

# Extrapolation Towards Imaginary 0-Nearest Neighbour and Its Improved Convergence Rate

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**Summary:** Proposed multiscale  $k$ -NN improves  
the convergence rate of  $k$ -NN.

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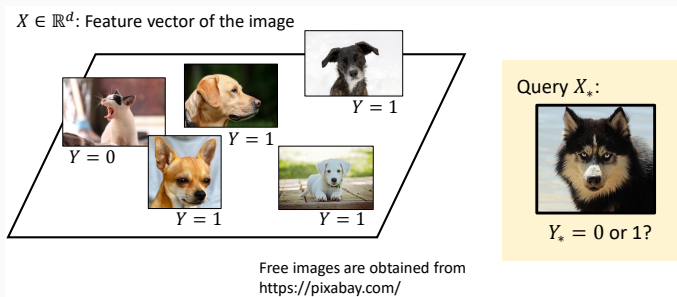
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## Preliminaries

# Classification problem

- Let  $X \in \mathbb{R}^d$ ,  $Y \in \{0, 1\}$  be random variables, where  $(X, Y) \sim \mathbb{Q}$ .
- Observations  $\mathcal{D}_n := \{(X_i, Y_i)\}_{i=1}^n$  are independent copies of  $(X, Y)$ .

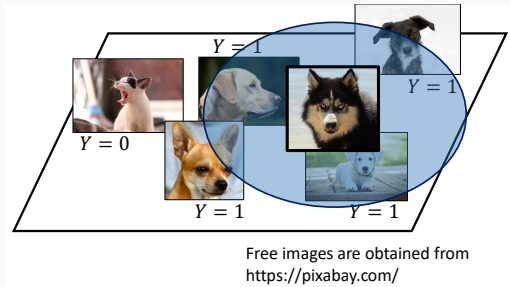


- We aim at obtaining a classifier  $\hat{g}_n : \mathbb{R}^d \rightarrow \{0, 1\}$  that minimizes

$$\mathbb{P}_{(X_*, Y_*) \sim \mathbb{Q}}(Y_* \neq \hat{g}_n(X_*)),$$

where  $X_*$  is a query, and  $\hat{g}_n$  is trained with the observations  $\mathcal{D}_n$ .

## $k$ -nearest neighbour ( $k$ -NN) classifier



- Rearrange the index such that

$$\|X_* - X_{(1)}\|_2 \leq \|X_* - X_{(2)}\|_2 \leq \dots \leq \|X_* - X_{(n)}\|_2.$$

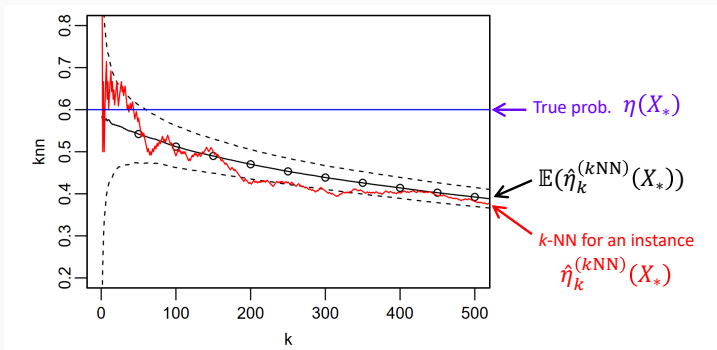
- $k$ -NN estimator is defined by the ratio

$$\hat{\eta}_k^{(kNN)}(X_*) := k^{-1} \sum_{i=1}^k Y_{(i)}.$$

- Hereinafter, we only consider plug-in classifier  $\hat{g}(X_*) = \mathbb{1}(\hat{\eta}(X_*) \geq 1/2)$  defined for estimators  $\hat{\eta}$ .

# Bias-variance tradeoff

- small  $k$ : 😊 small bias 😞 large variance
- large  $k$ : 😊 small variance 😞 large bias



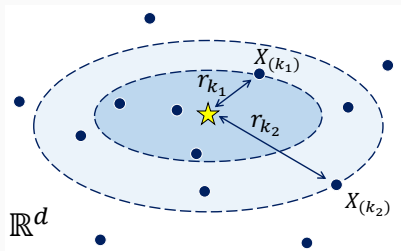
- **Conventional**: choose the best  $k$  value by considering the tradeoff.
- **Ours**: reduces the asymptotic bias!

