Divide and Conquer Kernel Ridge Regression

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Problem set-up

Goal Solve

$$\begin{aligned} \text{minimize} \quad & \mathbb{E}[(f(x) - y)^2] \\ \text{subject to} \quad & f \in \mathcal{H} \end{aligned}$$

where $(x, y) \sim \mathbb{P}$. $\mathcal{H}$ is a Reproducing Kernel Hilbert Space (RKHS).

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$\mathcal{H}$ defined by kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$:

$$\mathcal{H} = \{f : f = \sum_i \alpha_i k(x_i, \cdot), \ x_i \in \mathcal{X}\}.$$

Kernel regression review

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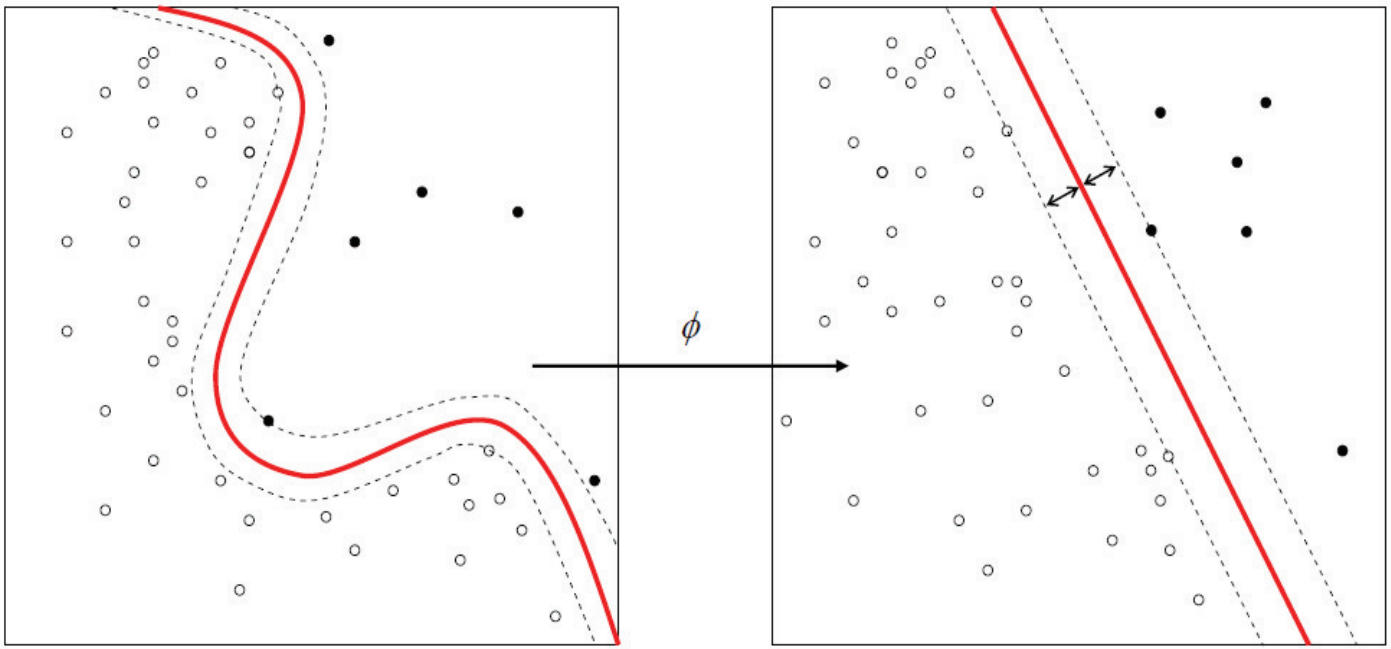
2. Map x onto a high-dimension space $x \Rightarrow \phi(x)$. Learn a model $f(x) = \theta^T \phi(x)$, so that f is non-linear function of x.



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4. k is the kernel function and should be easy to compute.

   Examples:

   - Polynomial kernel: $k(x, x') = (1 + x^T x')^d$.
   - Gaussian kernel: $k(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$.
   - Sobolev kernel in $\mathbb{R}^1$: $k(x, x') = 1 + \min(x, x')$.

