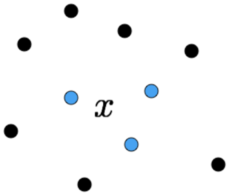
Nonparametric Analysis:
Nearest Neighbors and Friends



Samory Kpotufe
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Nonparametric Analysis:

Infinite capacity/number of parameters $\not\Rightarrow$ no Generalization

Which aspects of a procedure/data, $\Longrightarrow$ fast/slow Generalization

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k-Nearest Neighbor Approach:

Use the k closest datapoints to x *to infer* something about x.

Ubiquitous in ML (implicit at times):

Traditional ML: Classification, Regression, Density Estimation, Bandits, Manifold Learning, Clustering ...

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Of Practical Interest:

Which metric? Which values of k? Implementation and Tradeoffs?

A lot of recent insights towards these questions ...

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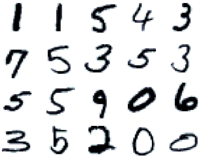
Basic Intuition:

Closest neighbors of x should be mostly of similar type $y = y(x)$ ...



... $y \leftarrow 5$

Prediction: **aggregate** Y values in **Neighborhood**(x)

Similar Intuition: Classification Trees, RBF networks, Kernel machines.

Results by various authors help formalize the above intuition

Posner, Fix, Hodges, Cover, Hart, Devroye, Lugosi, Hero, Nobel, Györfi, Kulkarni, Ben David, Shalev-Schwartz, Samworth, Gadat, H. Chen, Shah, von Luxburg, Hein, Chaudhuri, Dasgupta ...

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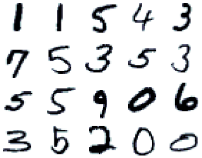

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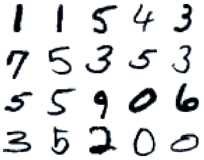

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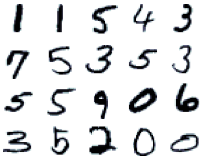 $\dots$ $x \equiv$  $\dots$ $y \leftarrow 5$

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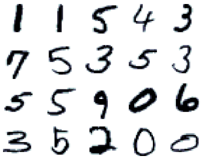

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Key questions:

1 **Statistical issues:** how well can NN perform?

- When is 1-NN enough?
- For k-NN, what should k be?
- Is there always a curse of dimension?

2 **Algorithmic issues:** how efficient can NN be?

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Examples:

- Direct Euclidean
- Deep Neural Representation (image, speech)
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- **PART I:** Basic Statistical Insights
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PART I: Basic Statistical Insights

- **Universality**
- Behavior of k-NN Distances
- From Regression to Classification
- Classification is easier than regression
- Multiclass and Mixed Costs

k-NN as a universal approach:

it can fit anything, provided k grows (but not too fast) with sample size!

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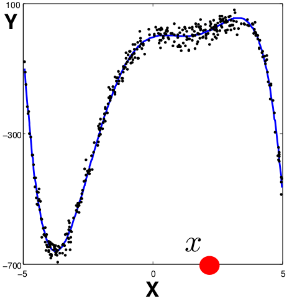
k-NN Regression

i.i.d. Data: $\{(X_i, Y_i)\}_{i=1}^n$,
$Y = f(X) +$ noise



Learn: $f_k(x) =$ avg (Y_i) of k-NN(x).

k-NN is universally consistent:

Suppose $\frac{k}{n} \to 0$ and $k \to \infty$, then $\mathbb{E}\,|f_k(X) - f(X)| \xrightarrow{n\to\infty} 0$

Any function f, $\mathbb{E}f^2 < \infty$, no matter how complex.

