






# Optimal Kernel Quantile Learning with Random Features

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# Introduction I

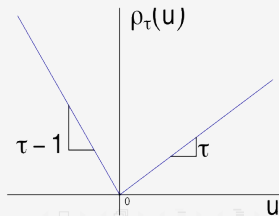
## Why Quantile Regression?

- Reason 1: Quantile regression allows us to study the impact of predictors on different quantiles of the response distribution, and thus provides a complete picture of the relationship between responses and covariates.
- Reason 2: Robust to outliers in response observations.
- Reason 3: Estimation and inference are distribution-free, and heterogeneity is usually allowed in quantile regression models.

## Loss Function

$$\rho_{\tau}(u) = u\{\tau - \mathcal{I}(u < 0)\},$$

where  $\mathcal{I}$  is the indicator function, and  $\tau$  is the quantile level.



# Introduction II



Figure 1: Financial Crisis

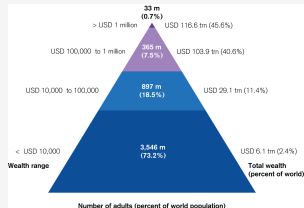


Figure 2: Income Pyramid



Figure 3: Powerful Typhoon



Figure 4: Air Pollution



## Introduction III

Suppose a random pair  $(x, y)$  is drawn from an unknown joint distribution  $\rho(x, y)$ , consider the following **quantile regression model**

$$y = f_{\tau}^*(x) + \varepsilon, \quad (1)$$

where

- $y \in \mathbb{R}$  is the scala response;
- $x \in \mathcal{X} \subset \mathbb{R}^p$  is the  $p$ -dimensional vector of the covariate;
- $\varepsilon$  is the model error which satisfies  $\mathbb{P}(\varepsilon_i < 0 | x) = \tau$  for  $\tau \in (0, 1)$ .

Model (1) implies the following model.

### Nonparametric quantile regression

$$Q_{\tau}(y_i | x) = f_{\tau}^*(x), \quad \tau \in (0, 1),$$

where  $Q_{\tau}(\cdot | x)$  refers to the  $\tau$ -th conditional quantile of the response  $y$  given the covariate  $x$ .



## Introduction IV

The method of kernel quantile regression (KQR) is based on the idea of a reproducing kernel Hilbert space.

### Reproducing Kernels

Any symmetric, bounded and positive semi-definite kernel function  $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  defines a reproducing kernel Hilbert space (RKHS), denoted by  $\mathcal{H}_K$ . An important property of  $\mathcal{H}_K$  is the **reproducing property** that for any  $f \in \mathcal{H}_K$ , there holds

$$\langle f, K(\mathbf{x}, \cdot) \rangle_K = f(\mathbf{x}),$$

where  $\langle \cdot, \cdot \rangle_K$  denotes the inner product in  $\mathcal{H}_K$ . Its equipped norm is defined as  $\| \cdot \|_K^2 = \langle \cdot, \cdot \rangle_K$ .





## Introduction V

Consider a standard supervised learning problem that we have a sample  $D = \{(x_i, y_i)\}_{i=1}^{|D|}$ , KQR estimates a function in the RKHS  $\mathcal{H}_K$  by minimizing the check loss function combined with a penalty based on the squared Hilbert norm

$$f_{D,\lambda} = \operatorname{argmin}_{f \in \mathcal{H}_K} \frac{1}{|D|} \sum_{i=1}^{|D|} \rho_\tau(y_i - f(x_i)) + \lambda \|f\|_K^2, \quad (2)$$

where  $|D|$  is the cardinality of  $D$  and  $\lambda$  is the regularization parameter controlling the model smoothness.





# Reviews and Motivation I

## Computation

According to the **representer theorem** (Wahba, 1990), the solution of this optimization task (2) is of finite form as given by  $f_{D,\lambda}(x) = \sum_{i=1}^{|D|} \alpha_i K(x, x_i) = \boldsymbol{\alpha}^T K_N(x)$ . With this solution plugged into (2), the optimization problem can be reformulated as

$$\hat{\boldsymbol{\alpha}} = \underset{\boldsymbol{\alpha} \in \mathbb{R}^{|D|}}{\operatorname{argmin}} \frac{1}{|D|} \sum_{i=1}^{|D|} \rho_{\tau}(y_i - \boldsymbol{\alpha}^T K_N(x_i)) + \lambda \boldsymbol{\alpha}^T K \boldsymbol{\alpha}, \quad (3)$$

where  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_{|D|})^T \in \mathbb{R}^{|D|}$  are the representer coefficients and  $K_N(x) = (K(x_1, x), \dots, K(x_{|D|}, x))^T \in \mathbb{R}^{|D|}$ , and  $K = \{K(x_i, x_j)\}_{i,j=1}^{|D|}$  is the Gram matrix.

- Dual optimization (Takeuchi et al., 2006; Feng et al., 2023);
- Path-following algorithm (Li et al., 2007);
- ADMM algorithm (Boyd et al., 2011; Wang et al., 2024).







## Reviews and Motivation II

### Existing issues

- The scalability of KQR for large datasets is limited due to the **expensive computational complexity** ( $\mathcal{O}(|D|^3)$ ) and **storage requirements** ( $\mathcal{O}(|D|^2)$ ) when  $|D|$  is large.
- The theoretical investigation of KQR is not clear and deep enough (**Suboptimal or capacity-independent**).
- Most work assume the **realizable setting**, i.e.,  $f_{\tau}^* \in \mathcal{H}_K$ , does KQR work in the **agnostic setting**, i.e.,  $f_{\rho} \notin \mathcal{H}_K$ ?

**Question:** Can we find some accelerated methods that can achieve a **optimal trade-off** between the computation and theory, especially in the agnostic settings?





