Tight Kernel Query Complexity of Kernel Ridge Regression and Kernel k-means Clustering

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Introduction

Given a kernel matrix \mathbf{K} , a regularization parameter λ , and a target vector \mathbf{z} , the kernel ridge regression (KRR) problem asks for the minimizer of the following objective function:

$$\boldsymbol{\alpha}_{\text{opt}} = \underset{\boldsymbol{\alpha} \in \mathbb{R}^n}{\operatorname{argmin}} \|\mathbf{K}\boldsymbol{\alpha} - \mathbf{z}\|_2^2 + \lambda \boldsymbol{\alpha}^{\mathsf{T}} \mathbf{K}\boldsymbol{\alpha}.$$
 (1)

We consider the problem of outputting approximate solutions, i.e.

$$\|\hat{\boldsymbol{\alpha}} - \boldsymbol{\alpha}_{\text{opt}}\|_{2} \le \varepsilon \|\boldsymbol{\alpha}_{\text{opt}}\|_{2} = \varepsilon \|(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{z}\|_{2}.$$
 (2)

How many kernel entries do we need to read in order to approximate KRR?

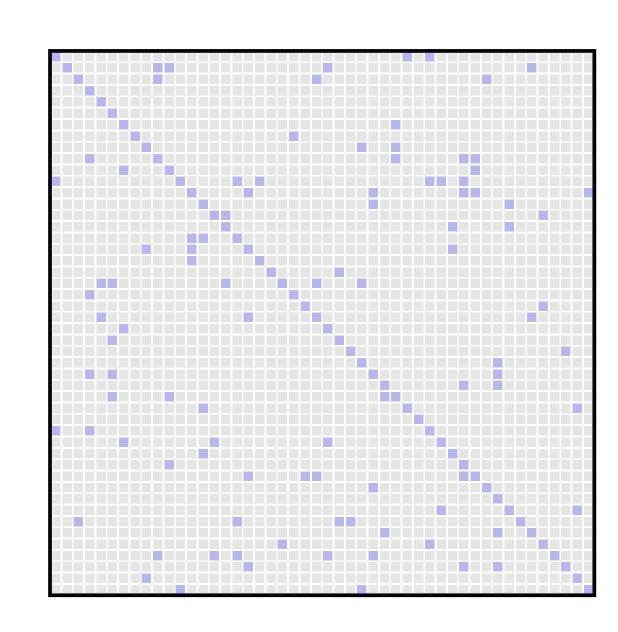


Figure 1: An algorithm might read the diagonal and sample some uniformly random entries.

The best known algorithms have kernel query complexity depending on the effective statistical dimension

$$d_{\text{eff}}^{\lambda}(\mathbf{K}) := \text{tr}\left(\mathbf{K}(\mathbf{K} + \lambda \mathbf{I}_n)^{-1}\right) = \sum_{i=1}^{\text{rank}(\mathbf{K})} \frac{\sigma_i^2}{\sigma_i^2 + \lambda}.$$
 (3)

For example, the following result is proved in [MM17] using an adaptive sampling techinque known as *ridge leverage score sampling*:

ALGORITHM FOR KRR [MM17]

There is an algorithm computing a $(1+\varepsilon)$ relative error KRR solution with probability at least 2/3 making $O(\frac{nd_{\text{eff}}^{\lambda}}{\varepsilon}\log\frac{d_{\text{eff}}^{\lambda}}{\varepsilon})$ kernel queries.

Main Result: KRR

The following open question was posed by El Alaoui and Mahoney [EAM15]:

Is the effective statistical dimension a lower bound on the kernel query complexity of KRR?

We answer this question affirmatively in our main result for KRR:

Lower Bound for KRR [FWY19]

Any algorithm computing a $(1+\varepsilon)$ relative error KRR solution with probability at least 2/3 makes at least $\Omega(\frac{nd_{\text{eff}}^{\lambda}}{\varepsilon})$ kernel queries.