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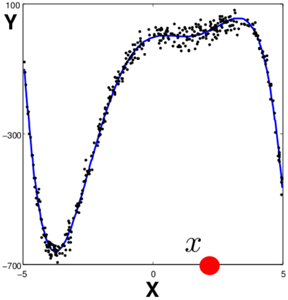

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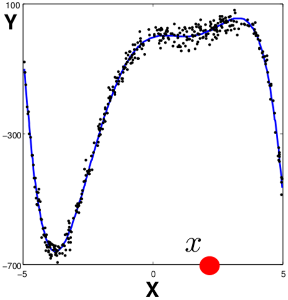

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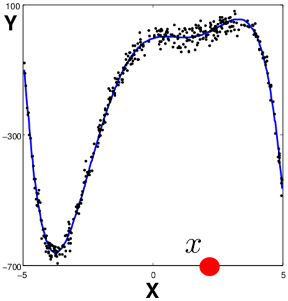

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Intuition:

- $\{X_{(i)}\}_1^k \to x$ as long as k is fixed or grows slow $(k/n \to 0)$
- Suppose f is continuous, then we also get $\{f(X_{(i)})\}_1^k \to f(x)$
- If $k \to \infty$, then $f_k(x) = \frac{1}{k} \sum (f(X_{(i)}) + \text{noise}) \to f(x)$

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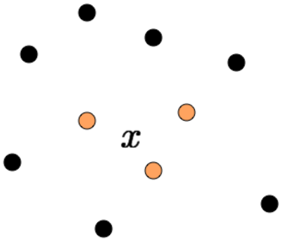

Consider the k-NN $\{X_{(i)}\}_1^k$ of some x

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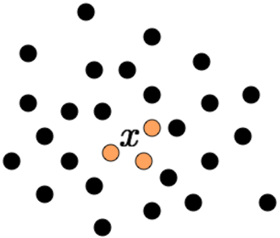

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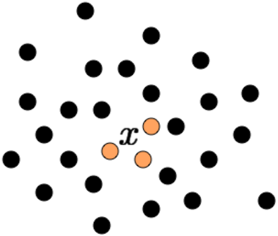

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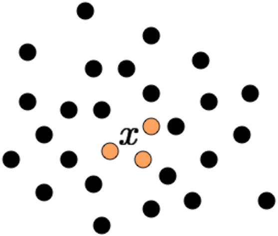

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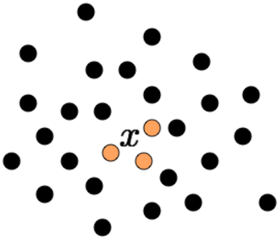

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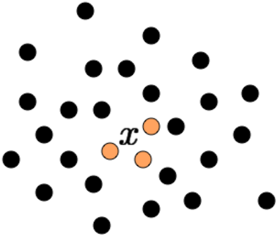

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Similar universality results for classification, density estimation, ...

Seminal results on k-NN consistency:

- [Fix, Hodges, 51]: classification + regularity, $\mathbb{R}^d$.
- [Cover, Hart, 65, 67, 68]: classification + regularity, any metric.
- [Stone, 77]: classification, universal, $\mathbb{R}^d$.
- [Devroye, Wagner, 77]: density estimation + regularity , $\mathbb{R}^d$.
- [Devroye, Gyorfi, Kryzak, Lugosi, 94]: regression, universal, $\mathbb{R}^d$.
- [Chaudhuri, Dasgupta, 14]: classification, *nice* metric/measure.

Main message: k should grow (not too fast) with n ... (e.g. $k \sim \log n$)

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PART I: Basic Statistical Insights

- Universality
- **Behavior of k-NN Distances**
- From Regression to Classification
- Classification is easier than regression
- Multiclass and Mixed Costs

Why k-NN Distances?

Recall Intuition:

Closest neighbors of x should be mostly of similar type $y = y(x)$ ...

So we hope that k-NN(x) are close to x ... depends on k ...

Formally: let $r_k(x) \equiv$ distance from x to k-th NN in i.i.d. $\{X_i\}_1^n$

Q: How small is $r_k(x) \equiv$ function of (P_X, k, n)?

