Self-Tuning in Nonparametric Regression

Samory Kpotufe
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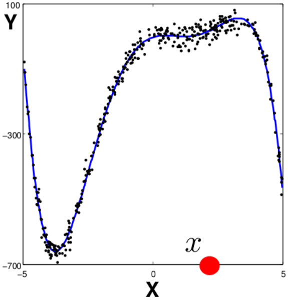
Local Regression

Data: $\{(X_i, Y_i)\}_{i=1}^n$, $Y = f(X) +$ noise
$f \in$ nonparametric $\mathcal{F}$, i.e. $\dim(\mathcal{F}) = \infty$.



Learn:
$f_n(x) =$ avg (Y_i) of Neighbors(x).
(e.g. k-NN, kernel, or tree-based reg.)

Quite basic $\Longrightarrow$ common in modern applications.

Sensitive to choice of Neighbors(x): k, band. h, tree cell size.
Goal: choose Neighbors(x) optimally!

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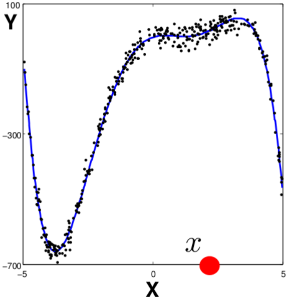

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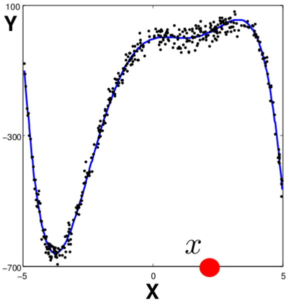

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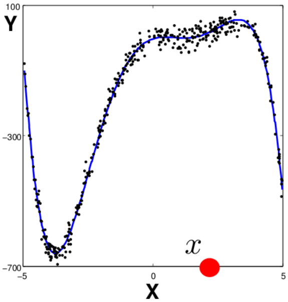

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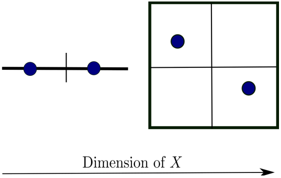

Performance would depend on dim(X) and how fast f varies ...
Suppose $X \in \mathbb{R}^D$, and $\forall x, x'$, $\quad |f(x) - f(x')| \leq \lambda \|x - x'\|^\alpha$.

Performance measure: $\|f_n - f\|^2_{2,P_X} \doteq \mathbb{E}_X |f_n(X) - f(X)|^2$.

Minimax global performance *(Stone 80-82)*

$$\|f_n - f\|^2_{2,P_X} \propto \lambda^{2D/(2\alpha+D)} \cdot n^{-2\alpha/(2\alpha+D)}.$$

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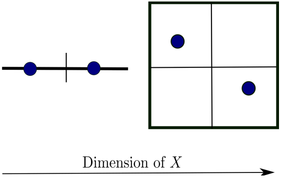

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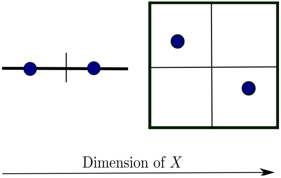

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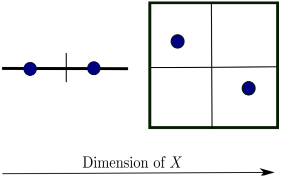

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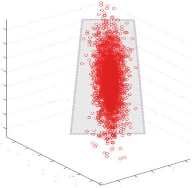

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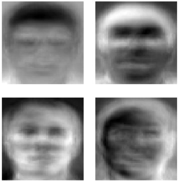

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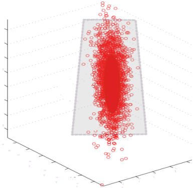

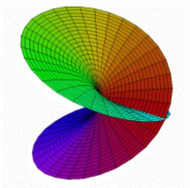

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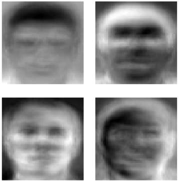

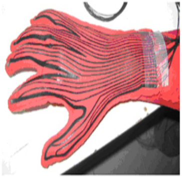

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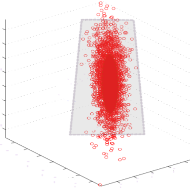

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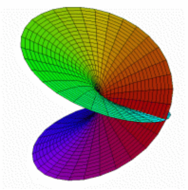