# Random Fourier Features I

The following classical theorem from harmonic analysis provides the key insight behind random feature mapping:

## Bochner's theorem

A continuous kernel  $K(\mathbf{x}, \mathbf{x}') = K(\mathbf{x} - \mathbf{x}')$  on  $\mathbb{R}^p$  is positive definite if and only if  $K(\mathbf{x} - \mathbf{x}')$  is the Fourier transform of a non-negative measure.

## Unbiased feature mapping

If a shift-invariant kernel  $K(\cdot, \cdot)$  is properly scaled, Bochner's theorem guarantees that its Fourier transform  $\pi(\boldsymbol{\omega})$  is a proper probability distribution. Define  $\phi(\mathbf{x}, \boldsymbol{\omega}) = e^{j\boldsymbol{\omega}^T \mathbf{x}}$  we have

$$K(\mathbf{x}, \mathbf{x}') = K(\mathbf{x} - \mathbf{x}') = \int_{\mathbb{R}^p} \pi(\boldsymbol{\omega}) e^{j\boldsymbol{\omega}^T (\mathbf{x} - \mathbf{x}')} d\boldsymbol{\omega} = \mathbb{E}_{\boldsymbol{\omega}} [\phi(\mathbf{x}, \boldsymbol{\omega}) \phi^*(\mathbf{x}', \boldsymbol{\omega})], \quad (4)$$

where  $*$  denoting the Hermitian transpose. So  $\phi(\mathbf{x}, \boldsymbol{\omega}) \phi^*(\mathbf{x}', \boldsymbol{\omega})$  is an **unbiased estimator** of  $K(\mathbf{x}, \mathbf{x}')$  when  $\boldsymbol{\omega}$  is drawn from  $\pi(\boldsymbol{\omega})$ .



## Random Fourier Features II

Since both  $\pi(\omega)$  and  $K(\cdot, \cdot)$  are real, the integral (4) converges when the complex exponentials are replaced with cosines.

### Real-valued feature mapping

A real-valued mapping that satisfies the condition  $K(x, x') = \mathbb{E}_{\omega} [\phi(x, \omega) \phi^*(x', \omega)]$  can be obtained by setting

$$\phi(x, \omega) = \sqrt{2} \cos(\omega^T x + b),$$

where  $\omega$  is drawn from  $\pi(\omega)$  and  $b$  is drawn uniformly from  $[0, 2\pi]$ .



# Random Fourier Features III

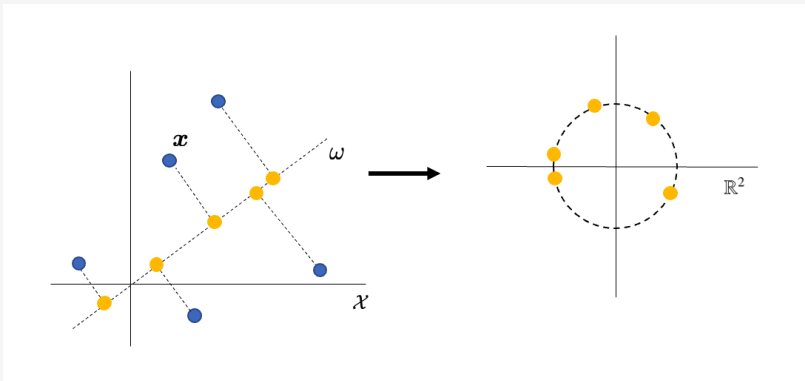


Figure 5: Random Fourier Features. Each component of the feature map  $\phi(x, \omega) = \sqrt{2} \cos(\omega^T x + b)$  projects  $x$  onto a random direction  $\omega$  drawn from the Fourier transform  $\pi(\omega)$ , and wraps this line onto the unit circle in  $\mathbb{R}^2$ . After transforming two points  $x$  and  $x'$  in this way, their inner product is an unbiased estimator of  $K(x, x')$ . The mapping additionally rotates this circle by a random amount  $b$  and projects the points onto the interval  $[0, 1]$  (Rahimi and Recht, 2007).



# Examples

Table 1: Some examples of shift invariant kernels and their Fourier transforms (Rahimi and Recht, 2007).

Kernel Name	$K(\Delta)$	$\pi(\omega)$
Gaussian Kernel	$e^{-\frac{\ \Delta\ _2^2}{2}}$	$(2\pi)^{\frac{D}{2}} e^{-\frac{\ \omega\ _2^2}{2}}$
Laplacian Kernel	$e^{-\ \Delta\ _1}$	$\prod_d \frac{1}{\pi(1+\omega_d^2)}$
Cauchy Kernel	$\prod_d \frac{1}{(1+\Delta_d^2)}$	$e^{-\ \omega\ _1}$



# Kernel Approximation

## Kernel approximation with random features

It is thus clear that we can adopt the standard Monte Carlo sampling method to estimate  $K(x, x')$  by

$$K_M(x, x') = \langle \phi_M(x, \omega), \phi_M(x', \omega) \rangle,$$

where  $\phi_M(x, \omega) = \frac{1}{\sqrt{M}}(\phi(x, \omega_1), \dots, \phi(x, \omega_M))^T$  is the feature map and  $\omega_1, \dots, \omega_M$  are independently sampled with respect to  $\pi$ .