Kernel ridge regression

Given finite samples $(x_1, y_1), \ldots, (x_N, y_N)$, minimize the empirical risk

$$\hat{f} = \operatorname*{argmin}_{f \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2$$

as the estimator of $f^* = \operatorname{argmin}_{f \in \mathcal{H}} \mathbb{E}[(f(x) - y)^2]$.

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This minimization problem has a closed-form solution:

$$\hat{f} = \sum_{i=1}^{N} \alpha_i k(x_i, \cdot), \quad \text{where} \quad \alpha = (K + \lambda N I)^{-1} y.$$

K is the $N \times N$ kernel matrix defined by $K_{ij} = k(x_i, x_j)$.

Think about large datasets

The matrix inversion $\alpha = (K + \lambda N I)^{-1} y$ takes $\mathcal{O}(N^3)$ time and $\mathcal{O}(N^2)$ memory space, which can be prohibitively expensive when N is large.

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1. Low-rank matrix approximation:
   - Kernel PCA [SSM98]
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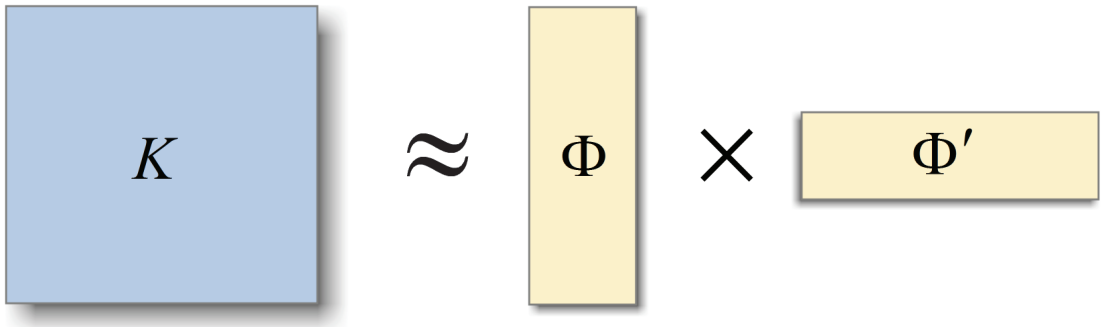

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Accuracy of approximate methods vs. exact algorithm is unknown.

Our main idea

Only keep the diagonal blocks, so that the matrix inversion is fast.

$$K = \begin{pmatrix} K_{11} & K_{12} & K_{13} & K_{14} & K_{15} & K_{16} \\ K_{21} & K_{22} & K_{23} & K_{24} & K_{25} & K_{26} \\ K_{31} & K_{32} & K_{33} & K_{34} & K_{35} & K_{36} \\ K_{41} & K_{42} & K_{43} & K_{44} & K_{45} & K_{46} \\ K_{51} & K_{52} & K_{53} & K_{54} & K_{55} & K_{56} \\ K_{61} & K_{62} & K_{63} & K_{64} & K_{65} & K_{66} \end{pmatrix}$$

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Block Diagonalize

Fast Kernel Ridge Regression (Fast-KRR)

Divide-and-conquer approach:

1. Divide samples $\{(x_1, y_1), \ldots, (x_N, y_N)\}$ uniformly at randomly into the m disjoint subsets $S_1, \ldots, S_m$.

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2. For each $i = 1, 2, \ldots, m$, compute the *local KRR estimate*

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$$\text{Time: } \mathcal{O}(N^3) \Rightarrow \mathcal{O}(N^3/m^2)$$
$$\text{Space: } \mathcal{O}(N^2) \Rightarrow \mathcal{O}(N^2/m^2).$$

Theoretical result

Theorem

With m splits, Fast-KRR achieves the mean square error:

$$\mathbb{E}[\|\bar{f} - f^*\|_2^2] \leq C\Big(\underbrace{\lambda \|f^*\|_{\mathcal{H}}^2}_{\text{squared bias}} + \underbrace{\frac{\gamma(\lambda)}{N}}_{\text{variance}} + \exp\big(-\frac{c \cdot N/m}{\gamma^2(\lambda)}\big)\Big)$$

We assume $\|f^*\|_{\mathcal{H}} < \infty$. There is an "oracle" extension to this result.