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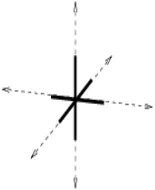
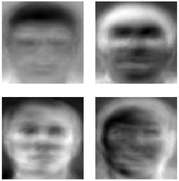
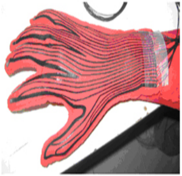
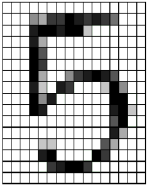


Sparse data







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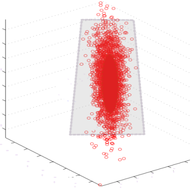

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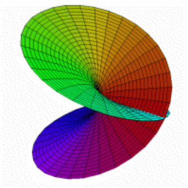

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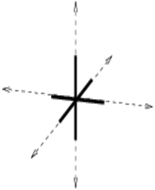

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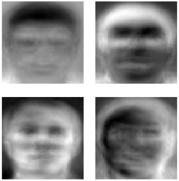

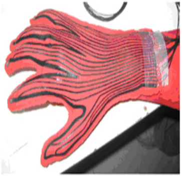

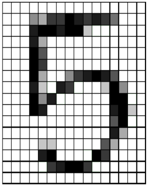

Basic approach: Manifold or Dictionary Learning/Regularization
(e.g. LLE, Isomap, Laplacian eigenmaps, kernel PCA, ...)

Basic approach introduces much more tuning!

Recent Alternative:
f_n **operates in** $\mathbb{R}^D$ **but adapts to the unknown** d **of** $\mathcal{X}$**.**

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Some work on adaptivity to intrinsic dimension:

- Kernel and local polynomial regression: Bickel and Li 2006, Lafferty and Wasserman 2007. Manifold dim.
- G-P regression: Yang and Dunson 2016. Manifold dim.
- Dyadic tree classification: Scott and Nowak 2006. Box dim.
- RP/dyadic tree regression: K. and Das. 2011. Doubling dim.
- 1-NN regression*: Kulkarni and Posner 1995. Metric dim.

Adaptivity to intrinsic d

Main insight: Key algorithmic quantities depend on d, not on D.

For Lipschitz f, $\quad \|f_{n,\epsilon} - f\|^2_{2,P_X} \approx \dfrac{\epsilon^{-d}}{n} + \epsilon^2.$

Cross-validate over ϵ for a good rate in terms of d.

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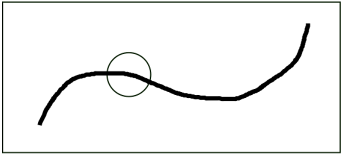
Kernel reg.: Avg. **mass of a ball** of radius ϵ is approx. ϵ^d



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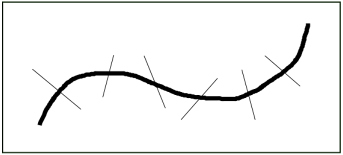

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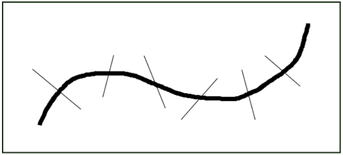

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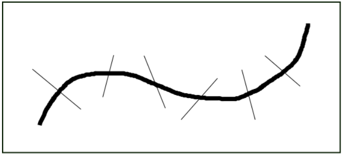

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Insights help with tuning under time-constraints.

Main Idea: compress data in a way that respects structure of $\mathcal{X}$.

- Online tuning for regression-trees. [Kpo. and Orabona 2013]
- Compressed Kernel regression. [Kpo. and Verma, 2017]
- Subsampled 1-NN's. [Xue and Kpo, Submitted]

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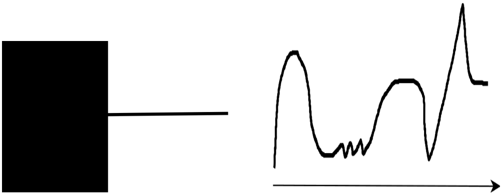
So far, we have viewed d as a global characteristic of $\mathcal{X}$ ...

Problem complexity is likely to depend on location!