**Remark:** In addition to the shift invariant kernel, any kernel has the following integral representation can use the above approximation,

$$K(x, x') = \int_{\Omega} \phi(x, \omega) \phi(x', \omega) d\pi(\omega),$$

(5)





# RKHS Approximation

## RKHS approximation with random features

Define a  $M$ -dimensional function space  $\mathcal{H}_M$  related to  $\phi_M(\mathbf{x})$  as

$$\mathcal{H}_M = \left\{ f \mid f(\mathbf{x}) = \mathbf{u}^T \phi_M(\mathbf{x}), \mathbf{x} \in \mathcal{X}, \mathbf{u} \in \mathbb{R}^M \right\}.$$

It thus clear that  $\mathcal{H}_M$  is a RKHS induced by kernel function  $K_M(\mathbf{x}, \mathbf{x}') = \langle \phi_M(\mathbf{x}, \boldsymbol{\omega}), \phi_M(\mathbf{x}', \boldsymbol{\omega}) \rangle$ . For  $f = \mathbf{u}^T \phi_M(\mathbf{x}) \in \mathcal{H}_M, g = \mathbf{z}^T \phi_M(\mathbf{x}) \in \mathcal{H}_M$ , we define their inner product in  $\mathcal{H}_M$  as  $\langle f, g \rangle_{\mathcal{H}_M} = \mathbf{u}^T \mathbf{z}$ . And the corresponding norm of  $f$  in  $\mathcal{H}_M$  is  $\|f\|_{\mathcal{H}_M} = \sqrt{\mathbf{u}^T \mathbf{u}} = \|\mathbf{u}\|_2$ .



# Illustration

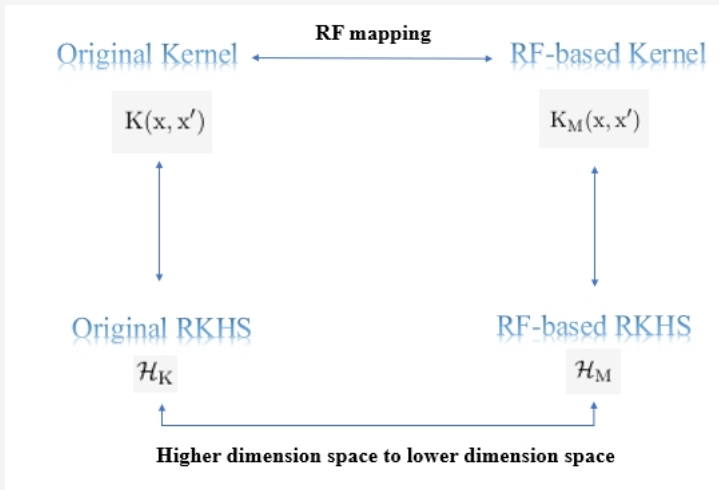


Figure 6: A simple illustration of kernel and RKHS approximation using RF.





# KQR with Random Features I

## KQR-RF

Different from KQR, KQR with random features (KQR-RF) estimates a function in the approximation RKHS  $\mathcal{H}_M$

$$f_{M,D,\lambda} = \operatorname{argmin}_{f \in \mathcal{H}_M} \frac{1}{|D|} \sum_{(x,y) \in D} \rho_\tau(y - f(x)) + \lambda \|f\|_{\mathcal{H}_M}^2, \quad (6)$$





## KQR with Random Features II

### Computation

According to the representer theorem, the solution of (3) with random features can be written as

$$f_{M,D,\lambda}(x) = \hat{u}^T \phi_M(x), \quad (7)$$

and the optimization problem becomes

$$\hat{u} = \underset{u \in \mathbb{R}^M}{\operatorname{argmin}} \frac{1}{|D|} \sum_{i=1}^{|D|} \rho_{\tau}(y_i - u^T \phi_M(x_i)) + \lambda u^T u. \quad (8)$$

Notably, leveraging random features allows us to reformulate the initial problem into linear quantile regression augmented by a ridge penalty, reducing the number of parameters to be  $M \ll |D|$ .





# Theoretical Goal

The objective of KQR-RF is to find an estimator that minimizes the following expected risk

$$\mathcal{E}(f) = \int_{\mathcal{X} \times \mathbb{R}} \rho_{\tau}(y - f(x)) d\rho(x, y),$$

and we evaluate the performance of KRR-RF by the **excess risk**  $\mathcal{E}(f) - \mathcal{E}(f_{\tau}^*)$ , or the  $L^2_{\rho_{\mathcal{X}}}$ -norm of the difference  $\|f - f_{\tau}^*\|_{\rho}^2$ .



# Definitions and Assumptions I

## Definition 1 (Integral operators)

For any  $f \in L^2_{\rho_{\mathcal{X}}}$ , we define the integral operators by the kernel  $K$  and  $K_M$  as

$$\begin{aligned} L_K f &= \int_{\mathcal{X}} K(x, \cdot) f(x) d\rho_{\mathcal{X}}, \\ L_M f &= \int_{\mathcal{X}} K_M(x, \cdot) f(x) d\rho_{\mathcal{X}}. \end{aligned}$$

## Definition 2 (Effective dimension)

For  $\lambda > 0$ , we define the effective dimension of kernel  $K$  and  $K_M$  as

$$\begin{aligned} \mathcal{N}(\lambda) &= \text{Tr}((L_K + \lambda I)^{-1} L_K), \\ \mathcal{N}_M(\lambda) &= \text{Tr}((L_M + \lambda I)^{-1} L_M). \end{aligned}$$



## Definitions and Assumptions II

### Assumption 1 (Bounded and continuous random features)

Assume kernel  $K$  has the integral representation defined in (5) with  $\phi$  bounded and continuous in both variables, that is, there exists some constant  $\kappa \geq 1$  such that  $|\phi(\mathbf{x}, \boldsymbol{\omega})| \leq \kappa$  for any  $\mathbf{x} \in \mathcal{X}$  and  $\boldsymbol{\omega} \in \Omega$ . The associated RKHS  $\mathcal{H}_K$  is separable.

### Assumption 2 (Source condition)

Suppose there exists  $R > 0$ ,  $r > 0$  and  $\mathbf{h}_\tau \in L_{\rho_X}^2$  such that

$$\mathbf{f}_\tau^* = L_K^r \mathbf{h}_\tau, \quad (9)$$

where  $\|\mathbf{h}_\tau\|_\rho \leq R$  and  $L_K^r$  is the  $r$ -th power of  $L_K$ .