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- $\gamma(\lambda)$ is the *effective dimensionality*: let $\mu_1 \geq \mu_2 \geq \ldots$ be the sequence of eigenvalues in kernel k's eigen-expansion, then

$$\gamma(\lambda) = \sum_{k=1}^{\infty} \mu_k/(\lambda + \mu_k).$$

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$$\gamma(\lambda) = \sum_{k=1}^{\infty} \mu_k/(\lambda + \mu_k).$$

- $\exp(-\frac{c \cdot N/m}{\gamma^2(\lambda)})$ is negligibly small when $m \lesssim N/\gamma^2(\lambda)$.

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Apply to specific kernels

Corollary

For polynomial kernel if $m \leq cN/\log N$ then

$$\mathbb{E}[\|\bar{f} - f^*\|_2^2] = \mathcal{O}\left(\frac{1}{N}\right) \qquad \text{(minimax optimal rate)}$$

Time: $\mathcal{O}(N^3) \Rightarrow \mathcal{O}(N \log^2 N)$ Space: $\mathcal{O}(N^2) \Rightarrow \mathcal{O}(\log^2 N)$

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For Gaussian kernel, if $m \leq cN/\log^2 N$ then

$$\mathbb{E}[\|\bar{f} - f^*\|_2^2] = \mathcal{O}\left(\frac{\sqrt{\log N}}{N}\right) \quad \text{(minimax optimal rate)}$$

Time: $\mathcal{O}(N^3) \Rightarrow \mathcal{O}(N \log^4 N)$ Space: $\mathcal{O}(N^2) \Rightarrow \mathcal{O}(\log^4 N)$

Apply to specific kernels

Corollary

For Sobolev kernel of smoothness ν, if $m \leq cN^{\frac{2\nu-1}{2\nu+1}} / \log N$ then

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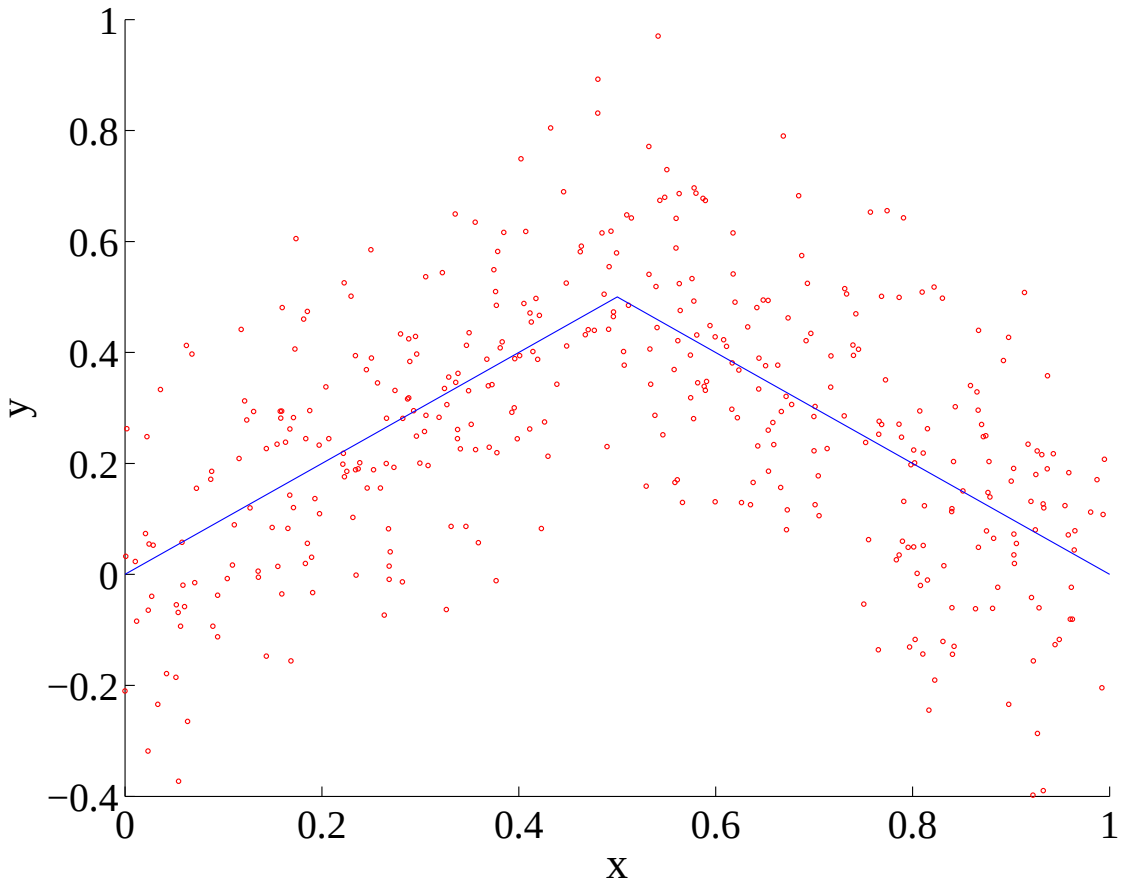
$$\text{Time: } \mathcal{O}(N^3) \Rightarrow \mathcal{O}(N^{\frac{2\nu+5}{2\nu+1}} \log^2 N)$$

