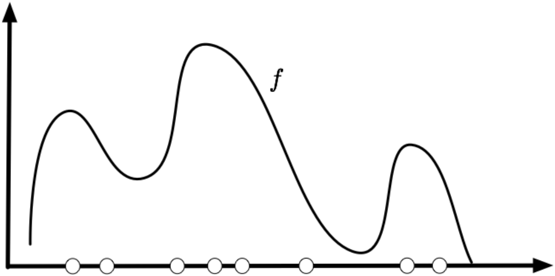
Optimal rates for k-NN density and mode estimation

Samory Kpotufe
ORFE, Princeton University

Joint work with **Sanjoy Dasgupta**, UCSD, CSE.

Goal:

Practical and Optimal estimator of all modes of f from $X_{1:n} \sim F^n$.



Rate-Optimal: single mode case ([S. Tsybakov, 90] ...).
Practical: mean-shift (hard to analyze ... see [Genovesee, ... Wasserman et.al., 13], [Arias-Castro et.al., 13] on consistency)

We derive a rate-optimal estimator based on k-NN graphs ...

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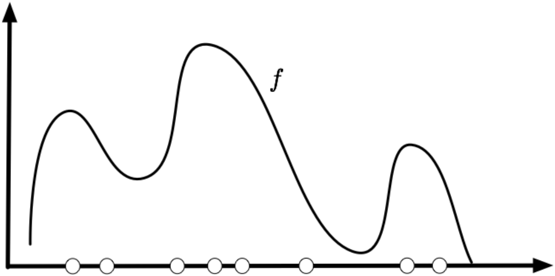

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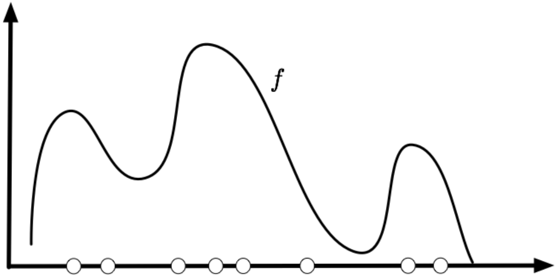

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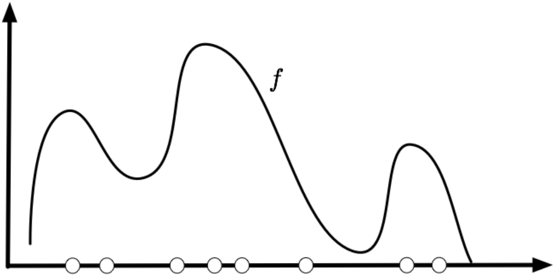

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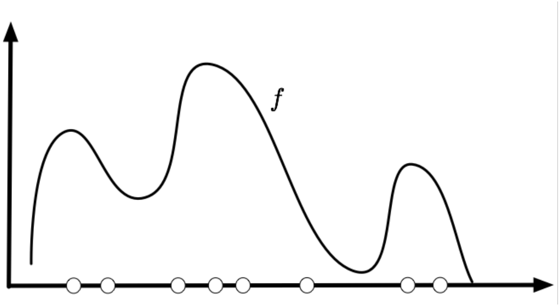

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Program of construction

- k**-NN density rates:**
  asymptotic $1/\sqrt{k}$ rates (e.g. [Biau, ..., Devroye et.al., 11]).
  We show high-prob. finite sample rates!
- **Single mode:**
  Common estimator in theory: $\hat{x} = \arg\sup_{x \in \mathbb{R}^d} \hat{f}(x)$.
  Practical estimator: $\tilde{x} = \arg\max_{x \in X_{1:n}} \hat{f}(x)$.
  Consistency of $\tilde{x}$ [Abraham, Biau, Cadre, 04]
  We show that $\tilde{x}$ is also minimax-optimal!
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- **k-NN density rates**
- Single mode rates
- Multiple modes rates

k-NN density estimate:

Define $r_k(x) \equiv$ distance from x to its kth neighbor in $X_{1:n}$.

$$f_k(x) \triangleq \frac{k}{n \cdot \mathrm{vol}\left(B(x, r_k(x))\right)} = \frac{k}{n \cdot v_d \cdot r_k(x)^d}.$$

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Devroye, Wagner, 77

Strong consistency.

Moore, Yackel, 76

$$\sqrt{k} \cdot \frac{(f_k(x) - f(x))}{f(x)} \xrightarrow{\mathcal{D}} \mathcal{N}(0,1),$$

provided $\nabla f < \infty$ on some $B(x)$, and $k \to \infty$, $k/n^{2/(2+d)} \to 0$.

Similar results by [Biau, Chazal, ... Devroye et. al., 2011]

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Express rates generally in terms of mod. of continuity at x:

$$\hat{r}(\epsilon, x) \triangleq \sup \left\{ r : \sup_{\|x-x'\| \leq r} f(x') \leq f(x) + \epsilon \right\}$$

$$\check{r}(\epsilon, x) \triangleq \sup \left\{ r : \sup_{\|x-x'\| \leq r} f(x') \geq f(x) - \epsilon \right\}$$

Why not just $r(\epsilon, x)$?