## Definitions and Assumptions III

### Remark

- The parameter  $r$  controls the size of the functional class of  $f_\tau^*$ . When  $r \in [1/2, 1]$ , the functional class  $\mathcal{C}$  is a subset of the assumed RKHS  $\mathcal{H}_K$ , so we have  $f_\tau^* \in \mathcal{H}_K$ . When  $r \in (0, 1/2)$ , the functional class  $\mathcal{C}$  is larger than the assumed RKHS  $\mathcal{H}_K$ , and there exists some cases where  $f_\tau^* \notin \mathcal{H}_K$ .
- Existing literature on KQR and kernel methods with Lipschitz continuous loss functions often assumes that  $r = 1/2$  (Bach, 2017; Sun et al., 2018; Li et al., 2021) or  $r \in [1/2, 1]$  (Lian, 2022), corresponding to the realizable setting  $f_\tau^* \in \mathcal{H}_K$ . However, our analysis further allows  $r \in (0, 1/2)$ , relating to the agnostic setting  $f_\tau^* \notin \mathcal{H}_K$ .

### Assumption 3 (Capacity condition)

For  $\lambda > 0$ , there exists  $Q > 0$  and  $\gamma \in [0, 1]$  such that

$$\mathcal{N}(\lambda) \leq Q^2 \lambda^{-\gamma}. \quad (10)$$



## Definitions and Assumptions IV

- For kernel ridge regression (KRR) and Kernel ridge regression with random features (KRR-RF), the **minimax optimal capacity-dependent rate** has been shown to be  $\mathcal{O}(|\mathcal{D}|^{\frac{2r}{2r+\gamma}})$  (Caponnetto and De Vito, 2007; Rudi and Rosasco, 2017).
- Whether KRR-RF can achieve the above optimal learning rate even under the agnostic settings?

### Assumption 4 (Adaptive self-calibration condition)

Let  $f_{y|x}(\cdot)$  denote the conditional density function of  $y$  given  $x$ . Suppose that  $\sup_{t \in \mathbb{R}} f_{y|x}(t) \leq c_1$  for  $c_1 > 0$ . Furthermore, there exist some universal constants  $\varepsilon, \varepsilon', c_2 > 0$  that are independent with  $x$  and  $y$ , such that for any  $y \in \mathcal{B}(f_\tau^*(x), \varepsilon)$  and  $|\delta| \leq \varepsilon'$ , the following inequality holds almost surely,

$$|F_{y|x}(y + \delta) - F_{y|x}(y)| \geq c_2 |\delta|, \quad (11)$$

where  $\mathcal{B}(f_\tau^*(x), \varepsilon) = \{y \mid |y - f_\tau^*(x)| \leq \varepsilon\}$  denotes the ball centered at  $f_\tau^*(x)$  with radius  $\varepsilon$ , and  $F_{y|x}(\cdot)$  is the cumulative distribution function of  $y$  given  $x$ .



## Definitions and Assumptions V

- For example, if  $y$  has a density that is bounded away from zero on some compact interval around  $f_{\tau}^*(x)$ , then Assumption 4 holds. **More importantly, we do not impose any moment condition on the distribution of  $y$ .**
- It is also worth noting that Assumption 3.6 is **weaker than** Condition 2 in He and Shi (1994) where the density function of  $y$  is lower bounded everywhere by some positive constant. It is also **weaker than** Condition D.1 in Belloni and Chernozhukov (2011) requiring the conditional density of  $Y$  given  $x$  to be continuously differentiable and bounded away from zero uniformly for all  $\tau \in (0, 1)$  and all  $x$  in the support  $\mathcal{X}$ .
- The special case when  $\varepsilon = 0$  aligning with the **self-calibration condition** also appeared in Shen et al. (2021); Madrid Padilla and Chatterjee (2022).







## Existing Theorem

### Theorem 19 of Li et al. (2021)

Assume there exists a function  $f_{\mathcal{H}}$  such that  $f_{\mathcal{H}} = \operatorname{argmin}_{f \in \mathcal{H}_K} \mathcal{E}(f)$ . Under some technical assumptions<sup>a</sup>, and  $\lambda = \mathcal{O}(|D|^{-1})$ , when the number of random features satisfies

$$M \gtrsim |D|^{\frac{\gamma}{2}} \log |D|,$$

and  $|D|$  is sufficiently large, there holds

$$\mathcal{E}(f_{M,D,\lambda}) - \mathcal{E}(f_{\mathcal{H}}) \asymp \|f_{M,D,\lambda} - f_{\mathcal{H}}\|_{\rho}^2 = \mathcal{O}(|D|^{-\frac{1}{2}}),$$

with probability near to 1.

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<sup>a</sup>Assumption 1, Assumption 2 with  $r = 1/2$ , eigenvalue decaying assumption (stronger than Assumption 3), and the local strongly convex assumption which can be derived from Assumption 4.





# Sharper Learning Rates for KQR-RF I

## Theorem 1

Under Assumptions 1-4, if  $r \in (0, 1]$ ,  $\gamma \in [0, 1]$ , and set  $\lambda = |D|^{-\frac{1}{2r+\gamma}}$ , when the number of random features satisfies

$$M \gtrsim |D|^{\frac{1}{2r+\gamma}}, \quad \text{for } r \in (0, 1/2);$$

$$M \gtrsim |D|^{\frac{(2r-1)\gamma+1}{2r+\gamma}}, \quad \text{for } r \in [1/2, 1],$$

and  $|D|$  is sufficiently large, there holds

$$\mathcal{E}(f_{M,D,\lambda}) - \mathcal{E}(f_{\tau}^*) \asymp \|f_{M,D,\lambda} - f_{\tau}^*\|_{\rho}^2 = \mathcal{O}(|D|^{-\frac{2r}{2r+\gamma}} \log^2 |D|),$$

with probability near to 1.