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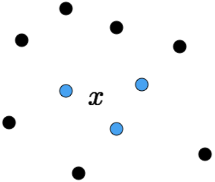

$$B_x \equiv B(x, r_k(x)) \equiv \text{smallest ball containing } k\text{-NN}(x)$$

- Assume no ties: $P_n(B_x) = k/n$.
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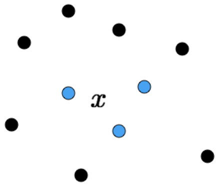

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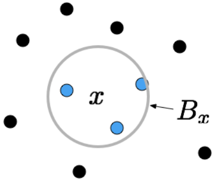

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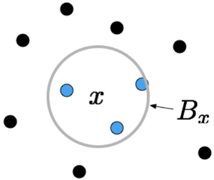

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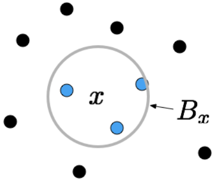

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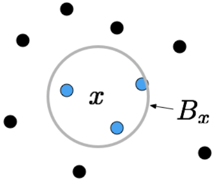

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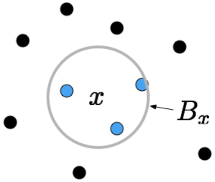

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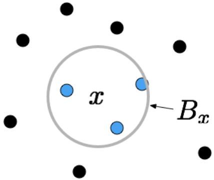

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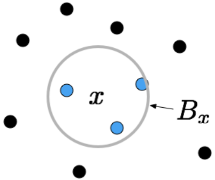

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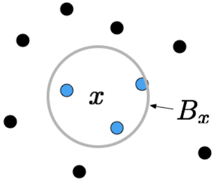

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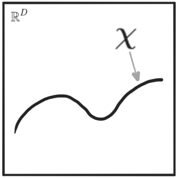

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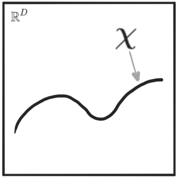

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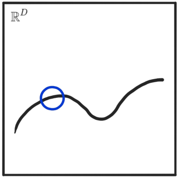

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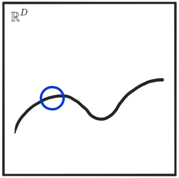

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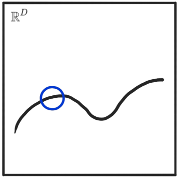

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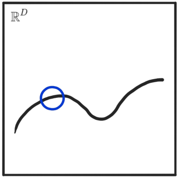

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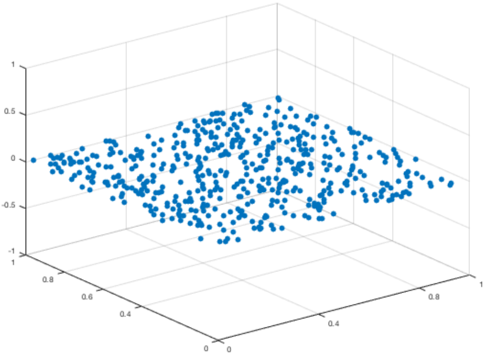

Embed $(d = 2)$-data into high-dimensional $\mathbb{R}^D$, $D \to \infty$

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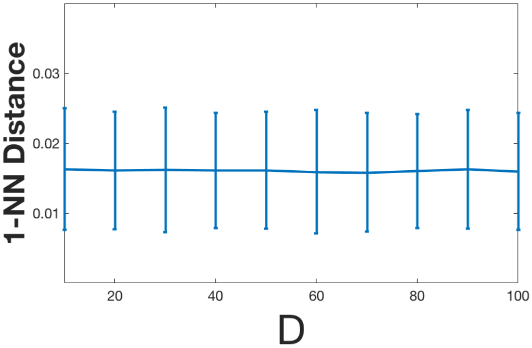

Fix $d = 2$: average NN distances are stable as D varies

Refined analysis for $r_k(x)$:

[J. Costa, A. Hero 04], [R. Samworth 12]

Implications:

$r_k(x)$ **adaptive to** d $\implies$ **NN methods adaptive to** d **...**

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PART I: Basic Statistical Insights

