

## 4033/5033 Assignment 2

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In this assignment, we will implement an efficient variant of KRR called accelerated kernel ridge regression (AKRR). Recall the optimal KRR model is expressed by all training points i.e.,  $\beta = \sum_{i=1}^n \alpha_i \phi(x_i)$ . AKRR approximates this model using a (random) subset of  $m$  training points i.e.,

$$\tilde{\beta} = \sum_{i=1}^m \alpha_i \phi(x_i), \quad (1)$$

where integer  $m$  is a hyperparameter and often  $m < n$ .

Other parts of AKRR are the same as KRR i.e., we plug (1) back to the following objective function

$$J(\tilde{\beta}) = \sum_{i=1}^n (\phi(x_i)^T \tilde{\beta} - y_i)^2 + \lambda \tilde{\beta}^T \tilde{\beta}, \quad (2)$$

to get a dual objective  $J(\tilde{\alpha})$  of  $\tilde{\alpha} = [\alpha_1, \dots, \alpha_m]^T$ .

Then, we solve  $\min_{\tilde{\alpha}} J(\tilde{\alpha})$  to get the optimal  $\tilde{\alpha}$  and predict the label of any point  $z$  as

$$\tilde{\beta}^T \phi(z) = \sum_{j=1}^m \alpha_j \phi(x_j)^T \phi(z) = \sum_{j=1}^m \alpha_j k(x_j, z). \quad (3)$$

### Part I: Theory

[Task 1] Derive the optimal  $\tilde{\alpha}$  for problem  $\min_{\tilde{\alpha}} J(\tilde{\alpha})$ . (tip: you may first derive a matrix form of  $J(\tilde{\alpha})$  using proper kernel matrices e.g.,  $\tilde{K} \in \mathbb{R}^{n \times m}$  where the  $m$  columns correspond to the  $m$  instances in (1)).

[Task 1 - Solution]

Defining the proper kernel matrices:

$$\tilde{K} \in \mathbb{R}^{n \times m}, (\tilde{K}_{ij}) = k(x_i, x_j),$$

and the basis-basis kernel

$$K_m \in \mathbb{R}^{m \times m}, (K_m)_{j\ell} = k(x_j, x_\ell)$$

Let  $\tilde{\alpha} = (\alpha_1, \dots, \alpha_m)^T$  and  $y = (y_1, \dots, y_n)^T$ .

Predictions on the training set are

$$\hat{y} = \tilde{K} \tilde{\alpha}$$

Now, for the optimality, differentiate and set to zero:

$\nabla_{\tilde{\alpha}} J = 2\tilde{K}^T(\tilde{K}\tilde{\alpha} - y) + 2\lambda K_m \tilde{\alpha} = 0$  Thus, the normal equations are:

$$(\tilde{K}^T \tilde{K} + \lambda K_m) \tilde{\alpha} = \tilde{K}^T y$$

and the closed form solution is

$$\tilde{\alpha} = (\tilde{K}^T \tilde{K} + \lambda K_m)^{-1} \tilde{K}^T y$$

[Task 2] Justify the computational complexity for computing the optimal  $\tilde{\alpha}$  is  $O(mnp + m^2n)$ . (tip: you just need to explain which part of the  $\tilde{\alpha}$  computation contributes to which term in the big O notation.)

[Task 2 - Solution]

1. Build the rectangular Kernel  $\tilde{K}$  of size  $n \times m$

- Evaluations of the  $n \cdot m$  kernel are needed.
- For common kernels that use an inner product or distance in  $R^p$  (whether linear, radial basis function, or polynomial), each evaluation is  $O(p)$ .
- Thus, the cost is  $\boxed{O(mnp)}$ .

2. Form the normal-equation pieces and right-hand side

- Compute  $\tilde{K}^T \tilde{K}$  (an  $m \times m$  Gram matrix of  $\tilde{K}$ ): each of the  $m^2$  entries is a dot product of two  $n$ -length columns  $\rightarrow O(n)$  each  $\rightarrow \boxed{O(m^2n)}$ .
- Compute  $\tilde{K}^T y : O(nm)$  (lower order than  $m^2n$ ).