$$\text{Space: } \mathcal{O}(N^2) \Rightarrow \mathcal{O}(N^{\frac{4}{2\nu+1}} \log^2 N)$$

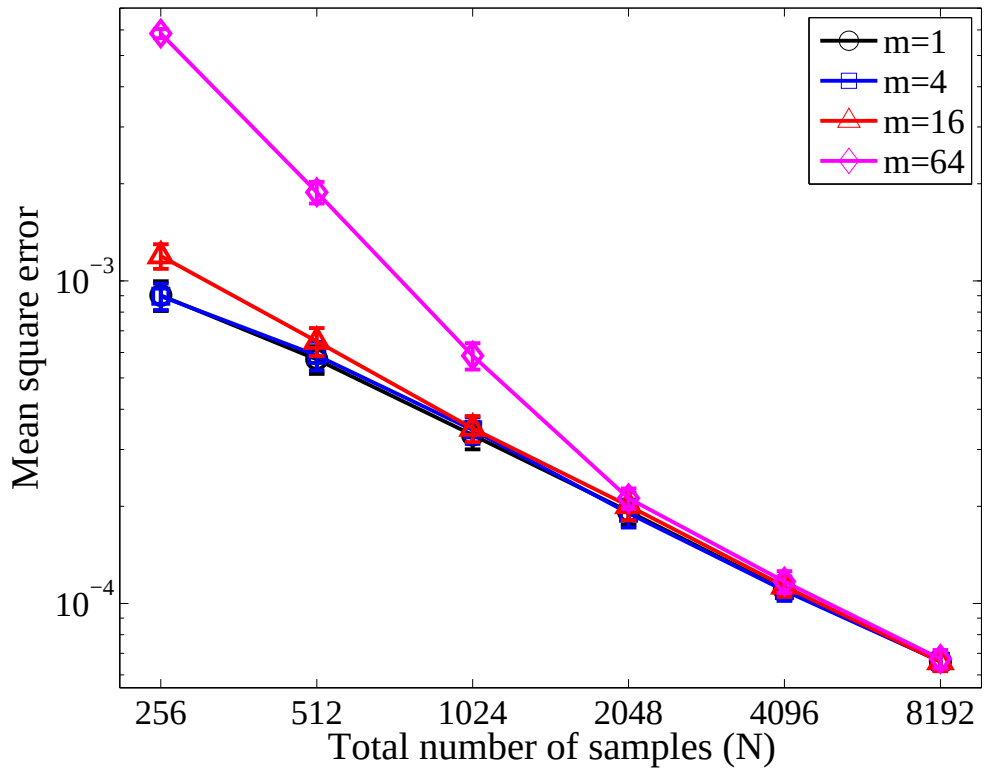
Simulation Study

Data (x, y) is generated by $y = \min(x, 1 - x) + \varepsilon$ where $\varepsilon \sim N(0, 0.2)$.



Compare Fast-KRR and exact KRR

We use a Sobolev kernel of smoothness-1 to fit the data.