- Universality
- Behavior of k-NN Distances
- **From Regression to Classification**
- Classification is easier than regression
- Multiclass and Mixed Costs

From bounds on $r_k(x)$ to error rates:

Program:

1. Regression bounds
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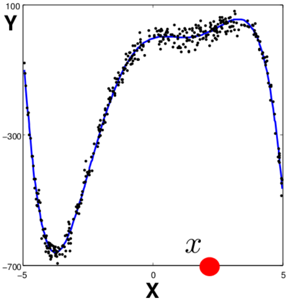
Data: $\{(X_i, Y_i)\}_{i=1}^n$, $Y = f(X) + \text{noise}$

Learn: $f_k(x) = \text{avg}\ (Y_i)$ of k-NN(x).



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... e.g., assume f is Lipschitz: $|f(x) - f(x')| \leq \lambda \cdot \rho(x, x')$.

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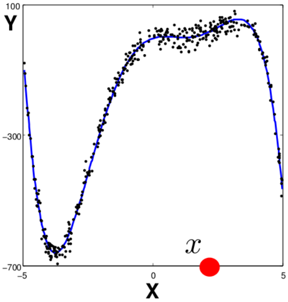

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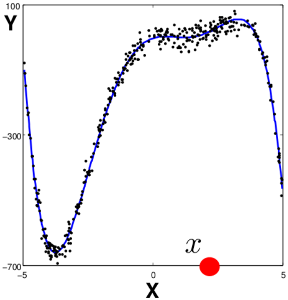

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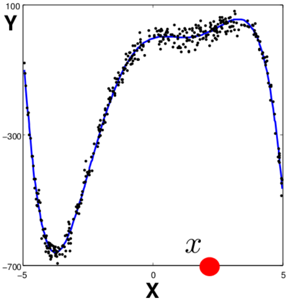

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Intuition: $\mathbb{E}\,|Z - c|^2 = \mathbb{E}\,|Z - \mathbb{E}Z|^2 + |c - \mathbb{E}Z|^2.$

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Step 2: *Bound the two terms*

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$$\mathrm{Var}(f_k(x)) = \frac{1}{k^2}\sum_{X_i \in k\text{-NN}(x)} \mathrm{Var}(Y_i) = \frac{\sigma_Y^2}{k}$$

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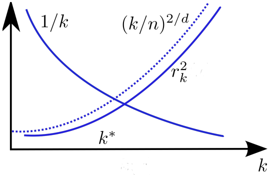

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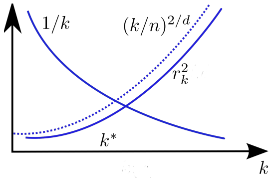

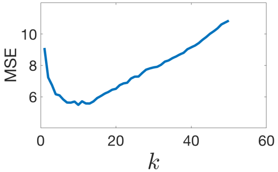

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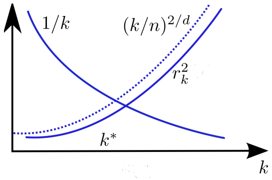

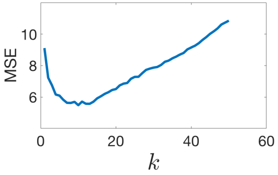

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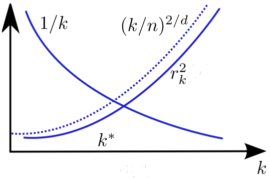

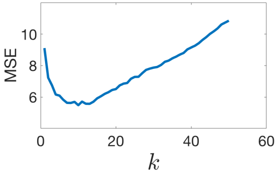

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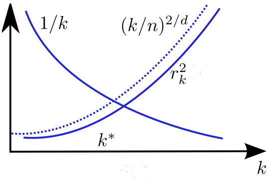

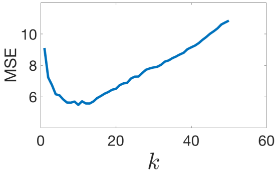

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- **Hölder continuity:** $|f(x) - f(x')| \leq \lambda \cdot \rho(x, x')^{\alpha}$.