**Proposal: multiscale  $k$ -NN**

## How to reduce the bias?: An overview

Consider a radius  $r_k := \|X_* - X_{(k)}\|_2$ , a ball  $B(X_*; r)$ , and  $\eta^{(\infty)}(B) := \mathbb{E}(Y \mid X \in B)$ , where Chaudhuri and Dasgupta (2014) proves that

$$\hat{\eta}_k^{(kNN)}(X_*) \approx \eta^{(\infty)}(B(X_*, r_k)) \quad (k = k_n \rightarrow \infty, n \rightarrow \infty \text{ and } k/n \rightarrow 0).$$



bias is due to  $r > 0 \Rightarrow$  (imaginary)  $r = 0$  is preferred:

$$\eta^{(\infty)}(B(X_*; r)) \rightarrow \eta(X_*) = \mathbb{E}[Y_* \mid X_*], \quad (r \rightarrow 0; \text{Federer (1967)})$$

To obtain **(imaginary) 0-NN estimator**, we extrapolate  $k$ -NN estimators

$$\hat{\eta}_{k_1}^{(kNN)}(X_*), \hat{\eta}_{k_2}^{(kNN)}(X_*), \dots, \hat{\eta}_{k_V}^{(kNN)}(X_*)$$

to  $r = 0$  via the radii  $r_{k_1}, r_{k_2}, \dots, r_{k_V}$ .



Consider a set  $\mathcal{F}$  of regression functions  $f : \mathbb{R} \rightarrow \mathbb{R}$  (e.g.,  $f(r) = \beta_0 + \beta_1 r$ ). By choosing  $V \in \mathbb{N}$  and  $1 \leq k_1 < k_2 < \dots < k_V \leq n$ , we conduct a regression

$$\hat{f} := \arg \min_{f \in \mathcal{F}} \sum_{v=1}^V \left( \hat{\eta}_{k_v}^{(kNN)} - f(r_{k_v}) \right)^2, \quad (r_k := \|X_* - X_{(k)}\|_2).$$

## Definition (Multiscale $k$ -NN)

We define a **multiscale  $k$ -NN** (MS- $k$ -NN) estimator

$$\hat{\eta}_{\mathbf{k}}^{(MSkNN)}(X_*) := \hat{f}(0)$$

where  $\mathbf{k} = (k_1, k_2, \dots, k_V)$ .

MS- $k$ -NN formally extrapolates  $k$ -NN estimators to  $r = 0$ .

# Comparison with existing estimators

## Comparison with $k$ -NN estimator

Roughly speaking, bias is reduced for  $\beta > 2$ :

$$k\text{-NN: } |\hat{\eta}_k^{(k\text{NN})}(X_*) - \eta(X_*)| \approx O(r_k^2),$$

$$\text{MS-}k\text{-NN: } |\hat{\eta}_k^{(\text{MS}k\text{NN})}(X_*) - \eta(X_*)| \approx O(r_k^\beta).$$

Variances are in the same order; overall, the convergence rate is reduced.

## Comparison with local polynomial (LP) estimator

LP and MS- $k$ -NN attain the **same optimal convergence rate**. However, MS- $k$ -NN requires **much less terms** than LP, to obtain the same rate.

LP:  $1 + d + d^2 + \dots + d^C$  coefficients, to estimate Taylor polynomial of  $\eta(X)$  (and extrapolate to  $X_*$ ),

MS- $k$ -NN:  $1 + C$  coefficients to be estimated.

Furthermore, MS- $k$ -NN is also expected to inherit the favorable properties of  $k$ -NN.

## Theories: convergence rate analysis

# Convergence rate of the excess risk

Given a classifier  $g : \mathbb{R}^d \rightarrow \{0, 1\}$ , we define a misclassification error rate  $L(g) := \mathbb{P}_{(X_*, Y_*) \sim \mathbb{Q}}(Y_* \neq g(X_*))$  and excess risk

$$\mathcal{E}(g) := L(g) - \inf_{g: \mathbb{R}^d \rightarrow \{0, 1\}} L(g).$$

## Convergence rate:

the order of  $\mathcal{E}(\hat{g}_n)$  w.r.t.  $n$ .