Proof sketch. To show the result, we consider a reduction to the problem of labeling the block size of each row of the following kernel matrix:

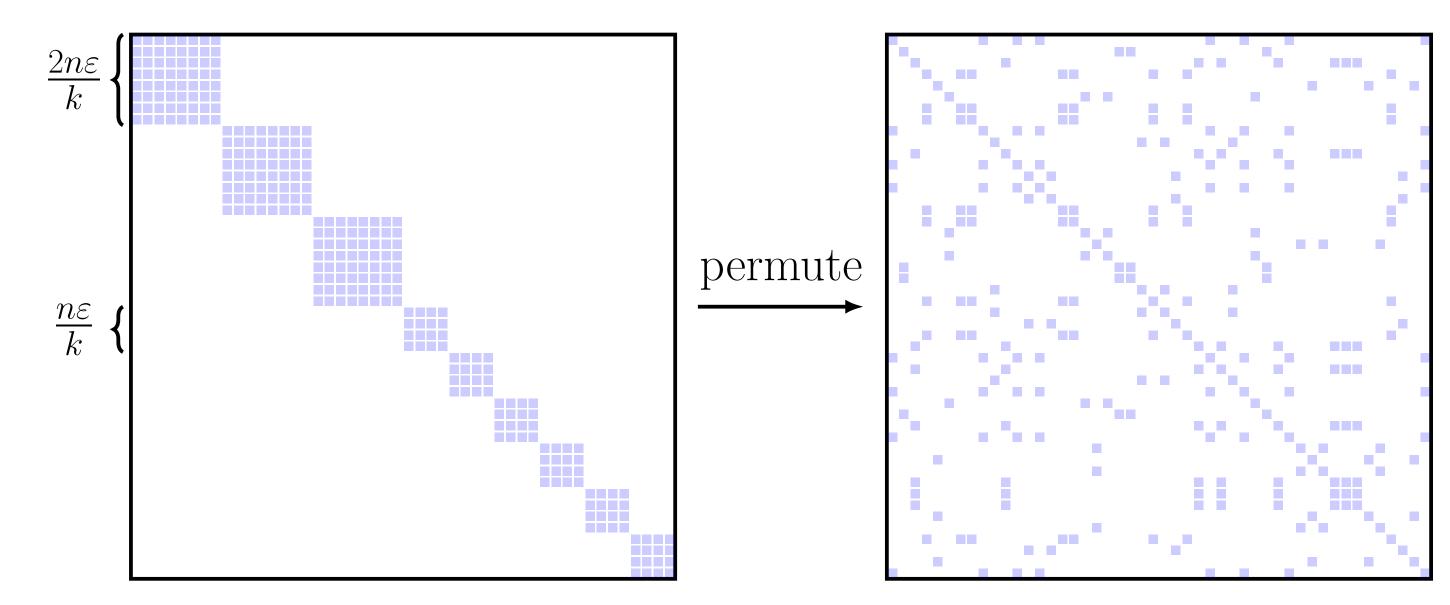


Figure 2: Hard input distribution for KRR: does the *i*th row have $\frac{2n\varepsilon}{k}$ or $\frac{n\varepsilon}{k}$ ones?

By standard arguments, this problem requires $\Omega(nk/\varepsilon)$ kernel queries. It is well-known that the exact solution to the KRR problem is

$$\boldsymbol{\alpha}_{\text{opt}} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{z}. \tag{4}$$

If we set $\mathbf{z} = \mathbf{1_n}$ and $\lambda = n/k$, then the *i*th coordinate of $\boldsymbol{\alpha}_{\mathrm{opt}}$ is

$$\mathbf{e}_{i}^{\mathsf{T}} \boldsymbol{\alpha}_{\mathrm{opt}} = \begin{cases} (2n\varepsilon/k + n/k)^{-1} = \frac{k/n}{1+2\varepsilon} & \text{if row } i \text{ has block size } 2n\varepsilon/k \\ (n\varepsilon/k + n/k)^{-1} = \frac{k/n}{1+\varepsilon} & \text{if row } i \text{ has block size } n\varepsilon/k \end{cases}$$

so a $(1+\varepsilon)$ relative error solution can distinguish these two cases. We also have $d_{\text{eff}}^{\lambda} = \Theta(k)$ so we conclude.

Main Result: KKMC

Next, we present our main result for kernel k-means clustering:

Lower Bound for KKMC [FWY19]

Any algorithm computing a $(1 + \varepsilon)$ relative error KKMC solution with probability at least 2/3 makes at least $\Omega(\frac{nk}{\varepsilon})$ kernel queries.

This result uses similar reductions as our KRR result, but the cost computations are much more involved. Our result matches the following algorithmic result of [MM17] (also based on ridge leverage score sampling) up to log factors:

ALGORITHM FOR KKMC [MM17]

There is an algorithm computing a $(1+\varepsilon)$ relative error KKMC solution with probability at least 2/3 making $O(\frac{nk}{\varepsilon}\log\frac{k}{\varepsilon})$ kernel queries.

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