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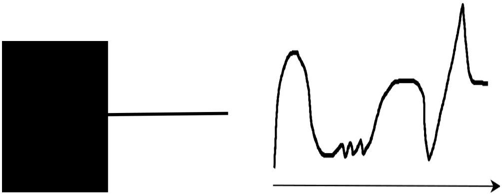

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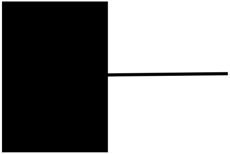

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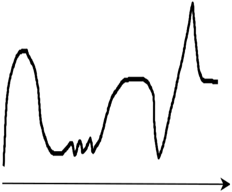

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NEXT:

I. Local notions of smoothness and dimension.

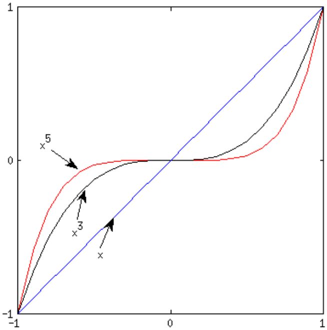
II. Local adaptivity to dimension: k-NN example.

III. Full local adaptivity: kernel example.

Local smoothness

Use local Hölder parameters $\lambda = \lambda(x), \alpha = \alpha(x)$ *on* $B(x, r)$*:*

For all $x' \in B(x, r)$, $\quad |f(x) - f(x')| \leq \lambda \rho(x, x')^{\alpha}$.



$f(x) = x^{\alpha}$ is flatter at $x = 0$ as α is increased.

Local dimension

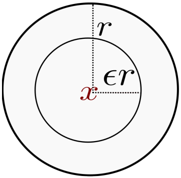


Figure: d-dimensional balls centered at x.

Volume growth: $\mathrm{vol}(B(x,r)) = C \cdot r^d = \epsilon^{-d} \cdot \mathrm{vol}(B(x,\epsilon r))$.

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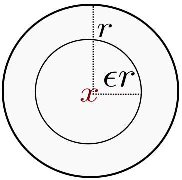

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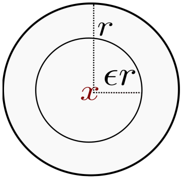

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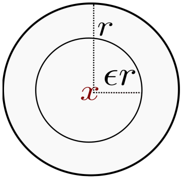


Figure: d-dimensional balls centered at x.

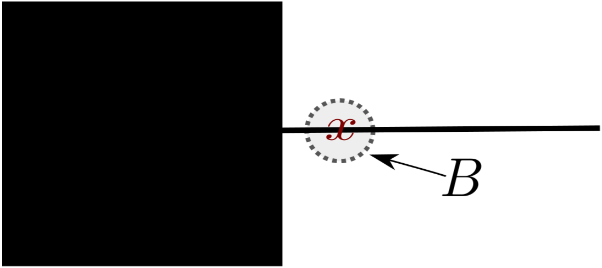
Volume growth: $\text{vol}(B(x,r)) = C \cdot r^d = \epsilon^{-d} \cdot \text{vol}(B(x,\epsilon r))$.

If P_X *is* $\mathcal{U}(B(x,r))$, *then* $P_X(B(x,r)) \lesssim \epsilon^{-d} \cdot P_X(B(x,\epsilon r))$.

Def.: P_X *is* (C,d)*-homogeneous on* $B(x,r)$ *if* $\forall r' \leq r, \epsilon > 0$,

$$P_X(B(x,r')) \leq C\epsilon^{-d} \cdot P_X(B(x,\epsilon r')).$$

The growth of P_X can capture the intrinsic dimension in $B(x)$.



Location of query x matters!

Size of neighborhood B matters!

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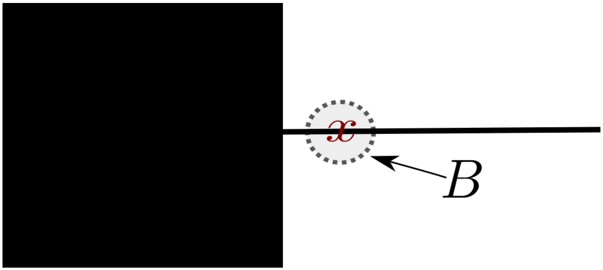