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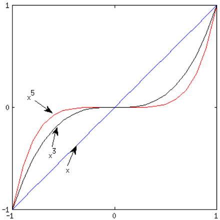

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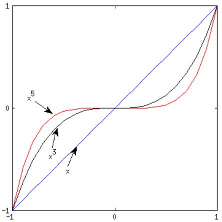

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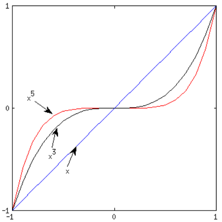

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From bounds on $r_k(x)$ to error rates:

Program:

1. ~~Regression bounds~~
2. Reduce Classification to Regression

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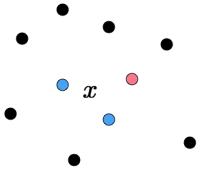
Data: $\{(X_i, Y_i)\}_{i=1}^n$, $Y \in \{0, 1\}$.

Learn: $h_k(x) =$ majority (Y_i) of k-NN(x).



Reduces to regression: let $f_k(x) =$ avg (Y_i) of k-NN(x)

... then: $h_k(x) \equiv \mathbb{1}\{f_k(x) \geq 1/2\}$.

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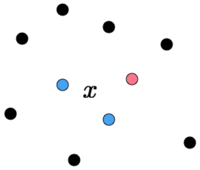

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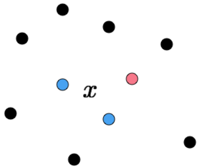

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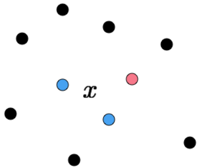

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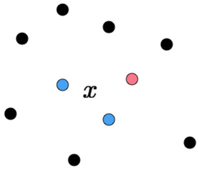

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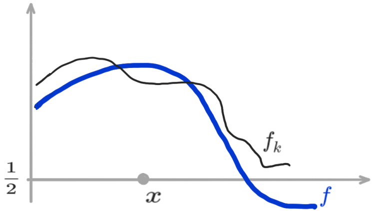

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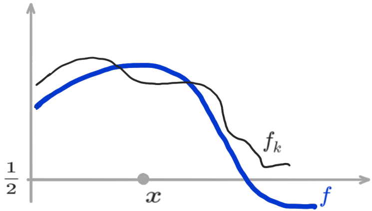

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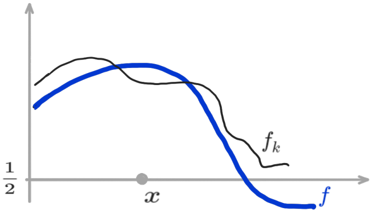

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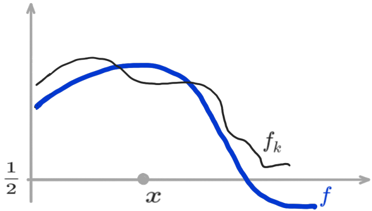

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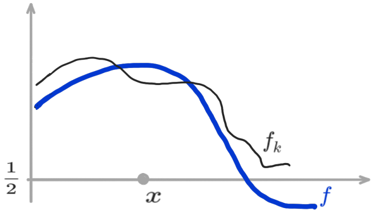

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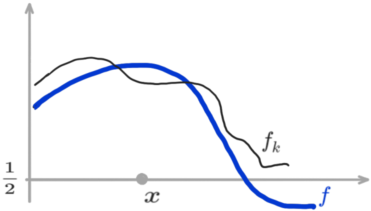

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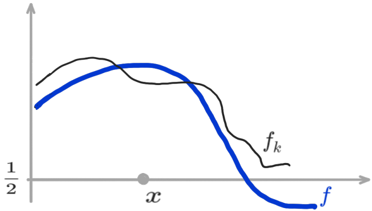

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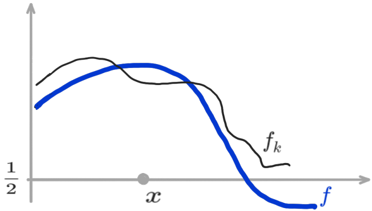

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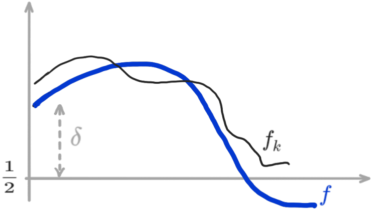

Suppose $|f(x) - 1/2| \geq \delta$ for most values x ...

