Asymptotic Properties of Nonparametric Estimation on Manifold

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Overview

1. Nonparametric Estimation and Manifolds
2. Manifold Learning
3. Data Model and Problem Statement
4. Results

Nonparametric Regression (univariate output)

Unknown function

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Kernel nonparametric estimator

$$\hat{f}(X) = \frac{\sum_{n=1}^{N} K_N(X, X_n) f(X_n)}{\sum_{n=1}^{N} K_N(X, X_n)},$$

where $K_N(X, X')$ is a weight (kernel) function.

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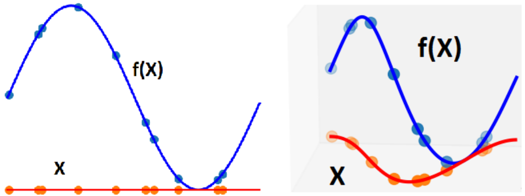

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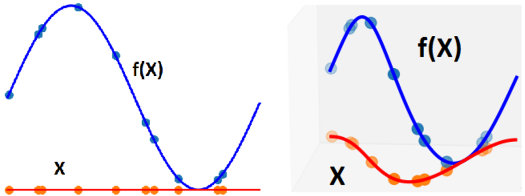

Wish: replace $N^{-\frac{2}{p+4}}$ with $N^{-\frac{2}{q+4}}$.

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- cost function in the **ML**: $\delta_\theta(X) = |X - g(h(X))|_p$.

Common scheme of the ML algorithms

First step: neighborhoods construction
For each $X_n \in \mathbb{X}_N$ point $X_i \in \mathbb{X}_N$ is in the neighborhood iff $|X_i - X_n|_p < \varepsilon$, where $\varepsilon = \varepsilon(N) > 0$.

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Second step: neighborhoods descriptions Chosen descriptions of the neighborhoods (local descriptions of the DM) are computed. Examples:

- barycentric coordinates of the "central" point X_n with respect to its nearest-neighbors (except itself);
- local PCA basis via local covariance

$$\Sigma(X) = \sum_{n=1}^{N} I(|X - X_n|_p < \varepsilon) \cdot (X_n - X) \cdot (X_n - X)^T.$$

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Third step: global description

Chosen global description of the DM is computed by solving some convex optimization problems under some normalization constraints. Usually low-dimensional sample features $\mathbb{Y}_N = h(\mathbb{X}_N) = \{y_1, \ldots, y_N\} \subset \mathbb{Y}_h$ are computed by minimization of chosen cost function $L(\mathbb{Y}_N|\mathbb{X}_N)$ over $\mathbb{Y}_N$.

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$$L_{LLE}(\mathbb{Y}_N|\mathbb{X}_N) = \sum_{n=1}^{N} \|y_n - \sum_{j=1} w_{n,j} y_{n,j}\|_F^2;$$

$$L_{LE}(\mathbb{Y}_N|\mathbb{X}_N) = \sum_{n,j=1}^{N} K(X_n, X_j) \cdot \|y_n - y_j\|_2^2;$$

$$L_{LTSA}(\mathbb{Y}_N|\mathbb{X}_N) =$$

$$= \sum_{j=1}^{N} \|(I_q - Q_{PCA}(X_n) \cdot Q_{PCA}^T(X_n)) \cdot H_n \cdot Y_{(n)}\|_F^2.$$

Fourth step: Out-of-Sample extension
The Feature sample $\mathbb{Y}_N$ gives the values of the Embedding mapping $h(X)$ only at sample points; a finding of low-dimensional features $h(X)$ for Out-of-Sample (OoS) points $X \in \mathbb{M} \setminus \mathbb{X}_N$ is usually called OoS-extension problem.