In order to elucidate the convergence rate, we employ

- $\alpha$ -margin condition,
- $\beta$ -Hölder condition, and
- $\gamma$ -neighbour average smoothness condition,

by referring to existing studies (see, e.g., Audibert and Tsybakov (2007), Samworth (2012) and Chaudhuri and Dasgupta (2014)).

## Definition ( $\alpha$ -margin condition)

If  $\exists L_\alpha > 0, \tilde{t} > 0, \alpha \geq 0$  such that

$$\mathbb{P}(|\eta(X) - 1/2| \leq t) \leq L_\alpha t^\alpha \quad (\forall t \in (0, \tilde{t}], X \in \mathcal{X}),$$

$\eta$  is said to be satisfying  $\alpha$ -margin condition.

$$\eta(X) = \mathbb{P}[Y = 1 | X]$$

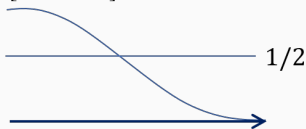


Figure: Small  $\alpha$

$$\eta(X) = \mathbb{P}[Y = 1 | X]$$

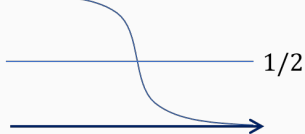


Figure: Large  $\alpha$

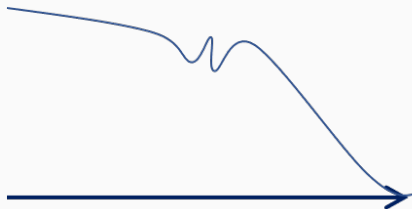
$\alpha$  is Large  $\Rightarrow$  only a few covariates are near boundary  $\Rightarrow$  classification is easy.  
 $\Rightarrow$  fast convergence

## Definition ( $\beta$ -Hölder condition)

Let  $\mathcal{T}_{q, X_*}[\eta]$  be the Taylor expansion of  $\eta$  of degree  $q \in \mathbb{N}_0$ . If  $\exists L_\beta > 0$  such that

$$|\eta(X) - \mathcal{T}_{\lfloor \beta \rfloor, X_*}[\eta](X)| \leq L_\beta \|X - X_*\|^\beta \quad (\forall X, X_* \in \mathcal{X}),$$

$\eta$  is said to be satisfying  $\beta$ -Hölder condition.



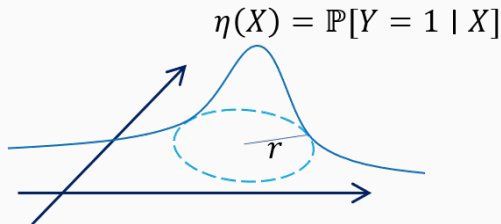
$\beta$  is large  $\Rightarrow \eta(X)$  is smooth  $\Rightarrow$  estimation of  $\eta$  is easy  
 $\Rightarrow$  fast convergence

## Definition ( $\gamma$ -neighbour average smoothness condition)

Let  $\eta^{(\infty)}(B) := \mathbb{E}[Y | X \in B]$ . If  $\exists L_\gamma, \gamma > 0$  such that

$$|\eta^{(\infty)}(B(X; r)) - \eta(X)| \leq L_\gamma r^\gamma \quad (\forall r > 0, X \in \mathcal{S}(\mu)),$$

$\eta$  is said to be satisfying  $\gamma$ -**neighbour average smoothness condition**.



$\gamma$  is large  $\Rightarrow$   $k$ -NN approximation  $\eta^{(\infty)}(B(X_*; r)) = \mathbb{E}[Y | X \in B(X_*; r)]$  converges to  $\mathbb{E}[Y | X_*]$  quickly  
 $\Rightarrow$  fast convergence

Definition (Strong density assumption (SDA) on pdf  $\mu$  of  $X$ )

If  $\exists \mu_{\min}, \mu_{\max} \in (0, \infty)$  such that  $\mu(X) \in [\mu_{\min}, \mu_{\max}]$  for all  $X \in \mathcal{X}$ ,  $\mu$  is said to be satisfying **strong density assumption (SDA)**.

Theorem (Chaudhuri and Dasgupta (2014) Theorem 4)

Let  $\mathcal{X}$  be a compact set, and assuming that (i)  $\eta$  satisfies  $\alpha$ - and  $\gamma$ -conditions, and (ii)  $\mu$  satisfies SDA, it holds with  $k_* \asymp n^{2\gamma/(2\gamma+d)}$  that

$$\mathcal{E}(\hat{g}_{k_*}^{(kNN)}) = O(n^{-(1+\alpha)\gamma/(2\gamma+d)}),$$

for (unweighted)  $k$ -NN plug-in classifier  $\hat{g}_{k_*}^{(kNN)}$ .