For $x = \arg\max f(x)$, $\hat{r}(\epsilon, x) = \infty$ while $\check{r}(\epsilon, x) < \infty$.

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Theorem 1.

W.p $> 1 - e^{-C}$, simult. $\forall x \in$ supp(f), $\forall \epsilon > 0$,

$$\left(1 - \frac{C}{\sqrt{k}}\right)(f(x) - \epsilon) \le f_k(x) \le \left(1 + \frac{C}{\sqrt{k}}\right)(f(x) + \epsilon),$$

provided $\ln n/n \lesssim k/n \lesssim v_d \cdot r(\epsilon, x)^d \cdot (f(x) - \epsilon)$.

$\therefore$ **optimal (local) rates under smoothness conditions.**
If f is α-Hölder at x, i.e. $\forall x', |f(x') - f(x)| \le L \|x - x'\|^\alpha$, then

$$|f_k(x) - f(x)| = O\left(n^{-\alpha/(2\alpha+d)}\right), \quad \text{for } k = \Theta(n^{2\alpha/(2\alpha+d)}).$$

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Proof idea:

$$f_k(x) = \frac{k}{n \cdot v_d \cdot r_k(x)^d}.$$

Express $r_k(x)$ in terms of $f(x)$:

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- If $F(B(x,r)) \approx k/n$ then $r \approx (k/n \cdot f(x))^{1/d}$.
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- k-NN density rates
- **Single mode rates**
- Multiple modes rates

Most commonly studied

$\hat{x} = \arg\sup_{x \in \mathbb{R}^d} f_n(x)$

Recursive estimates (One sample at the time)

[L. Devroye 79], [S. Tsybakov, 90 (optimal for Hölder classes.)]

Direct estimates

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A.2 (global): level sets of f have single CC.

Theorem 2. Let $\tilde{x} = \arg max_{x \in X_{1:n}} f_k(x)$. W.h.p. we have

$$\|\tilde{x} - x\| \lesssim k^{-1/4}, \quad \text{provided } \ln n \lesssim k \lesssim n^{4/(4+d)}.$$

Constants depend on $f(x)$ and $\nabla^2 f(x)$. (OPTIMAL, see Tsyb.90)

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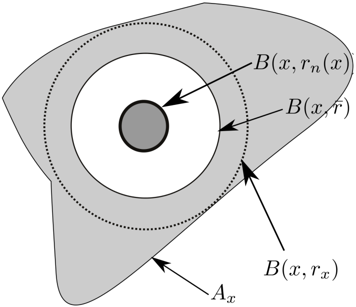

$\nabla^2 f(x) \prec 0$: $\exists$ a level set A_x:

$$c \|x - x'\|^2 \leq f(x) - f(x') \leq C \|x - x'\|^2.$$

Theorem 1 allows for different rates near or far from x:

$\min_{B(x, r_n(x))} f_k > \max_{\mathcal{X} \setminus B(x, \bar{r})} f_k$

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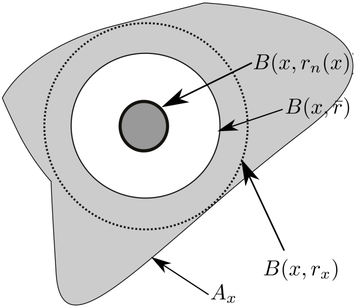

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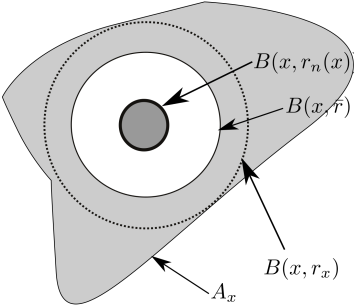

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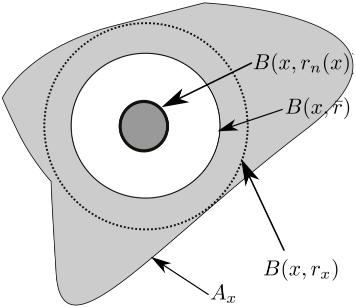


$\nabla^2 f(x) \prec 0 :$ $\exists$ a level set A_x:

$$c\,\|x - x'\|^2 \leq f(x) - f(x') \leq C\,\|x - x'\|^2.$$

Theorem 1 allows for different rates near or far from x:
$\min_{B(x,r_n(x))} f_k \;>\; \max_{\mathcal{X}\setminus B(x,\bar{r})} f_k$

Outline:

- k-NN density rates
- Single mode rates
- **Multiple modes rates**

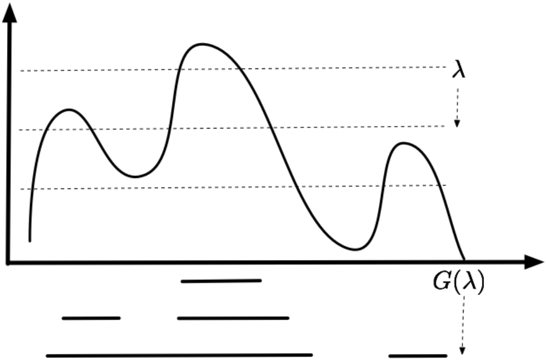
Setup:

Modes: $\mathcal{M} \equiv \{x : \exists r > 0, \forall x' \in B(x, r),\ f(x') < f(x)\}$.