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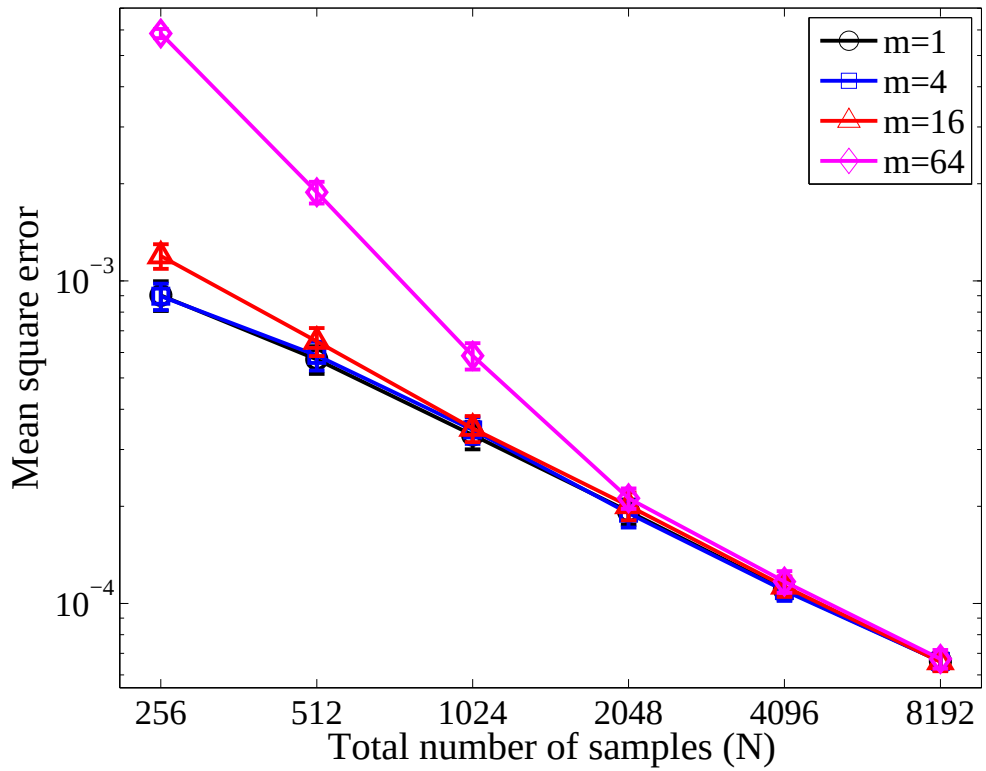
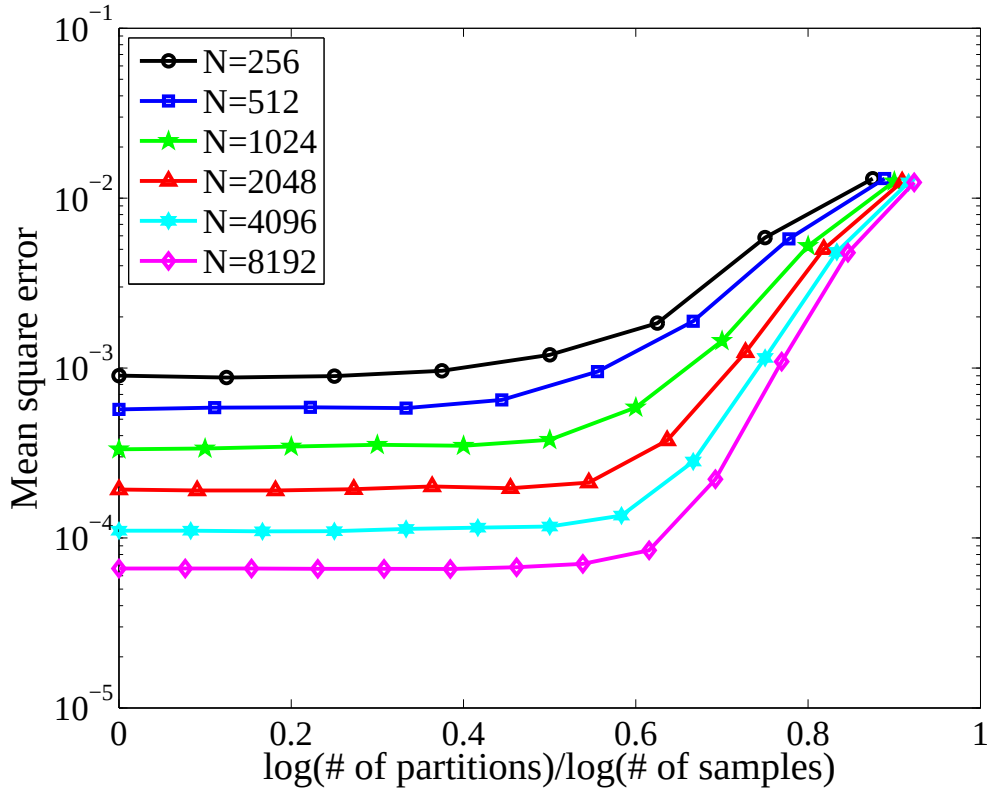