- A natural question:  $\gamma = \beta$  if  $\beta$ -Hölder condition is employed instead of  $\gamma$ -?



Answer is **No**.

### Theorem (Okuno and Shimodaira (2020) Theorem 1)

Let  $\eta(X) := \mathbb{E}(Y | X)$  and let  $\mu$  be the p.d.f. of  $X$ . Assuming that

- (1) both of  $\mu$  and  $\eta\mu$  are  $\beta (> 0)$ -Hölder,
- (2) support of  $\mu$  is compact,
- (3)  $k = k_n \rightarrow \infty, k/n \rightarrow 0, n \rightarrow \infty$ .

Then, for some  $b_2^*, \dots, b_{\lfloor \beta/2 \rfloor}^* \in \mathbb{R}$ , it holds that

$$\eta^{(\infty)}(B(X_*, r_k)) = \eta(X_*) + \underbrace{b_1^* r_k^2 + b_2^* r_k^4 + \dots + b_{\lfloor \beta/2 \rfloor}^* r_k^{2\lfloor \beta/2 \rfloor}}_{\text{bias}} + O(r_k^\beta),$$

and  $b_1^* = \frac{1}{2d+4} \frac{1}{\mu(X_*)} \{ \Delta[\eta(X_*)\mu(X_*)] - \eta(X_*)\Delta\mu(X_*) \}$  with the Laplacian operator  $\Delta$ .

If  $\beta$ -Hölder condition is assumed instead of  $\gamma$ -, we have

$$\gamma = \min\{\beta, 2\},$$

indicating that  $\mathcal{E}(\hat{g}_{k_*}^{(kNN)}) = O(n^{-2(1+\alpha)/(4+d)})$  even for sufficiently smooth  $\eta$ .

Audibert and Tsybakov (2007) Theorem 3.5 proves the optimal rate for plug-in classifiers: considering  $\beta(> 0)$ -Hölder function  $\eta$ , there exists  $L > 0$  such that

$$\inf_{g:\text{plug-in classifier}} \sup_{\eta, \mu} \mathcal{E}(g) \geq L \cdot n^{-(1+\alpha)\beta/(2\beta+d)}.$$

Table: Convergence rates for  $\alpha = 1, \beta = 2u$  ( $u \in \mathbb{N}$ )

$k$ -NN	$O(n^{-4/(4+d)})$	Chaudhuri and Dasgupta (2014)
Local linear	$O(n^{-4/(4+d)})$	Hall and Kang (2005)
Local polynomial	$O(n^{-2\beta/(2\beta+d)})$	Audibert and Tsybakov (2007)
<b>Multiscale <math>k</math>-NN</b>	$O(n^{-2\beta/(2\beta+d)})$	Okuno and Shimodaira (2020)

## Another implication of Theorem 1

Okuno and Shimodaira (2020) Theorem 1:

$$\underbrace{\eta^{(\infty)}(B(X_*, r_k))}_{\text{kNN estimator}} = \eta(X_*) + \underbrace{b_1^* r_k^2 + b_2^* r_k^4 + \cdots + b_{\lfloor \beta/2 \rfloor}^* r_k^{2\lfloor \beta/2 \rfloor}}_{\text{bias}} + O(r_k^\beta)$$

leads to a regression function

$$f_C(r; \mathbf{b}) := b_0 + b_1 r^2 + b_2 r^4 + \cdots + b_C r^{2C} \quad (C = \lfloor \beta/2 \rfloor).$$

The function  $f_C$  approximates the bias term, and extrapolation to  $r = 0$  yields

$$f_C(0; \hat{\mathbf{b}}) = \hat{b}_0 \approx \eta(X_*).$$

Therefore, we may employ a set of even-degree polynomials

$$\mathcal{F}_C := \{b_0 + b_1 r^2 + b_2 r^4 + \cdots + b_C r^{2C} \mid b_0, b_1, \dots, b_C \in \mathbb{R}\}.$$