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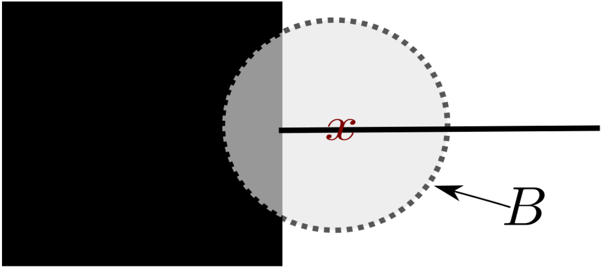

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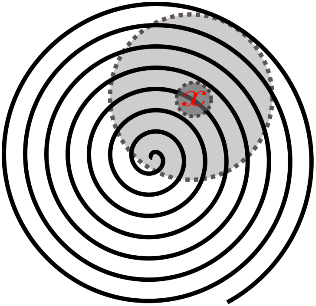

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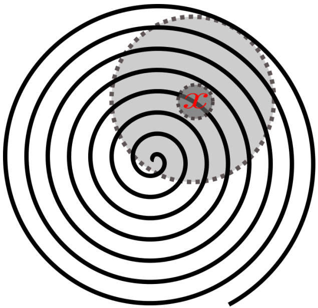
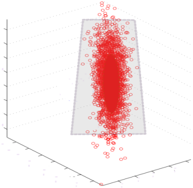
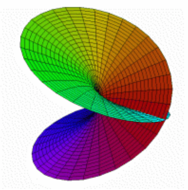


For k-NN, or kernel reg, size of B depends on n and (k or h).

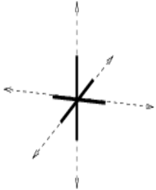
The growth of $P_X(B)$ can capture the intrinsic dimension locally.



Linear data



Manifold data



Sparse data

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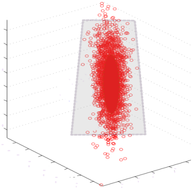

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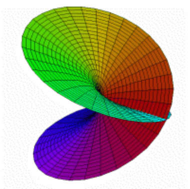

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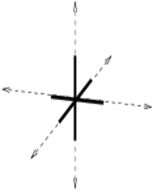

Sparse data

$\mathcal{X}$ can be a collection of subspaces of various dimensions.

Intrinsic d tightly captures the minimax rate:

Theorem: Consider a metric measure space $(\mathcal{X}, \rho, \mu)$, such that for all $x \in \mathcal{X}, r > 0, \epsilon > 0$, we have $\mu(B(x,r)) \approx \epsilon^{-d}\mu(B(x, \epsilon r))$. Then, for any regressor f_n, there exists $P_{X,Y}$, where $P_X = \mu$ and $f(x) = \mathbb{E}\, Y|x$ is λ-Lipschitz, such that

$$\mathop{\mathbb{E}}_{\mathcal{P}^n_{X,Y}} \|f_n - f\|^2_{2,\mu} \gtrsim \lambda^{2d/(2+d)} \cdot n^{-2/(2+d)}.$$

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NEXT:

I. Local notions of smoothness and dimension.

II. Local adaptivity to dimension: k-NN example.

III. Full local adaptivity: kernel example.

Main Assumptions:

- $X \in$ metric space $(\mathcal{X}, \rho)$.
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k-NN regression: $f_n(x) =$ weighted avg (Y_i) of k-NN(x).

Suppose $\mathcal{X} \subset \mathbb{R}^D$, the learner operates in $\mathbb{R}^D$!
No dimensionality reduction, no dimension estimation!

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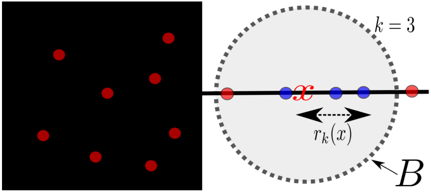
Bias-Variance tradeoff

$$\mathop{\mathbb{E}}_{(X_i,Y_i)_1^n} |f_n(x) - f(x)|^2 = \underbrace{\mathbb{E}\, |f_n(x) - \mathbb{E}\, f_n(x)|^2}_{\text{Variance}} + \underbrace{|\mathbb{E}\, f_n(x) - f(x)|^2}_{\text{Bias}^2}.$$

General intuition:

Fix $n \gtrsim k \gtrsim \log n$, and consider neighborhood $B(x)$ of dim. d.



