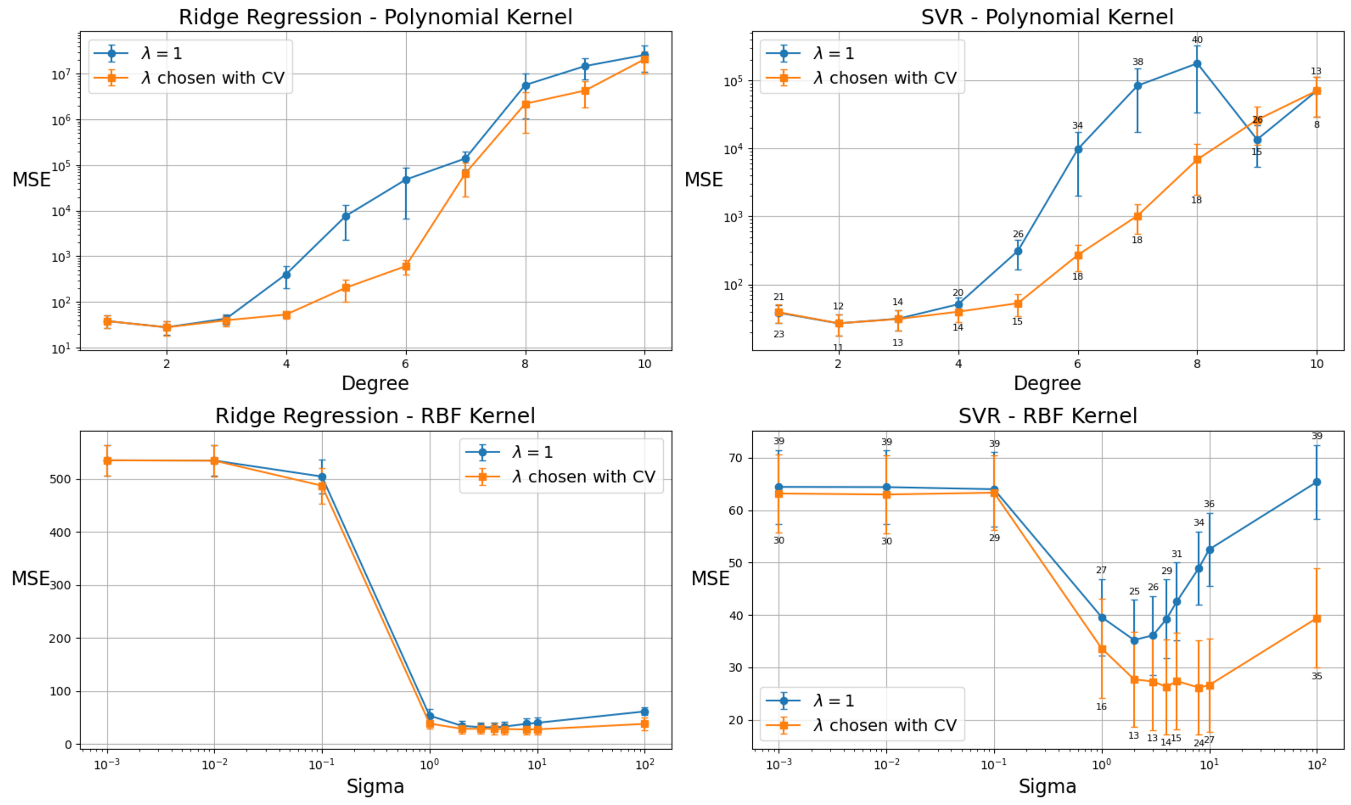

Figure 2. Comparison of models at different parameter values

III. Part 3

For this part, we used a subset of 1000 images from the UTKFace dataset, which is commonly used for age prediction from facial images. All images were resized to (128×128) pixels. To evaluate our methods, we performed a train-validation-test split in a 60%-20%-20% ratio.

As a baseline, we used a naive attribute representation where each image is flattened into a raw pixel vector. We applied kernelized ridge regression for learning, since it offers significantly faster training times compared to SVR. For this baseline, we used the standard RBF kernel.

In our improved method, we enhanced the RBF kernel by first extracting Histogram of Oriented Gradients (HOG) features from the images, and then computing the RBF kernel on these feature vectors.

Hyperparameter tuning for both methods was performed using grid search. Once the optimal parameters were identified, we retrained the models using the combined training and validation sets. For evaluation, we computed the Mean Squared Error (MSE) on the test set and estimated the uncertainty using asymptotic normality.

The results are shown in Table II. It is evident that the HOG-enhanced representation significantly outperforms the naive raw pixel approach.

Representation	MSE	Std. Error
Naive attribute representation	195.46	24.29
HOG-Enhanced representation	137.79	24.62

Table II
Comparison of the naive attribute representation with our implementation