## MS- $k$ -NN attains the optimal rate!

With user-specified  $\ell_1 = 1 < \ell_2 < \dots < \ell_V < \infty$ , we consider

$$(C1) \quad k_1 \asymp n^{2\beta/(2\beta+d)},$$

$$(C2) \quad k_v := \min\{k \in [n] \mid \|X_{(k)} - X_*\|_2 \geq \ell_v r_{k_1}\} \text{ for } v = 2, 3, \dots, V,$$

$$(C3) \quad \exists L_Z > 0 \text{ such that } \left\| \frac{(I - \mathcal{P}_R)\mathbf{1}}{\mathbf{1}^\top (I - \mathcal{P}_R)\mathbf{1}} \right\|_\infty \leq L_Z \text{ for } \mathbf{R} = (\ell_i^{2j})_{ij}, \mathcal{P}_R = \mathbf{R}(\mathbf{R}^\top \mathbf{R})^{-1} \mathbf{R}^\top.$$

### Theorem (Okuno and Shimodaira (2020) Theorem 2)

Assuming that (i)  $\mu, \eta\mu$  are  $\beta$ -Hölder<sup>1</sup>, (ii)  $\mu$  satisfies SDA, (iii)  $C := \lfloor \beta/2 \rfloor \leq V - 1$ , and (iv) (C-1)–(C-3) are satisfied. Then, MS- $k$ -NN plug-in classifier attains the optimal rate

$$\mathcal{E}(\hat{g}_{k_*}^{(\text{MSkNN})}) = O(n^{-(1+\alpha)\beta/(2\beta+d)}).$$

<sup>1</sup>For  $k$ -NN, only  $\eta$  is assumed to be  $\beta$ -Hölder (Chaudhuri and Dasgupta, 2014)

## Weighted $k$ -NN

# MS- $k$ -NN = weighted $k$ -NN with real-valued weights

Consider a **weighted**  $k$ -NN estimator

$$\hat{\eta}_{k,w}^{(k\text{NN})}(X_*) = \sum_{i=1}^k w_i Y_{(i)}$$

with weights  $\sum_{i=1}^k w_i = 1$ . Then, MS- $k$ -NN is equivalent to the weighted  $k$ -NN equipped with  $k = k_V$  and **real-valued weights**

$$w_i := \sum_{v:i \leq k_V} \frac{z_v}{k_V} \in \mathbb{R} \ (\forall i \in [k_V]), \quad \mathbf{z} = (z_1, z_2, \dots, z_V) := \frac{(I - \mathcal{P}_R)\mathbf{1}}{\mathbf{1}^\top (I - \mathcal{P}_R)\mathbf{1}} \in \mathbb{R}^V.$$

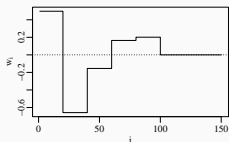


Figure:  $V = 5$

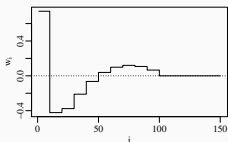


Figure:  $V = 10$

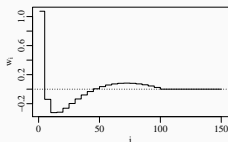


Figure:  $V = 20$

- **Negative weights** are essential for eradicating the bias.

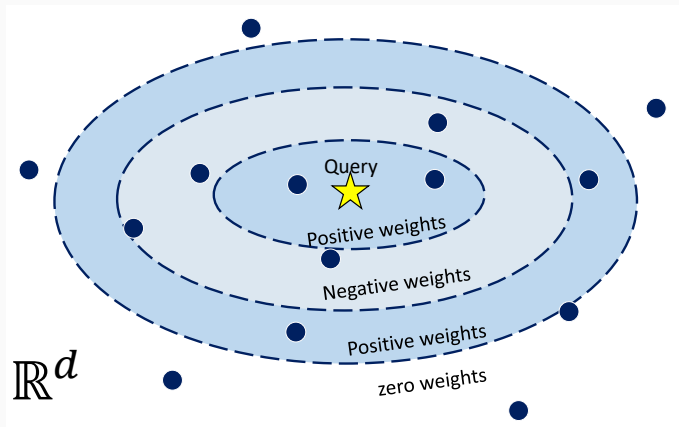


Figure: (Implicit) weights obtained in multiscale  $k$ -NN

## Other (existing) real-valued weights

Only one existing study that considers  $k$ -NN with real-valued weights is Samworth (2012); it proves for  $\alpha = 1, k_* \asymp n^{2\beta/(2\beta+d)}$  that

$$\inf_{\mathbf{w} \in \mathcal{W}} \mathcal{E}(\hat{g}_{k_*, \mathbf{w}}^{(k\text{NN})}) = O(n^{-(1+\alpha)\beta/(2\beta+d)}) \text{ for a conditioned set } \mathcal{W} \subseteq \mathbb{R}^{k_*}.$$