Rate of convergence of $f_n(x)$ depends on:

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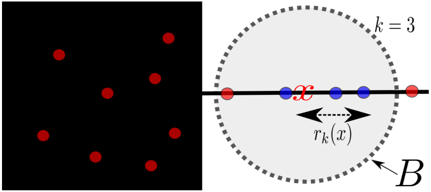

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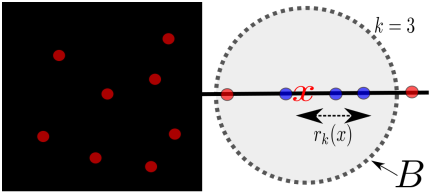

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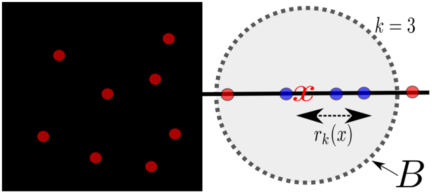

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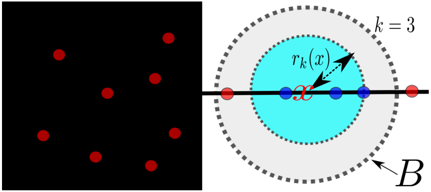

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Remember: Cross-valid. or dim. estimation at x are impractical.

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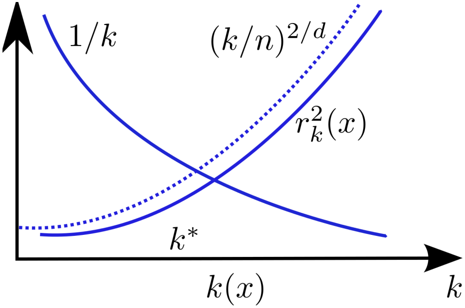

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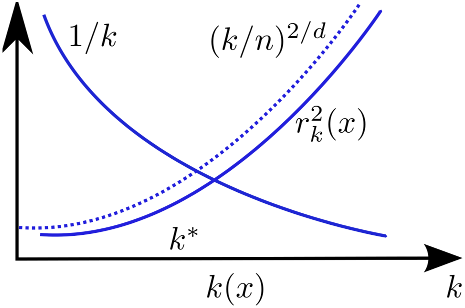

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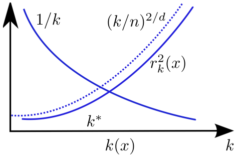

Theorem: Suppose $k(x)$ is chosen as above. The following holds w.h.p. simultaneously for all x.
Consider any B centered at x, s.t. $P_X(B) \gtrsim n^{-1/3}$. Suppose P_X is (C, d)-homogeneous on B. We have

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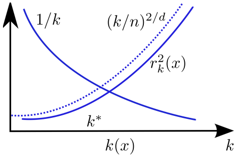

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(Recent work with Vikas Garg)

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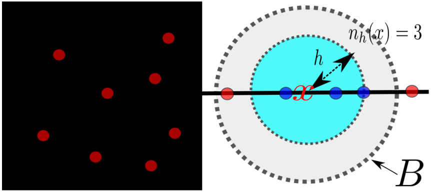

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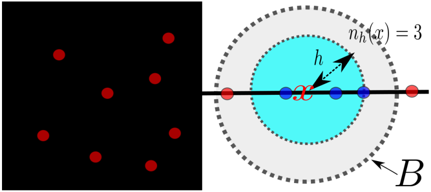

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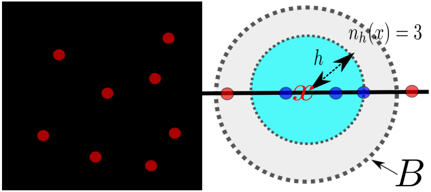

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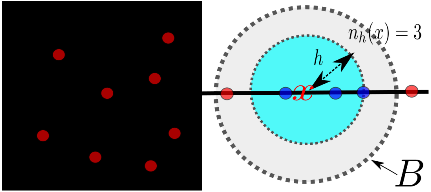

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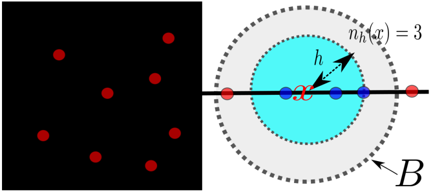

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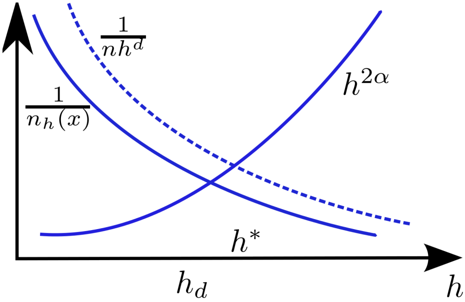
Suppose we know $\alpha(x)$ but not $d(x)$.