# Sharper Learning Rates for KQR-RF II

- The capacity-dependent learning rates obtained in Theorem 1 align with those of KRR (Caponnetto and De Vito, 2007) and KRR-RF (Rudi and Rosasco, 2017), which is **minimax optimal** and thus can not be improved any further.
- Compared to Lian (2022), we relax the regularity condition from  $r \in [1/2, 1]$  to  $r \in (0, 1]$ , covering a wider range of scenarios.

## Remark

Theorem 1 uses **the naive uniform sampling strategy** for the random features (generate  $\phi(x, \omega)$  with  $\pi(\omega)$ ), which is independent of the training samples. This may lead to an unnecessary burden in computation. Inspired by **the data-dependent sampling strategy** Bach (2017); Avron et al. (2017); Rudi and Rosasco (2017), we aim to demonstrate in the upcoming section how these strategies enable attaining optimal learning rates across all agnostic settings  $r \in (0, 1]$  with a **reduced number of random features** in the next section.





# Refined Analysis: Beyond Uniform Sampling I

## Assumption 5 (Compatibility condition)

Define the maximum dimension of random features as

$$\mathcal{N}_\infty(\lambda) = \sup_{\omega \in \Omega} \left\| (L_K + \lambda I)^{-1/2} \phi(\cdot, \omega) \right\|_{\rho_X}^2, \quad (12)$$

where  $\lambda > 0$ . There exist constants  $\alpha \in [0, 1]$  and  $F > 0$ , such that  $\mathcal{N}_\infty(\lambda) \leq F\lambda^{-\alpha}$ .

Recall the definition of  $\mathcal{N}(\lambda)$  in Definition 2.  $\mathcal{N}(\lambda)$  and  $\mathcal{N}_\infty(\lambda)$  measure the average and supreme capacities of  $\mathcal{H}_K$ , respectively, so we have

$$\mathcal{N}(\lambda) = \mathbb{E}_\omega \left\| (L_K + \lambda I)^{-1/2} \phi(\cdot, \omega) \right\|_{\rho_X}^2 \leq \sup_{\omega \in \Omega} \left\| (L_K + \lambda I)^{-1/2} \phi(\cdot, \omega) \right\|_{\rho_X}^2 = \mathcal{N}_\infty(\lambda),$$

where  $\mathbb{E}_\omega$  denotes the expectation taking over  $\omega$ .



# Refined Analysis: Beyond Uniform Sampling II

## Theorem 2

Under Assumptions 1-5, if  $r \in (0, 1]$ ,  $\gamma \in [0, 1]$ , and set  $\lambda = |D|^{-\frac{1}{2r+\gamma}}$ , when the number of random features satisfies

$$M \gtrsim |D|^{\frac{\alpha}{2r+\gamma}}, \quad \text{for } r \in (0, 1/2);$$

$$M \gtrsim |D|^{\frac{(2r-1)(1+\gamma-\alpha)+\alpha}{2r+\gamma}}, \quad \text{for } r \in [1/2, 1],$$

and  $|D|$  is sufficiently large, there holds

$$\mathcal{E}(f_{M,D,\lambda}) - \mathcal{E}(f_{\tau}^*) \asymp \|f_{M,D,\lambda} - f_{\tau}^*\|_{\rho}^2 = \mathcal{O}(|D|^{-\frac{2r}{2r+\gamma}} \log^2 |D|),$$

with probability near to 1.

## Refined Analysis: Beyond Uniform Sampling III

- The above capacity-dependent learning rate is the same as that of Theorem 1, while the required number of random features reduces from  $\mathcal{O}(|D|^{\frac{1}{2r+\gamma}})$  to  $\mathcal{O}(|D|^{\frac{\alpha}{2r+\gamma}})$  when  $r \in (0, 1/2)$  and  $\mathcal{O}(|D|^{\frac{(2r-1)\gamma+1}{2r+\gamma}})$  to  $\mathcal{O}(|D|^{\frac{(2r-1)(1+\gamma-\alpha)+\alpha}{2r+\gamma}})$  when  $r \in [1/2, 1]$ , owing to the additional Assumption 5.
- By adopting a favorable sampling strategy called **leverage scores sampling strategy**, we can further reduce the required number of random features and achieve the optimal learning rates across the entire range of  $r \in (0, 1]$ .

### Leverage scores sampling

Given the integral representation of kernel  $K$  as stated in (5), we adopt the leverage scores sampling strategy (Bach, 2017; Avron et al., 2017) by employing an importance ratio denoted as  $q(\omega) = l_\lambda(\omega) / \int_{\omega} l_\lambda(\omega) d\pi(\omega)$ , where  $l_\lambda(\omega) = \|(L_K + \lambda I)^{-1/2} \phi(\cdot, \omega)\|_{\rho_X}^2$ . Consequently, the random features are computed as  $\phi_1(x, \omega) = [q(\omega)]^{-1/2} \phi(x, \omega)$  and exhibit a distribution  $\pi_1(\omega) = q(\omega)\pi(\omega)$ .



## Refined Analysis: Beyond Uniform Sampling IV

- As pointed out in Rudi and Rosasco (2017), the random features provide the integral representation of  $K$  and satisfy Assumption 5 with  $\alpha = \gamma$  indicating that  $\mathcal{N}(\lambda) = \mathcal{N}_\infty(\lambda)$ .

### Corollary 1

Under Assumptions 1-5, if random features are sampled according to the leverage scores sampling strategy,  $r \in (0, 1]$ ,  $\gamma \in [0, 1]$ , and set  $\lambda = |D|^{-\frac{1}{2r+\gamma}}$ , when the number of random features satisfies

$$\begin{aligned} M &\gtrsim |D|^{\frac{\gamma}{2r+\gamma}}, \quad \text{for } r \in (0, 1/2); \\ M &\gtrsim |D|^{\frac{2r+\gamma-1}{2r+\gamma}}, \quad \text{for } r \in [1/2, 1], \end{aligned}$$

and  $|D|$  is sufficiently large, there holds

$$\mathcal{E}(f_{M,D,\lambda}) - \mathcal{E}(f_\tau^*) \asymp \|f_{M,D,\lambda} - f_\tau^*\|_\rho^2 = \mathcal{O}(|D|^{-\frac{2r}{2r+\gamma}} \log^2 |D|),$$

with probability near to 1.