Then $|f_k - f| \leq \delta$ implies $h_k = h^*$ often ... no need for $f_k \approx f$.

Tsybakov's noise condition: $\mathbb{P}_X(|f - 1/2| < \delta) \leq \delta^\beta$

If $|f_k - f| \leq \delta_n$, then $\mathbb{P}_X(h_k \neq h^*) \leq \mathbb{P}_X(|f - 1/2| < \delta_n) \leq \delta_n^\beta$.

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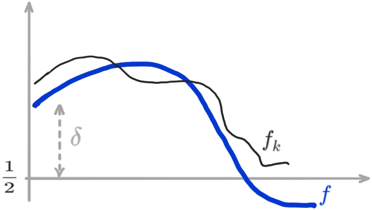

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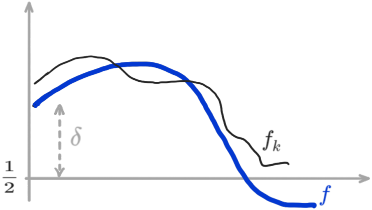

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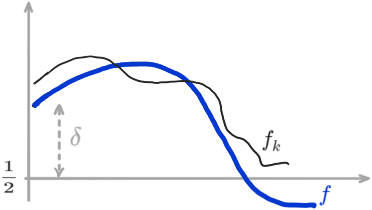

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Technical Remarks:

- Above rates assume $P_X \equiv$ Uniform.
([Chaudhuri, Dasgupta 14] [Gadat et al 14]).
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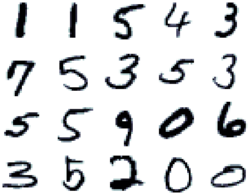
- **Multiclass and Mixed Costs**

k-NN extends naturally to multiclass



Data: $\{(X_i, Y_i)\}_{i=1}^n$, $Y \in \{1, , \ldots, L\}$.

Learn: $h_k(x) =$ majority (Y_i) of k-NN(x).

Reduction: let $f_k^y(x) =$ proportion $(Y = y)$ out of k-NN(x)

It estimates $f^y(x) = \mathbb{P}(Y = y|x)$.

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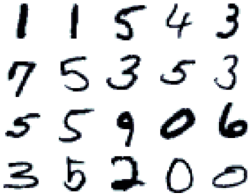

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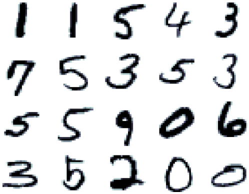

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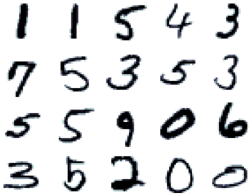

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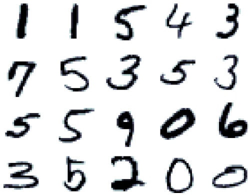

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- **Noise margin:** At any x, we want $f^{(1)}(x) \gg f^{(2)}(x)$ ...

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Then: $\quad \mathbb{E}\, \mathcal{E}(h_k) \lesssim (n/\log L)^{-(\beta+1)/(2+d)}$, for $k = \Theta(n^{2/(2+d)})$.

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$y \hookleftarrow$ Expected cost when y is wrong $\neq 1 - \mathbb{P}(Y = y)$

Natural extensions of previous insights considered in [Reeve, Brown 17]

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Continuity of $f(x) = \mathbb{E}[Y|x]$ is unnatural in classification ...

- **Piecewise Smoothness:** Ben-David, Scott, Nowak, Castro ... (k-NN not well-understood in these settings)
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End of Part I