Monitor $\frac{1}{n_h(x)}$ and $h^{2\alpha}$.



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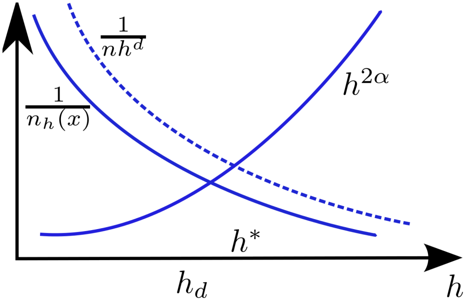

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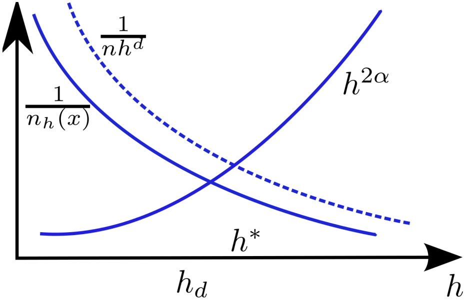

For every $h < h*$, $\frac{1}{nh^d} > h^{2\alpha}$ therefore for such h

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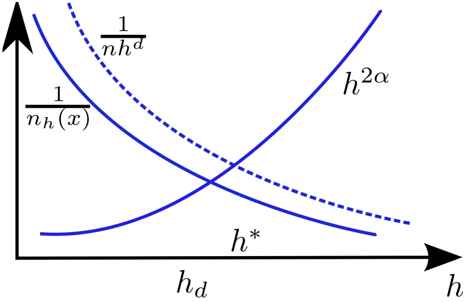

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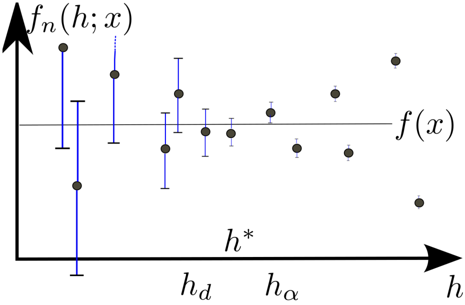

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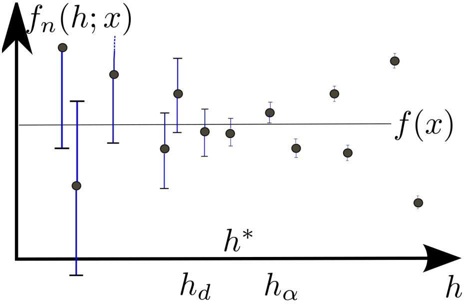

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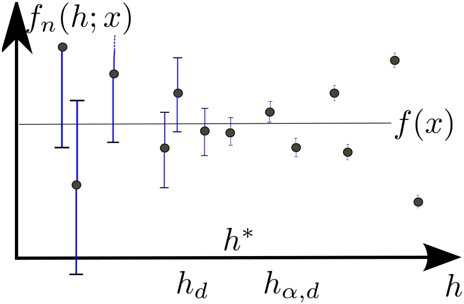

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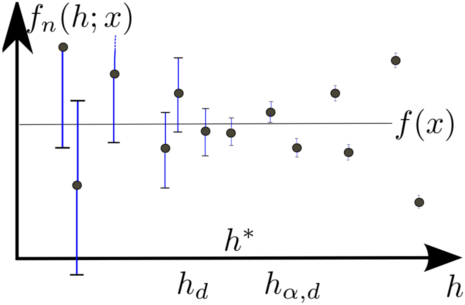

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Choosing $h_{\alpha,d}(x)$- Result

Tightness assumption on $d(x)$: $\exists r_0$, $\forall x \in \mathcal{X}, \exists C, C', d$ such that $\forall r \leq r_0, \quad Cr^d \leq P_X(B(x,r)) \leq C'r^d$.