# Refined Analysis: Beyond Uniform Sampling V

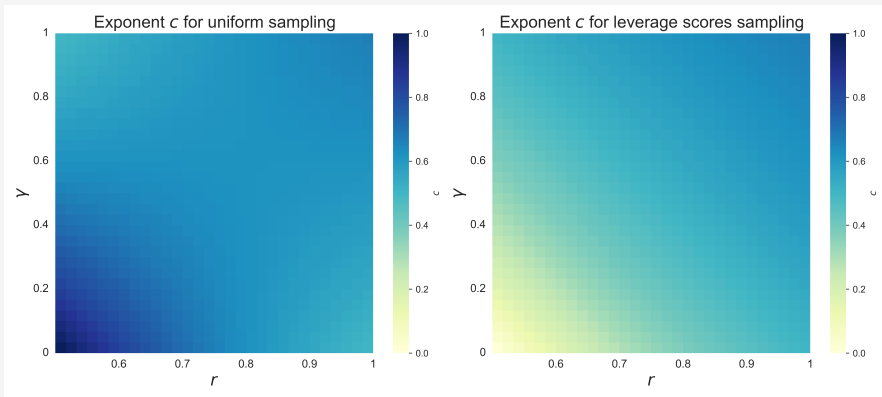


Figure 7: Comparison between the number of random features  $M = \mathcal{O}(|D|^c)$  required for uniform sampling ( $\alpha = 1$ , left) and leverage scores sampling ( $\alpha = \gamma$ , right) in the realizable case.



# Refined Analysis: Beyond Uniform Sampling VI

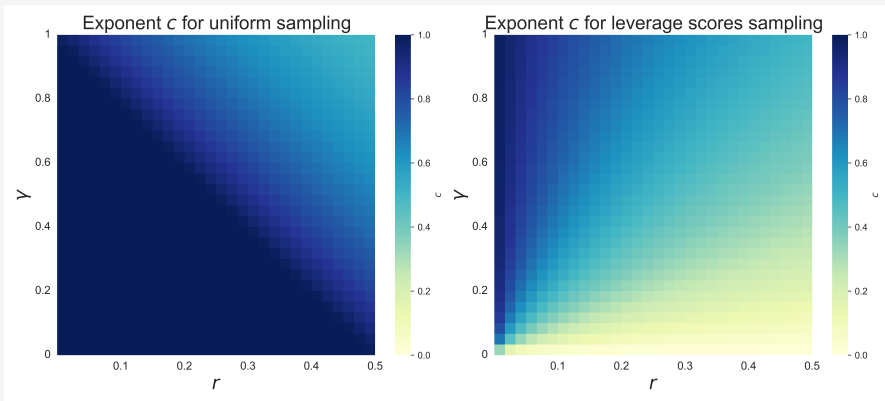


Figure 8: Comparison between the number of random features  $M = \mathcal{O}(|D|^c)$  required for uniform sampling ( $\alpha = 1$ , left) and leverage scores sampling ( $\alpha = \gamma$ , right) in the agnostic case.

# Comparisons to the Related Work

Table 2: Summary of conditions for derived learning rates in different methods.

Methods	Regularity condition	Capacity condition	Random centers M	Learning rate
KRR (Caponnetto and De Vito, 2007)	$r \in [1/2, 1]$	$\gamma \in [0, 1]$	$\times$	$ D ^{-\frac{2r}{2r+\gamma}}$
KRR (Zhang et al., 2023)	$r \in (0, 1]$	$\gamma \in [0, 1]$	$\times$	$ D ^{-\frac{2r}{2r+\gamma}}$
KRR-RF-Uniform (Rudi and Rosasco, 2017)	$r \in [1/2, 1]$	$\gamma \in [0, 1]$	$ D ^{-\frac{(2r-1)\gamma+1}{2r+\gamma}}$	$ D ^{-\frac{2r}{2r+\gamma}}$
KRR-RF-Leverage (Rudi and Rosasco, 2017)	$r \in [1/2, 1]$	$\gamma \in [0, 1]$	$ D ^{-\frac{2r+\gamma-1}{2r+\gamma}}$	$ D ^{-\frac{2r}{2r+\gamma}}$
KRR-RF-Uniform (Li et al., 2023)	$r \in (0, 1], 2r + \gamma \geq 1$	$\gamma \in [0, 1]$	$ D ^{-\frac{1}{2r+\gamma}}$	$ D ^{-\frac{2r}{2r+\gamma}}$
KRR-RF-Leverage (Li et al., 2023)	$r \in (0, 1]$	$\gamma \in [0, 1]$	$ D ^{-\frac{\gamma}{2r+\gamma}}$	$ D ^{-\frac{2r}{2r+\gamma}}$
KQR (Lian, 2022)	$r \in [1/2, 1]$	$\gamma \in [0, 1]$	$\times$	$ D ^{-\frac{2r}{2r+\gamma}}$
Lip-RF-Uniform (Rahimi and Recht, 2008)	$r = 1/2$	$\gamma \in [0, 1]$	$ D $	$ D ^{-1/2}$
Lip-RF-Leverage Bach (2017)	$r = 1/2$	$\gamma \in [0, 1]$	$ D ^{\frac{1}{2}}$	$ D ^{-1/2}$
Lip-RF-Uniform (Li et al., 2021)	$r = 1/2$	$\gamma \in [0, 1]$	$ D $	$ D ^{-1/2}$
Lip-RF-Leverage (Li et al., 2021)	$r = 1/2$	$\gamma \in [0, 1]$	$ D ^{\frac{1}{2}}$	$ D ^{-1/2}$
KSVM-RF (Sun et al., 2018)	$r = 1/2$	$\gamma \in [0, 1]$	$ D ^{\frac{2\gamma}{2\gamma+1}}$	$ D ^{-\frac{1}{2\gamma+1}}$
KQR-RF (Theorem 2)	$r \in (0, 1]$	$\gamma \in [0, 1]$	$ D ^{\frac{\alpha}{2r+\gamma}}, r \in (0, 1/2)$ $ D ^{\frac{(2r-1)(1+\gamma-\alpha)+\alpha}{2r+\gamma}}, r \in [1/2, 1]$	$ D ^{-\frac{2r}{2r+\gamma}}$
KQR-RF-Uniform (Theorem 1)	$r \in (0, 1]$	$\gamma \in [0, 1]$	$ D ^{\frac{1}{2r+\gamma}}, r \in (0, 1/2)$ $ D ^{\frac{(2r-1)\gamma+1}{2r+\gamma}}, r \in [1/2, 1]$	$ D ^{-\frac{2r}{2r+\gamma}}$
KQR-RF-Leverage (Corollary 1)	$r \in (0, 1]$	$\gamma \in [0, 1]$	$ D ^{\frac{\gamma}{2r+\gamma}}, r \in (0, 1/2)$ $ D ^{\frac{2r+\gamma-1}{2r+\gamma}}, r \in [1/2, 1]$	$ D ^{-\frac{2r}{2r+\gamma}}$