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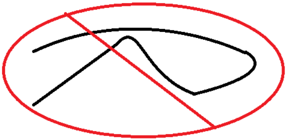
- no short circuits



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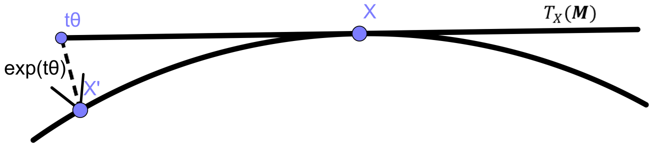
Function assumption

- $f \in C^2(\overline{\mathbb{M}})$ (*).

Data Model. Local Coordinates



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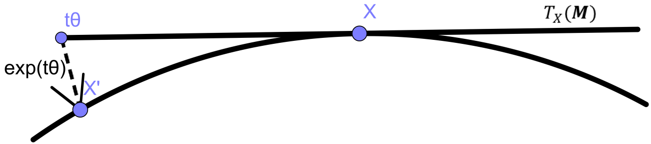

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Kernel assumptions

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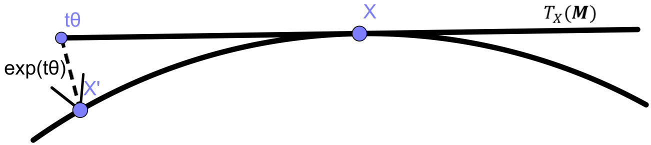

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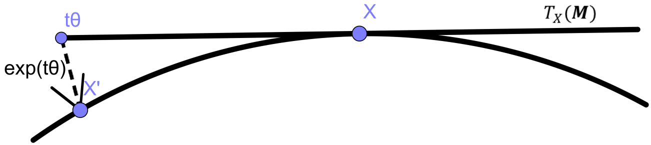

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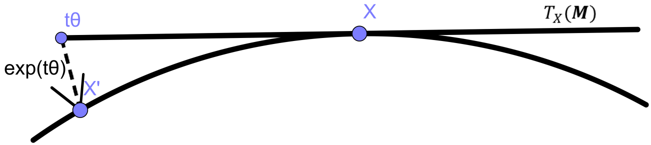

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- $\inf_{X \in \mathbb{M}} \int_{S_q} \int_{1/2}^{1} K(X, \theta, z) z^{q-1} d\theta dt \geq C_{K,1/2} > 0$.

Data Model. Parameter

For the neighborhood parameter $\varepsilon = \varepsilon(N) > 0$ it is assumed that

- For $N \to \infty$: $\varepsilon \to 0$;
- For $N \to \infty$: $N \cdot \varepsilon^q \to \infty$;
- For $N \to \infty$: $N \cdot \varepsilon^{q+4} \to 0$.

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and of its average

$$F_N = \frac{1}{N} \sum_{n=1}^{N} F_N(X_n).$$

Limits

$$\overline{F}(X) = \frac{\int_{S^{q-1}} \rho_{E,m}(X,\theta)\phi(X,\theta)d\theta}{\int_{S^{q-1}} \rho_{E,0}(X,\theta)d\theta},$$

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where S^{q-1} is sphere in q-dimensional space,

$$\rho_{E,m}(X,\theta) = \int_0^1 K(X,\theta,t)\, t^{q+m-1}dt.$$

Limits for $F(X'|X) = f(X')$

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$$f(X') = f(X) \cdot t^0 + O(t).$$

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Results-1

Statement 1 ($F_N(X)$ consistency). For each $X \in \mathbb{M}$ as $N \to \infty$

$$\mathbb{E}F_N(X) \to \overline{F}(X);$$
$$N\varepsilon^q \cdot \mathtt{Var}F_N(X) \to d(X);$$
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Theorem 1 (central limit for $F_N(X)$). For each $X \in \mathbb{M}$ as $N \to \infty$

$$\sqrt{N\varepsilon^q} \cdot \big(F_N(X) - \overline{F}(X)\big) \to^D N(m(X), d(X)),$$

where $m(X)$ and $d(X)$ are explicit functions, $m(X) \equiv 0$ for d:2, $\to^D$ is convergence in distribution.