Samworth (2012) shows equations of the optimal weights by minimizing Taylor series of the excess risk; solutions are obtained only for  $\beta = 2, 4$ . For  $\beta = 4$ ,

$$w_i = (a_0 + a_i \delta_i^{(1)} + \dots + a_u \delta_i^{(u)}) / k_*$$

with  $\delta_i^{(\ell)} := i^{1+2\ell/d} - (i-1)^{1+2\ell/d} (\forall \ell \in [u]), a_0 \in \mathbb{R}, a_1 := \frac{1}{k_*^{2/d}} \left\{ \frac{(d+4)^2}{4} - \frac{2(d+4)}{d+2} a_0 \right\}$ ,

and  $a_2 := \frac{1-a_0-k_*^{2/d} a_1}{k_*^{4/d}}$ .

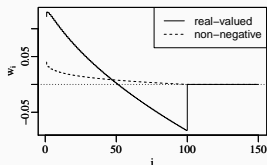


Figure: Optimal real-valued weights in Samworth (2012)

- cf. Samworth (2012) also proves the rate  $O(n^{-4/(4+d)})$  for non-negative weights, which is the same as unweighted  $k$ -NN.



## Numerical experiments

We perform

- (1) unweighted  $k$ -NN ( $w_i = 1/k$ )
- (2) weighted  $k$ -NN with *non-negative* weights  $w_i \geq 0$
- (3) weighted  $k$ -NN with *real-valued* weights  $w_i \in \mathbb{R}$
- (4) (**Proposal**) MS- $k$ -NN extrapolated via  $r(k)$
- (5) (**Modificaiton**) MS- $k$ -NN extrapolated via  $\log k$

on 13 datasets obtained from UCI ML Repository (Dua and Graff, 2017).

- Divided into: 70% for training, 30% for test.
- Sample mean and standard deviation of the prediction accuracy on 10 times experiments are computed.
- Regression in MS- $k$ -NN is ridge regularized with  $\lambda = 10^{-4}$ .
- $V = 5, k := n_{\text{train}}^{4/(4+d)}, k_1 = k/V, k_2 = 2k/V, \dots, k_V = k$ .

# Prediction accuracy

- $n$ : number of observations
- $d$ : dimension of  $X$
- $m$ : number of categories

Table: Best scores are **bolded**, and second best scores are underlined.