Theorem: Suppose $h_{\alpha,d}(x)$ is chosen as described. Let $n \geq N(r_0)$. The following holds w.h.p. simultaneously for all x. Let d, α, λ be the local problem parameters on $B(x, r_0)$. We have

$$|f_n(x) - f(x)|^2 \lesssim \lambda^{2d/(2\alpha+d)} \left(\frac{\ln n}{n}\right)^{2\alpha/(2\alpha+d)}.$$

The rate is optimal.

Choosing $h_{\alpha,d}(x)$*- Result*

Tightness assumption on $d(x)$**:** $\exists r_0$, $\forall x \in \mathcal{X}, \exists C, C', d$ such that $\forall r \leq r_0, \quad Cr^d \leq P_X(B(x,r)) \leq C'r^d$.

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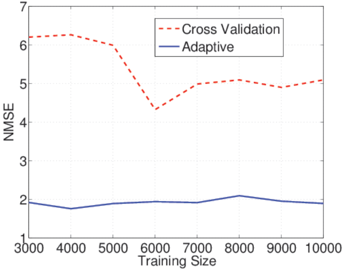
Simulation on data with mixed spatial complexity



... the approach is promising, but remains expensive!

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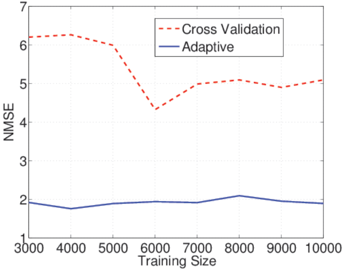
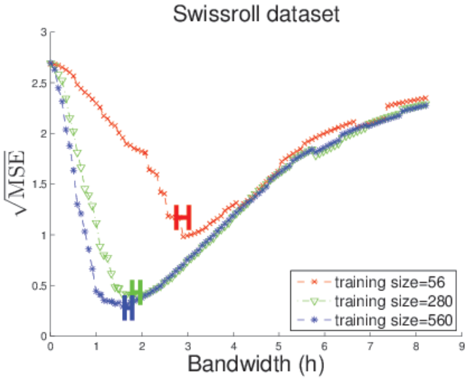


... the approach is promising, but remains expensive!

Future direction:

Cheaper tree-based kernel implementations.

Initial experiments with tree-based kernel:

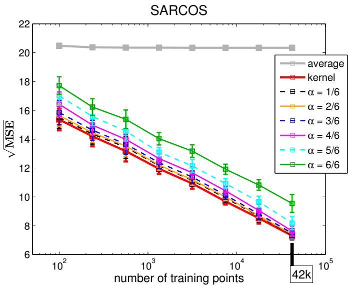


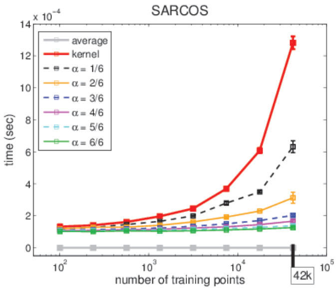
Without CValidation: automatically detect interval containing h^*.

Current directions:

Tradeoffs via data compression/quantization.

Estimating Robotic Torque:



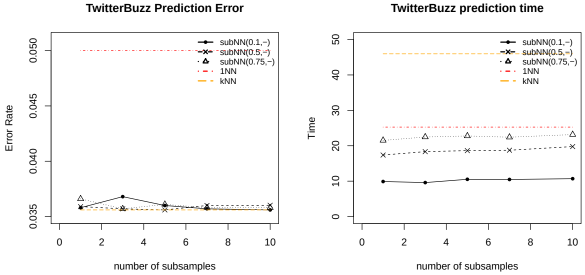


Tradeoffs can be controlled by some α.

Current directions:

Tradeoffs via subsampling ...

Predicting Viral Tweets:



Denoised subsamples of 1-NN's: fast and accurate.

Other directions:

- **Combine** adaptive tuning **with representation learning**.
- Adaptive **conf. bands** (à la Belloni, Chernozukov, Lepski, Wasserman?)
- **Other procedures** (kernel machines, rand. forests, neural nets)

...

TAKE HOME MESSAGE:

- We can adapt to intrinsic $d(\mathcal{X})$ without preprocessing.
- Local-learners can self-tune optimally to local $d(x)$ and $\alpha(x)$.

Results extend to plug-in classification!

Many potential future directions!

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Thank you!