Advanced Statistical Methods.
P4-E1-K3.
Pointwise derivative estimation.

Evgeny Lagutin

Skoltech Data Science

March 21, 2022

github.com/sverdoot/pointwise-derivative-estimation

Data generation

We observe sample $S_n=\{(X_i,Y_i):1\leq i\leq n\}$ where $X_i=\frac{i}{n},\ i\in\{1,\dots,n\}$

$$Y_i = f^*(X_i) + \varepsilon_i, \ \varepsilon_i \sim \mathcal{N}(0, 1), \quad 1 \le i \le n,$$

$$\psi_j(x) = \begin{cases} 1, & \text{if } j = 0\\ \sin(\pi(j+1)x), & \text{if } j \text{ is odd}\\ \cos(\pi j x), & \text{if } j \text{ is even.} \end{cases}$$

The true function f^* is then equal to

$$f(x) = c_1 \psi_1(x) + \dots + c_n \psi_n(x)$$

where the coefficients c_1, \ldots, c_n are chosen randomly: with γ_j i.i.d. standard normal,

$$c_j = \begin{cases} \gamma_j, & 1 \le j \le 10\\ \frac{\gamma_j}{(j-10)^2}, & 11 \le j \le n \end{cases}$$

Data generation

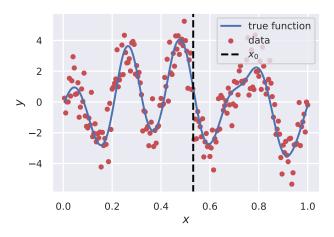


Figure 1: Function and sampled data

$$x_0 = 0.532$$

Local polynomial smoothing

Gaussian kernel: $K(x) = \exp(-x^2/2)$ Localizing weights: $w_i(x) = K\left(\frac{1}{m}(X_i - x)\right)$

$$\tilde{\theta}(x) = \mathcal{S}(x)\mathbf{Y}$$

$$S(x) = \{\Psi(x)W(x)\Psi(x)^{\top}\}^{-1}\Psi(x)W(x)$$

$$W(x) = \operatorname{diag}(\{w_i(x)\}_{i=1}^n)$$

$$\Psi(x) = \begin{pmatrix} 1 & \dots & 1 \\ (X_1 - x) & \dots & (X_n - x) \end{pmatrix}$$

Let $(\mathcal{S}(x))_j$ be a \mathbb{R}^n vector constructed of j's row of $\mathcal{S}(x)$, then

$$\hat{f}(x_0) = \tilde{\theta}_0(x_0) = (\mathcal{S}(x_0))_0^{\top} \mathbf{Y}$$
$$\hat{f}'(x_0) = \tilde{\theta}_1(x_0) = (\mathcal{S}(x_0))_1^{\top} \mathbf{Y}$$

Unbiased risk estimation

Homogeneous noise: $\varepsilon_i \sim \mathcal{N}(0, \sigma^2 I_n), \quad 1 \leq i \leq n, \quad \sigma = 1.$

$$\mathcal{R}_{m} = \|\mathbf{b}_{m}\|^{2} + \sigma^{2}\mathbf{p}_{m} = \|\mathcal{K}_{m}\mathbf{f} - \mathbf{f}\|^{2} + \sigma^{2}\operatorname{tr}(\mathcal{K}_{m}\mathcal{K}_{m}^{\top})$$

$$\tilde{\mathcal{R}}_{m} = \|\mathcal{K}_{m}\mathbf{Y} - \mathbf{Y}\|^{2} + 2\sigma^{2}\operatorname{tr}(\mathcal{K}_{m})$$

$$\mathbb{E}\tilde{\mathcal{R}}_{m} = \mathcal{R}_{m} + \sigma^{2}n = \|\mathcal{K}_{m}\mathbf{f} - \mathbf{f}\|^{2} + \sigma^{2}\operatorname{tr}(\mathcal{K}_{m}\mathcal{K}_{m}^{\top}) + \sigma^{2}n$$

$$\mathcal{K}_{m} = \begin{pmatrix} (\mathcal{S}(X_{1}))_{0} \\ \cdots \\ (\mathcal{S}(X_{m}))_{s} \end{pmatrix} \in \mathbb{R}^{n \times n}$$

Unbiased risk estimation for linear model

Bandwidth	Function estimate	True value	Derivative estimate	True value	Unbiased risk
0.00028	0.196	0.898	-101	-86	225

Table 1: Result for chosen bandwidth

True risk I

$$\mathcal{R}(\hat{f}) = \mathbb{E}((f^{*})'(x_{0}) - \hat{f}'(x_{0}))^{2} = \mathbb{E}((f^{*})'(x_{0}) - S(\mathcal{S}(x_{0}))_{1}^{\top} \mathbf{Y})^{2} = \\
\mathbb{E}\left((f^{*})'(x_{0}) - (\mathcal{S}(x_{0}))_{1}^{\top} (\mathbf{f} + \boldsymbol{\varepsilon})\right)^{2} = \\
\left((f^{*})'(x_{0}) - (\mathcal{S}(x_{0}))_{1}^{\top} \mathbf{f}\right)^{2} + (\mathcal{S}(x_{0}))_{1}^{\top} \mathbb{E}\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^{\top} (\mathcal{S}(x_{0}))_{1} - \\
2(f^{*})'(x_{0}) (\mathcal{S}(x_{0}))_{1}^{\top} (x_{0})\mathbb{E}\boldsymbol{\varepsilon} = \\
\left((f^{*})'(x_{0}) - (\mathcal{S}(x_{0}))_{1}^{\top} \mathbf{f}\right)^{2} + \sigma^{2} \| (\mathcal{S}(x_{0}))_{1} \|^{2}$$

True risk II

$$(S(x_0))_1^{\top} = \frac{1}{D} \left[w_i(x_0) \sum_{j=1}^n w_j(x_0) (X_i - X_j) \right]_{i=1}^n$$

$$D = \left[\sum_{i=1}^n w_i(x_0) \right] \left[\sum_{i=1}^n w_i(x_0) (X_i - x_0)^2 \right] - \left[\sum_{i=1}^n w_i(x_0) (X_i - x_0) \right]^2$$

True risk

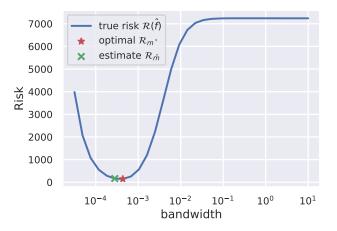


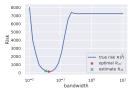
Figure 2: Dependence of true risk on bandwidth.

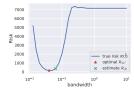
Comparison

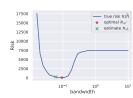
Oracle	Oracle	Chosen	Estimate
bandwidth	risk	bandwidth	risk
0.00043	144	0.00028	163

Table 2: Comparison with oracle

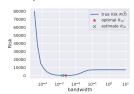
Additional results



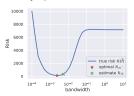




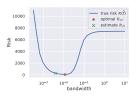
(a) Rectangular kernel, locally linear est.



(b) Rectangular kernel, locally quadratic est.



(c) Rectangular kernel, locally cubic est.



(d) Epanechnikov kernel, (e) Epanechnikov kernel, (f) Epanechnikov kernel, locally linear est.

locally quadratic est.

locally cubic est.