3. Solve the  $m \times m$  linear system

- Using Cholesky on  $\tilde{K}^T \tilde{K} + \lambda K_m : O(m^3)$ .
- In the intended regime  $n \geq m$ , the  $O(m^2n)$  term dominates  $O(m^3)$ , so it's absorbed by  $m^2n$ .

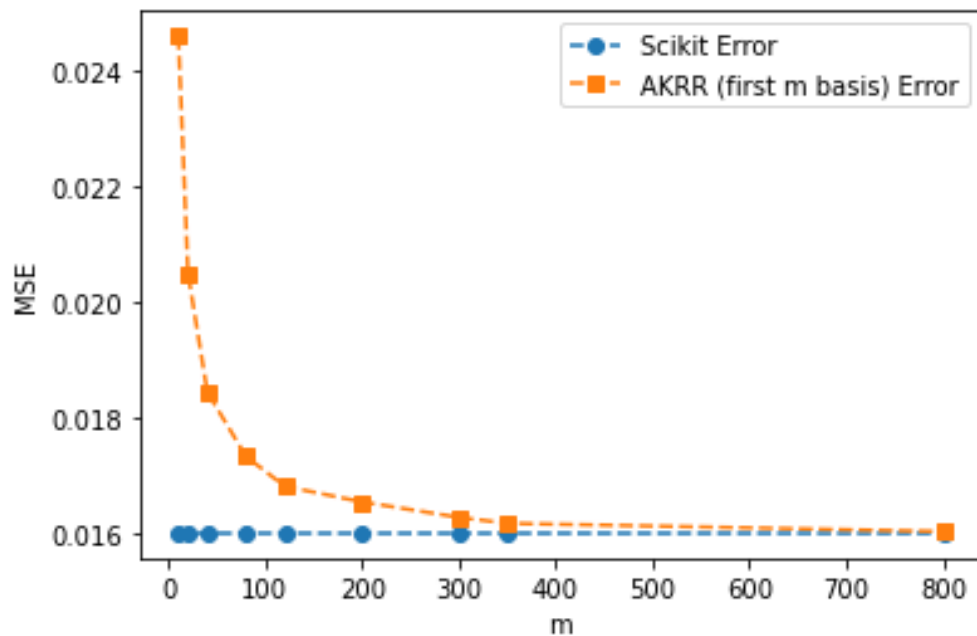
Putting the dominant terms together:  $\boxed{O(mnp) + O(m^2n)}$ .

- $O(mnp) \leftarrow$  building  $\tilde{K}$  (kernel evaluations).
- $O(m^2n) \leftarrow$  forming  $\tilde{K}^T \tilde{K}$  (and it dominates the linear-solve in the common  $n \geq m$ ) setting.

## Part II: Implementation

Implement AKRR based on 'hw3\_akrr.py'. Below are some instructions.

- Given a training set, simply choose the first  $m$  instances to express  $\tilde{\beta}$  for AKRR.
- Use RBF kernel and pick a proper  $\gamma$  by yourself for the kernel. Also pick a proper  $\lambda$  by yourself.
- Report testing MSE versus  $m$  in Figure 1. Pick at least five values of  $m$  by yourself which can provide a comprehensive picture of its impact on model performance. A KRR with RBF kernel from scikit-learn is given in the template. Do not remove it. Give it the same  $\gamma$  and  $\lambda$  you chose for AKRR. Figure 1 should contain a curve of AKRR error and a line of KRR error (which should not change as  $m$  increases).



**Fig. 1.** Testing Error versus  $m$  for AKRR and KRR.

#### Submission Instruction

Please submit two files to Canvas.

- (i) Submit 'hw3.pdf'. It should contain your answers to all questions in this document. A latex template 'hw2\_Latex.txt' is provided.
- (ii) Submit 'hw2\_akrr.py'. It should be the code that generates Figure 1.