Fast-KRR's performance is very close to exact KRR for $m \leq 16$.

Threshold for data partitioning

Mean square error is plotted for varied choices of m.



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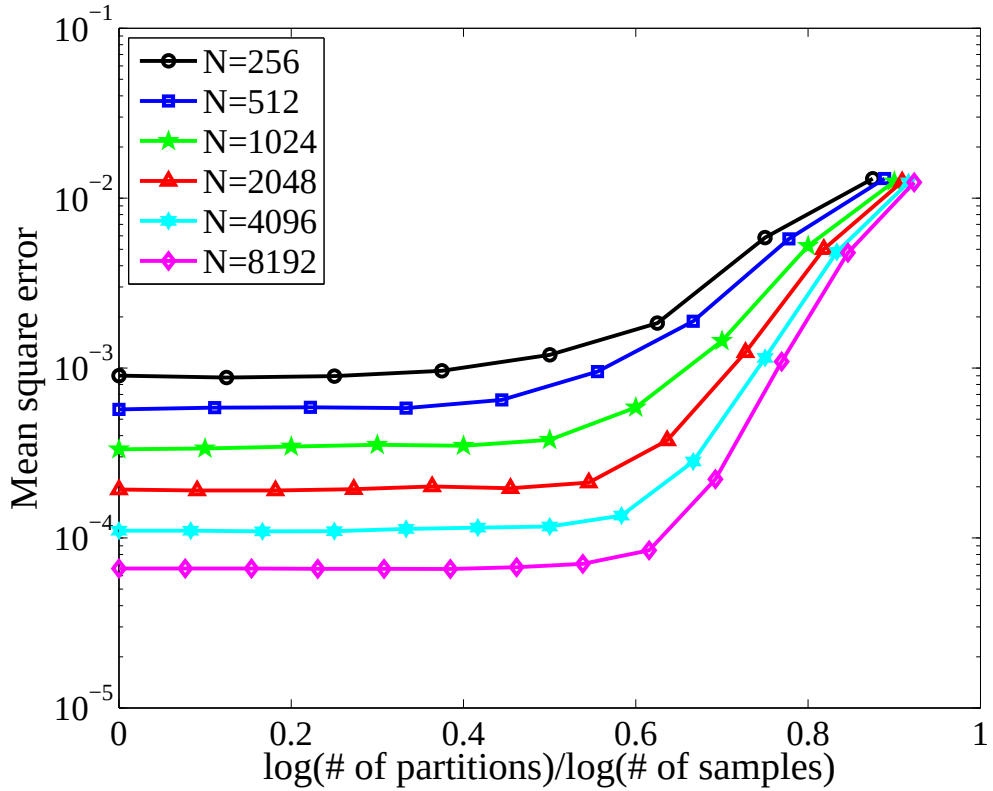

As long as $m \lesssim N^{0.45}$, the accuracy is not hurt.

Summary

- Divide-and-conquer approach for kernel ridge regression reduces time and space complexity.
- Optimal accuracy is retained.
- Polynomially time complexity in for Sobolev space kernels, nearly linear complexity for finite-rank kernels and Gaussian kernels.

Open Problems

- How to choose optimal partition number in practice?
- Lower bound for sub-sampling rate?
- Does divide-and-conquer work for other kernel-based methods?