## Spline kernel

We consider the spline kernel of order  $q$ , defined as

$$\Lambda_q(x, x') = \sum_{k=-\infty}^{\infty} e^{2\pi i k x} e^{-2\pi i k x'} |k|^{-q},$$

where  $x, x' \in [0, 1]$ , and  $q \in \mathbb{R}$ . According to the property of spline kernel, we have

$$\int_0^1 \Lambda_q(x, z) \Lambda_{q'}(x', z) dz = \Lambda_{q+q'}(x, x'),$$

for any  $q, q' \in \mathbb{R}$ . Consequently, for  $r \in (0, 1]$  and  $\gamma \in [0, 1]$ , let  $K(x, x') = \Lambda_{\frac{1}{\gamma}}(x, x')$ , and its corresponding random feature is  $\phi(x, w) = \Lambda_{\frac{1}{2\gamma}}(x, w)$  with  $w \sim U(0, 1)$ .





## Simulation Study II

### Simulation setting

Data are generated from the following model

$$y = \Lambda_{\frac{r}{\gamma} + \frac{1}{2}}(x, 0) + \varepsilon,$$

where  $\varepsilon \sim N(0, 0.01)$  and  $x \sim U(0, 1)$ .

To graphically show the true and estimated quantile function, we consider three different settings:

- ❶ worst case ( $r = 0, \gamma = 1$ );
- ❷ general case ( $r = 1/2, \gamma = 1$ );
- ❸ most benign case ( $r = 1, \gamma = 0$ ).



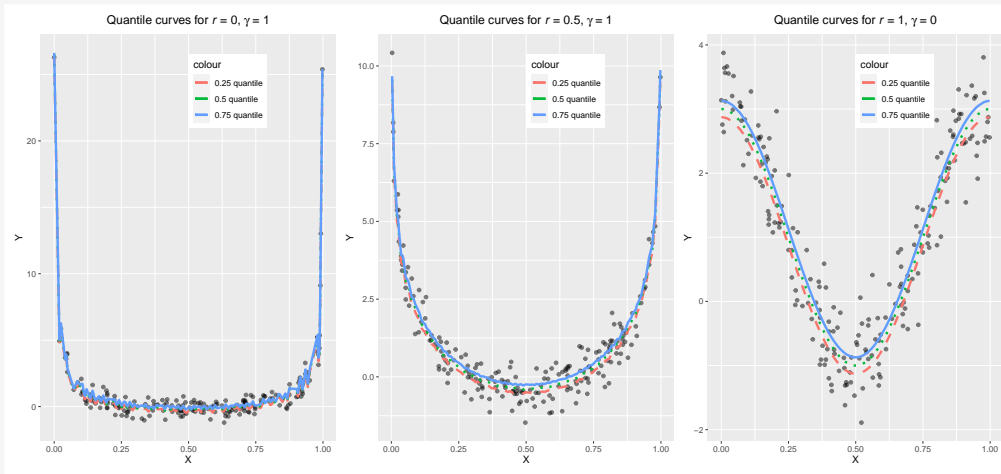


Figure 9: True quantile curves for  $r = 0, \gamma = 1$  (left),  $r = 1/2, \gamma = 1$  (middle), and  $r = 1, \gamma = 0$  (right).

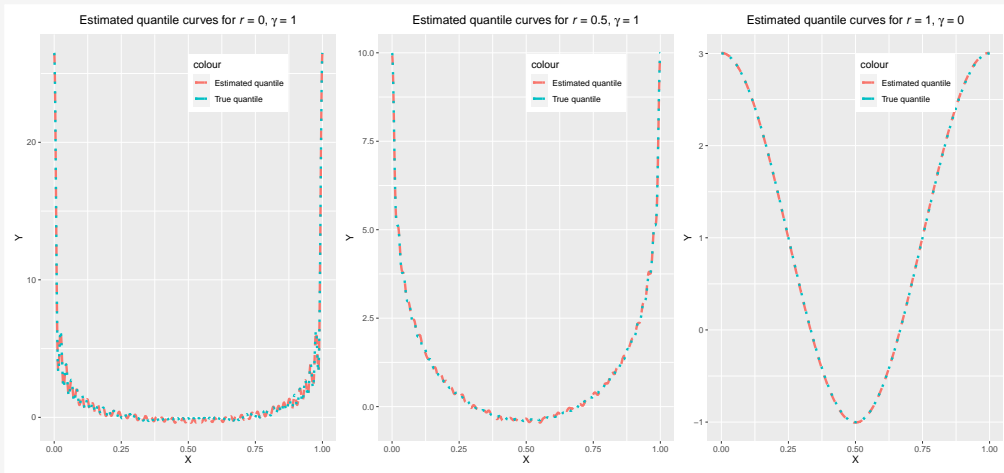


Figure 10: Estimated and true quantile curves for  $r = 0, \gamma = 1$  (left),  $r = 1/2, \gamma = 1$  (middle), and  $r = 1, \gamma = 0$  (right) when  $\tau = 0.5$ .