Dataset	$n$	$d$	$m$	$k$ -NN			MS- $k$ -NN	
				$w_i = 1/k$	$w_i \geq 0$	$w_i \in \mathbb{R}$	via $r(k)$	via $\log k$
Iris	150	4	3	$0.83 \pm 0.04$	$0.92 \pm 0.05$	$0.92 \pm 0.04$	$0.93 \pm 0.04$	<b><math>0.96 \pm 0.04</math></b>
Glass iden.	213	9	6	$0.58 \pm 0.06$	<u><math>0.64 \pm 0.06</math></u>	<b><math>0.67 \pm 0.05</math></b>	<u><math>0.64 \pm 0.05</math></u>	<u><math>0.64 \pm 0.05</math></u>
Ecoli	335	7	8	$0.80 \pm 0.03$	<b><u><math>0.85 \pm 0.03</math></u></b>	<u><math>0.84 \pm 0.02</math></u>	<b><math>0.85 \pm 0.02</math></b>	<u><math>0.84 \pm 0.02</math></u>
Diabetes	768	8	2	<b><math>0.75 \pm 0.03</math></b>	<u><math>0.74 \pm 0.03</math></u>	$0.70 \pm 0.04$	<b><math>0.75 \pm 0.03</math></b>	$0.71 \pm 0.03$
Biodeg.	1054	41	2	<u><math>0.84 \pm 0.02</math></u>	<b><math>0.86 \pm 0.03</math></b>	$0.79 \pm 0.02$	<b><math>0.86 \pm 0.02</math></b>	$0.80 \pm 0.02$
Banknote	1371	4	2	$0.95 \pm 0.01$	<u><math>0.98 \pm 0.01</math></u>	$0.97 \pm 0.01$	<u><math>0.98 \pm 0.01</math></u>	<b><math>0.99 \pm 0.00</math></b>
Yeast	1484	8	10	<u><math>0.57 \pm 0.02</math></u>	<b><math>0.58 \pm 0.02</math></b>	$0.54 \pm 0.03$	<b><math>0.58 \pm 0.02</math></b>	$0.54 \pm 0.02$
Wire. local.	2000	7	4	<u><math>0.97 \pm 0.00</math></u>	<b><math>0.98 \pm 0.00</math></b>	<b><math>0.98 \pm 0.01</math></b>	<b><math>0.98 \pm 0.00</math></b>	<b><math>0.98 \pm 0.01</math></b>
Spambase	4600	57	2	<u><math>0.90 \pm 0.01</math></u>	<b><math>0.91 \pm 0.00</math></b>	$0.86 \pm 0.01$	<b><math>0.91 \pm 0.00</math></b>	$0.87 \pm 0.01$
Robot navi.	5455	24	4	$0.81 \pm 0.01$	<b><math>0.86 \pm 0.01</math></b>	$0.81 \pm 0.01$	<u><math>0.84 \pm 0.01</math></u>	<u><math>0.84 \pm 0.01</math></u>
Page blocks	5473	10	5	<u><math>0.95 \pm 0.01</math></u>	<u><math>0.95 \pm 0.01</math></u>	<b><math>0.96 \pm 0.01</math></b>	<b><math>0.96 \pm 0.01</math></b>	<b><math>0.96 \pm 0.01</math></b>
MAGIC	19020	10	2	$0.82 \pm 0.00$	$0.82 \pm 0.00$	<b><math>0.84 \pm 0.01</math></b>	<u><math>0.83 \pm 0.00</math></u>	<u><math>0.83 \pm 0.00</math></u>
Avila	20867	10	12	$0.63 \pm 0.01$	$0.68 \pm 0.01$	<b><math>0.70 \pm 0.01</math></b>	<u><math>0.69 \pm 0.00</math></u>	<b><math>0.70 \pm 0.01</math></b>

## Some remarks

# Non-asymptotic regression function specification

Okuno and Shimodaira (2020) Theorem 1 proves that

$$\eta^{(\infty)}(B(X_*; r_k)) = \eta(X_*) + \sum_{c=1}^{\lfloor \beta/2 \rfloor} r_k^{2\lfloor \beta/2 \rfloor} + O(r_k^\beta).$$

for **small**  $r_k \approx 0$  (as  $k/n \rightarrow 0, n \rightarrow \infty$ ).

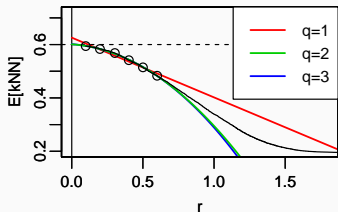


Figure:  $\delta = 0.1$

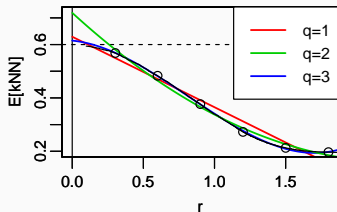


Figure:  $\delta = 0.3$

Figure: Monte-Carlo expectation of  $k$ -NN estimators (black line), and the polynomials of degrees  $q = 1, 2, 3$  trained on  $r = \delta, 2\delta, \dots, 6\delta$ .

# Sigmoid-based functions

- Even degree polynomials  $b_0 + b_1r_1^2 + \dots + b_cr^{2c} : \mathbb{R} \rightarrow \mathbb{R}$  can be replaced with

$$\sigma \left( b_0 + b_1r_1^2 + \dots + b_cr^{2c} \right) : \mathbb{R} \rightarrow [0, 1]$$

using the sigmoid function  $\sigma(z) = (1 + \exp(-z))^{-1}$ , to attain the optimal rate. (These two functions are essentially equivalent for small  $r \approx 0$ .)