Theorem 2 (large deviation probability for $F_N(X)$). For each ε-bounded from manifold boundary point $X \in \mathbb{M}_\varepsilon$, and for each $N > N_0$ and $\varepsilon < \varepsilon_0$ and $z \in [0, 1]$

$$P\left(\left|F_N(X) - \overline{F}(X)\right| \geq z + \varepsilon \cdot I(d \neq 2) \cdot C_{LD1} + \varepsilon^2 \cdot C_{LD2}\right) \leq 4 \cdot \exp\left(-\frac{z^2 \cdot N\varepsilon^q}{\sigma^2(X)}\right),$$

where $N_0, \varepsilon_0, C_{LD1}, C_{LD2}$ are positive constants, $\sigma^2(X)$ is bounded function.

Note for Results-2

The optimal rate in **Theorem 2** is ε^2 for

$$\begin{cases} z^2 = \frac{1}{N\varepsilon^q} \\ z = \varepsilon^2 \end{cases}$$

and it equals to $N^{-\frac{2}{q+4}}$.
Such rate is equal to the rate for classical case (where $p \mapsto q$).

Theorem 3 (uniform large deviation probability for $F_N(X)$). For each $z \in [0, 1]$, for $N > N_0$, $\varepsilon < \varepsilon_0$ for each ε-bounded from manifold boundary point $X \in \mathbb{M}_\varepsilon$

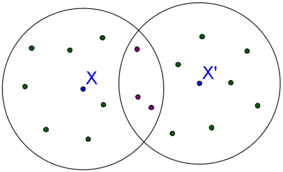
$$P\left(\sup_{X \in \mathbb{M}_\varepsilon} \left|F_N(X) - \overline{F}(X)\right| \geq z + \varepsilon \cdot I(d \not\vdots 2) \cdot C_{LD1} + \varepsilon^2 \cdot \tilde{C}_{LD2}\right) \leq$$

$$\leq 4 \cdot \left(\frac{2a\sqrt{p}}{\varepsilon^3}\right)^p \cdot \exp\left(-\frac{z^2 \cdot N\varepsilon^q}{C_\sigma}\right)$$

$$+ \left(\frac{6a\sqrt{p}}{\varepsilon}\right)^p \cdot \exp\left(-1/16 \cdot N\varepsilon^q V_q p_{\min}^2 / (9 p_{\max})\right),$$

where $a, N_0, \varepsilon_0, C_{LD1}, \tilde{C}_{LD2}, p_{\min}, p_{\max}$ are positive constants.

Results-4



Statement 2 (F_N consistency). For $N \to \infty$:

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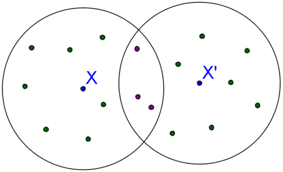

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Theorem 4 (large deviation probability for F_N). Exist positive constants $N_{U,0}$, $C_{U,1}$, $C_{U,2}$, $C_{U,p}$ such that for $z \in [0,1]$ and $N > N_{U,0}$:

$$P\left(\left|F_N - \overline{F}\right| \geq z + \varepsilon \cdot I(d \not\vdots 2) \cdot C_{U,1} + \varepsilon^2 \cdot C_{U,2}\right) \leq \exp\left(-z^2 \cdot N\varepsilon^q \cdot C_{U,p}\right).$$

Relations with Other Papers

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Relations with Other Papers

1. [Singer&Wu2012] local consistency and large deviation for local covariance (without explicit form for limit function)
2. [Gine&Koltchinskii2006] asymptotic expansion for squared gradient (not nonparametric, but sample mean)
3. [Belkin et.al. 2004, 2006, 2010] consistency for Laplace-Beltrami operator.

Conclusions

- specific for Manifold Learning nonparametric estimation on the manifold and its average are considered
- asymptotic expansion and uniform large deviation results are obtained for the considered nonparametric estimates
- the results could be used for the manifold learning algorithms analysis (already are used to get properties of Manifold Learning optimization procedures [Yanovich2017]).