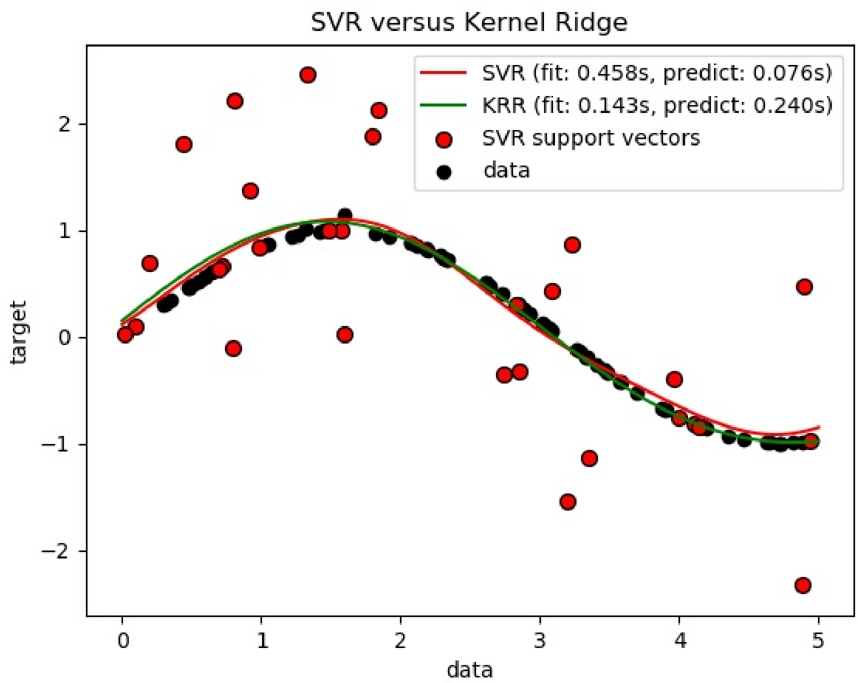
1.3. Kernel ridge regression

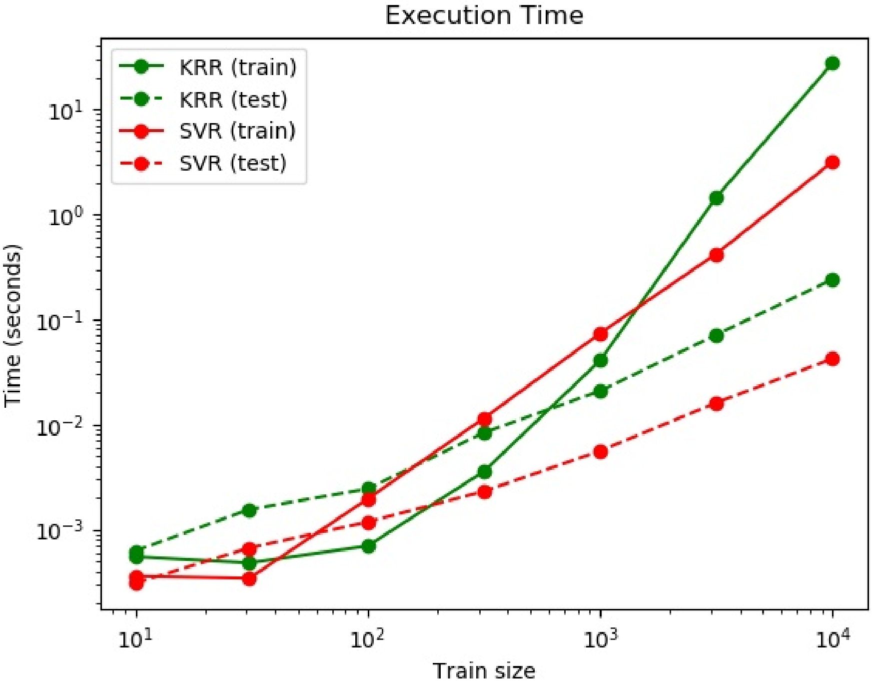
Kernel ridge regression (KRR) [M2012] combines Ridge regression and classification (linear least squares with l2-norm regularization) with the kernel trick. It thus learns a linear function in the space induced by the respective kernel and the data. For non-linear kernels, this corresponds to a non-linear function in the original space.

The form of the model learned by `KernelRidge` is identical to support vector regression (`SVR`). However, different loss functions are used: KRR uses squared error loss while support vector regression uses ϵ-insensitive loss, both combined with l2 regularization. In contrast to `SVR`, fitting `KernelRidge` can be done in closed-form and is typically faster for medium-sized datasets. On the other hand, the learned model is non-sparse and thus slower than SVR, which learns a sparse model for $\epsilon > 0$, at prediction-time.

The following figure compares `KernelRidge` and `SVR` on an artificial dataset, which consists of a sinusoidal target function and strong noise added to every fifth datapoint. The learned model of `KernelRidge` and `SVR` is plotted, where both complexity/regularization and bandwidth of the RBF kernel have been optimized using grid-search. The learned functions are very similar; however, fitting `KernelRidge` is approx. seven times faster than fitting `SVR` (both with grid-search). However, prediction of 100000 target values is more than three times faster with SVR since it has learned a sparse model using only approx. 1/3 of the 100 training datapoints as support vectors.



The next figure compares the time for fitting and prediction of `KernelRidge` and `SVR` for different sizes of the training set. Fitting `KernelRidge` is faster than `SVR` for medium-sized training sets (less than 1000 samples); however, for larger training sets `SVR` scales better. With regard to prediction time, `SVR` is faster than `KernelRidge` for all sizes of the training set because of the learned sparse solution. Note that the degree of sparsity and thus the prediction time depends on the parameters ϵ and C of the `SVR`; $\epsilon = 0$ would correspond to a dense model.



References:

[M2012] "Machine Learning: A Probabilistic Perspective" Murphy, K. P. - chapter 14.4.3, pp. 492-493, The MIT Press, 2012

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