— q=1 (poly)   - - q=1 (sigm)   — q=2 (poly)   - - q=2 (sigm)   — q=3 (poly)   - - q=3 (sigm)   — q=4 (poly)   - - q=4 (sigm)

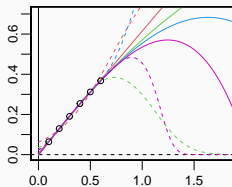


Figure:  $\delta = 0.1$

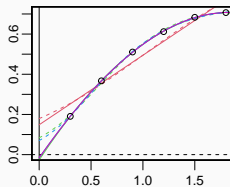


Figure:  $\delta = 0.3$

Figure: Sigmoid-based functions (dot lines).

$$\eta^{(\infty)}(B(X_*; r)) = \mathbb{E}[Y \mid X \in B(X_*; r)] = \frac{\int_{B(X_*; r)} \eta(X) \mu(X) dX}{\int_{B(X_*; r)} \mu(X) dX}$$

- To apply Taylor-expansion,  $\mu, \eta\mu$  are assumed to be  $\beta$ -Hölder in Theorem 1:

$$\eta^{(\infty)}(B(X_*; r)) = \sum_{c=0}^C b_c^* r^{2c} + O(r^\beta).$$

- If  $\mu, \eta\mu$  are polynomial, we have a non-asymptotic expansion:

$$\eta^{(\infty)}(B(X_*; r)) = \mathbb{1}(C_1 - C_2 \geq 0) \sum_{c=0}^{C_1 - C_2} b_c^* r^{2c} + \frac{\sum_{c=0}^{C_2 - 1} \gamma_c^{(1)} r^{2c}}{\sum_{c=0}^{C_2} \gamma_c^{(2)} r^{2c}}$$

for some  $\{b_c^*\}, \{\gamma_c^{(1)}\}, \{\gamma_c^{(2)}\} \subset \mathbb{R}$ .

# Dependence on $k$ -NN estimators

$k$ -NN estimators  $\hat{\eta}_{k_1}^{(kNN)}$ ,  $\hat{\eta}_{k_2}^{(kNN)}$ ,  $\dots$ ,  $\hat{\eta}_{k_V}^{(kNN)}$  are dependent.

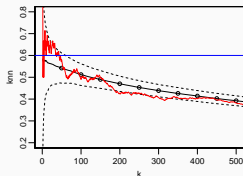


Figure:  $k$ -NN

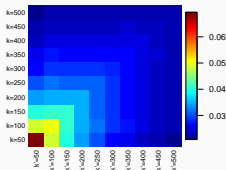


Figure: covariance<sup>1/2</sup>

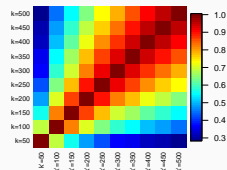


Figure: Correlation

Figure: Dependence of  $k$ -NN estimators computed via Monte-Carlo simulation.

- Dependence can be considered in the regression.



- Cross-validation is conducted for choosing the parameters  $k_1, k_2, \dots, k_V$ .
- Instead of choosing  $1 \leq k_1 < k_2 < \dots < k_V \leq n$ , we may employ  $k_1 = 1, k_2 = 2, \dots, k_{V'} = V'$  ( $V \ll V'$ ; for avoiding parameter selection): empirically better performance in some cases.

## Conclusion

# Conclusion

- To obtain **(imaginary) 0-NN estimator**,  $k$ -NN estimators  $\hat{\eta}_{k_1}, \hat{\eta}_{k_2}, \dots, \hat{\eta}_{k_V}$  are extrapolated to  $r = 0$  via radius  $r_k := \|X_{(k)} - X_*\|_2$ .
- Obtained multiscale  $k$ -NN (MS- $k$ -NN) estimator reduces the bias of  $k$ -NN, and **it attains the optimal rate**.
- MS- $k$ -NN is equivalent to weighted  $k$ -NN with some real-valued weights.
- Weights are automatically determined via regression (in MS- $k$ -NN); they are different from Samworth (2012), which solves entangled equations.

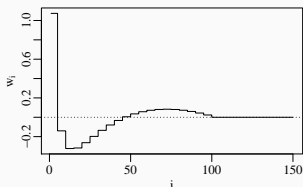


Figure: Ours ( $V = 20$ )

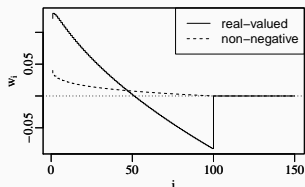


Figure: Samworth (2012)

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