# Learning Rates Validation

- To validate the derived learning rates, i.e.,  $\mathcal{E}(f_{M,D,\lambda}) - \mathcal{E}(f_{\tau}^*) = \mathcal{O}(|D|^{-\frac{2r}{2r+\gamma}})$ , we estimate the log-transformed excess risk on the testing data and compared it with the theoretical one. We consider two agnostic cases ( $r = 0.2, \gamma = 0.1$  and  $r = 0.4, \gamma = 0.2$ ) and two realizable cases ( $r = 0.5, \gamma = 0.1$  and  $r = 0.8, \gamma = 0.2$ ) for better illustration.



# Results III

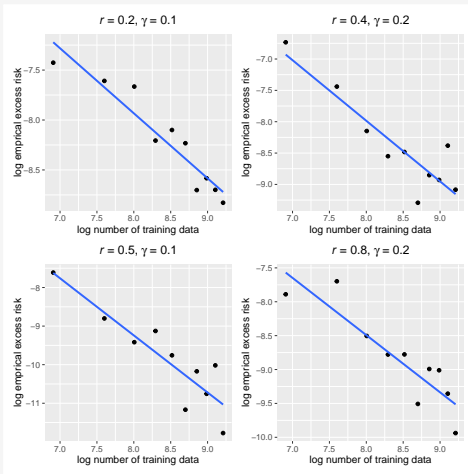


Figure 11: Log empirical excess risk for  $r = 0.2, \gamma = 0.1$  (left top),  $r = 0.4, \gamma = 0.2$  (right top),  $r = 0.5, \gamma = 0.1$  (left bottom) and  $r = 0.8, \gamma = 0.2$  (right bottom) when  $\tau = 0.5$ .





## Discussion

- **First two figures** shows that KQR-RF can estimate the quantile functions very well both in realizable and agnostic settings.
- **Last figure** that the data points are uniformly distributed on both sides of a straight line, which verifies the derived learning rate. To further investigate the constants in the big- $\mathcal{O}$  bounds, we calculate the slope of each learning curve and compare it to  $-\frac{2r}{2r+\gamma}$ . The slope constants are **0.81, 1.21, 1.63, 0.95** in four scenarios. This also highlights our contribution in deriving the sharper and capacity-dependent learning rates.



谢谢!  
Thank You!





# References

- Avron, H., Clarkson, K. L., and Woodruff, D. P. (2017). Faster kernel ridge regression using sketching and preconditioning. *SIAM Journal on Matrix Analysis and Applications*, 38(4):1116–1138.
- Bach, F. (2017). On the equivalence between kernel quadrature rules and random feature expansions. *The Journal of Machine Learning Research*, 18(1):714–751.
- Belloni, A. and Chernozhukov, V. (2011).  $\ell_1$ -penalized quantile regression in high-dimensional sparse models. *The Annals of Statistics*, 39(1):82.
- Boyd, S., Parikh, N., Chu, E., Peleato, B., and Eckstein, J. (2011). Distributed optimization and statistical learning via the alternating direction method of multipliers. *Foundations and Trends® in Machine learning*, 3(1):1–122.
- Caponnetto, A. and De Vito, E. (2007). Optimal rates for the regularized least-squares algorithm. *Foundations of Computational Mathematics*, 7:331–368.
- Feng, X., He, X., Wang, C., Wang, C., and Zhang, J. (2023). Towards a unified analysis of kernel-based methods under covariate shift. *Advances in Neural Information Processing Systems*, 36:73839–73851.
- He, X. and Shi, P. (1994). Convergence rate of b-spline estimators of nonparametric conditional quantile functions. *Journal of Nonparametric Statistics*, 3(3-4):299–308.
- Li, J., Liu, Y., and Wang, W. (2023). Optimal convergence for agnostic kernel learning with random features. *IEEE Transactions on Neural Networks and Learning Systems*, 28:1–11.
- Li, Y., Liu, Y., and Zhu, J. (2007). Quantile regression in reproducing kernel Hilbert spaces. *Journal of the American Statistical Association*, 102(477):255–268.
- Li, Z., Ton, J.-F., Oglic, D., and Sejdinovic, D. (2021). Towards a unified analysis of random fourier features. *The Journal of Machine Learning Research*, 22(1):4887–4937.
- Lian, H. (2022). Distributed learning of conditional quantiles in the reproducing kernel hilbert space. *Advances in Neural Information Processing Systems*, 35:11686–11696.
- Madrid Padilla, O. H. and Chatterjee, S. (2022). Risk bounds for quantile trend filtering. *Biometrika*, 109(3):751–768.
- Rahimi, A. and Recht, B. (2007). Random features for large-scale kernel machines. *Advances in Neural Information Processing Systems*, 20:1177–1184.
- Rahimi, A. and Recht, B. (2008). Weighted sums of random kitchen sinks: Replacing minimization with randomization in learning. *Advances in Neural Information Processing Systems*, 21:1313–1320.
- Rudi, A. and Rosasco, L. (2017). Generalization properties of learning with random features. *Advances in Neural Information Processing Systems*, 30:3215–3225.
- Shen, G., Jiao, Y., Lin, Y., Horowitz, J. L., and Huang, J. (2021). Deep quantile regression: Mitigating the curse of dimensionality