A.1 (local) $\forall x \in \mathcal{M},\ \nabla^2 f(x) \prec 0.$

A.2 (global) Any CC of any level set of f contains a mode in $\mathcal{M}$.

ALGO: As f_k goes down, pick a new mode as a new *bump* appears.



Identifying CCs of level sets:

CCs of subgraphs of a k-NN graph [Chau., Das., Kpo., v Lux., 14]

How to identify false modes in f_k?

Remove all *bumps* of height $\lesssim |f_k - f| \approx 1/\sqrt{k}$.

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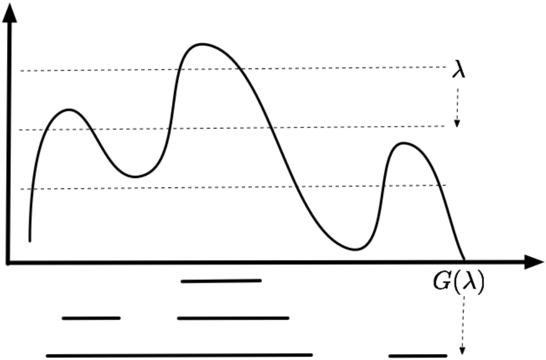

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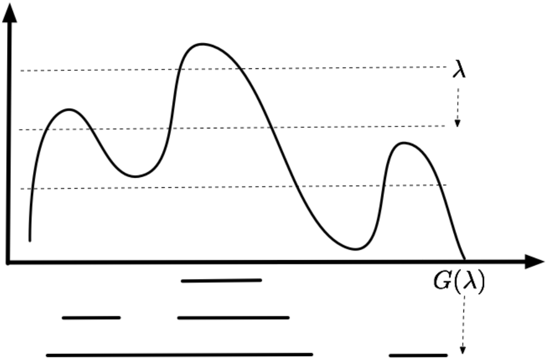

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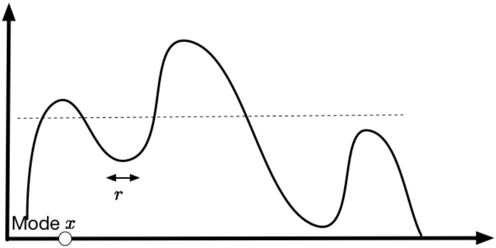
Identifying good modes



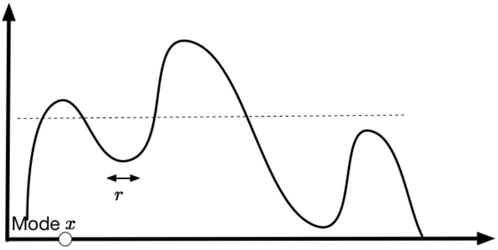
x is r-salient: separated from other modes by valley of radius r.

Theorem 3. Suppose $x \in \mathcal{M}$ is r-salient. Let $n \geq N(x)$. W.h.p. $\exists \tilde{x} \in \mathcal{M}_n$ s.t.

$$\|\tilde{x} - x\| \lesssim k^{-1/4}, \quad \text{provided } \ln n / r^4 \lesssim k \lesssim n^{4/(4+d)}.$$

Constants depend on $f(x)$ and $\nabla^2 f(x)$.

Identifying good modes



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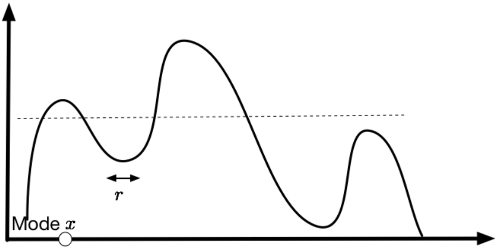

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Pruning bad modes

Theorem 4. Suppose f is Lipschitz. Assume $k \geq \ln n$. Let $\lambda_0 = \Theta(\ln n/k)$. All modes in $\mathcal{M}_n$ at f_k-level $\lambda > \lambda_0$ can be assigned to *distinct* modes in $\mathcal{M}$ at f-level $\approx \lambda_0$.

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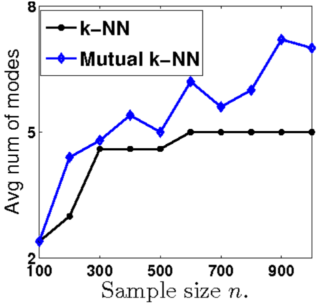

TRUTH: 5-modes mixture $\sum_{i=1}^{5} 0.2\mathcal{N}(2\sqrt{d}e_i, I_d)$

Merci!