Model selection for fast density estimation

László (Laci) Györfi¹

¹Department of Computer Science and Information Theory Budapest University of Technology and Economics Budapest, Hungary

July 17, 2008

e-mail: gyorfi@szit.bme.hu www.szit.bme.hu/~gyorfi

・ 同 ト ・ ヨ ト ・ ヨ ト

\mathbb{R}^d -valued i.i.d. random vectors X_1, \ldots, X_n

・ロト ・回ト ・ヨト ・ヨト

 \mathbb{R}^{d} -valued i.i.d. random vectors X_{1}, \ldots, X_{n} distributed according to unknown probability measure μ with density f

同 と く き と く き と

 \mathbb{R}^{d} -valued i.i.d. random vectors X_{1}, \ldots, X_{n} distributed according to unknown probability measure μ with density fThe L_{1} norm

$$\|f-g\|:=\int_{\mathbb{R}^d}|f(x)-g(x)|dx$$

回 と く ヨ と く ヨ と

 \mathbb{R}^{d} -valued i.i.d. random vectors X_{1}, \ldots, X_{n} distributed according to unknown probability measure μ with density fThe L_{1} norm

$$\|f-g\| := \int_{\mathbb{R}^d} |f(x)-g(x)| dx = 2 \sup_A \left| \int_A f(x) dx - \int_A g(x) dx \right|$$

回 と く ヨ と く ヨ と

For a kernel function K and bandwidth h > 0, let f_n be the kernel density estimate with sample size n:

$$f_n(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{x-X_i}{h}\right).$$

・ 回 ト ・ ヨ ト ・ ヨ ト

Density-free consistency

lf

$$\lim_{n\to\infty}h_n=0$$

 and

$$\lim_{n\to\infty}nh_n^d=\infty$$

回 と く ヨ と く ヨ と

Density-free consistency

lf

$$\lim_{n\to\infty}h_n=0$$

and

$$\lim_{n\to\infty}nh_n^d=\infty$$

then, for any density f,

$$\lim_{n\to\infty}\mathbf{E}\|f-f_n\|=0$$

and

$$\lim_{n\to\infty}\|f-f_n\|=0 \text{ a.s.}$$

回 と く ヨ と く ヨ と

If the density f has a compact support and is twice differentiable, then

$$\mathbf{E}(\|f_n-f\|) \leq \frac{c_1}{\sqrt{nh_n^d}} + c_2 h_n^2.$$

回下 ・ヨト ・ヨト

If the density f has a compact support and is twice differentiable, then

$$\mathbf{E}(\|f_n-f\|) \leq \frac{c_1}{\sqrt{nh_n^d}} + c_2h_n^2.$$

If $h_n = cn^{-1/(d+4)}$ then

$$\mathbf{E}(||f_n - f||) \le Cn^{-2/(d+4)}.$$

回 と くほ と くほ とう

If the density f has a compact support and is twice differentiable, then

$$\mathbf{E}(\|f_n-f\|) \leq \frac{c_1}{\sqrt{nh_n^d}} + c_2h_n^2.$$

If $h_n = cn^{-1/(d+4)}$ then

$$\mathbf{E}(||f_n - f||) \le Cn^{-2/(d+4)}.$$

TOO SLOW.

回 と く ヨ と く ヨ と

Model selection for density estimation

We wish to estimate a density f on \mathbb{R}^d

白 と く ヨ と く ヨ と …

We wish to estimate a density f on \mathbb{R}^d that belongs to a parametric family, \mathcal{F}_k , where k is unknown,

ヨット イヨット イヨッ

We wish to estimate a density f on \mathbb{R}^d that belongs to a parametric family, \mathcal{F}_k , where k is unknown, but $\mathcal{F}_k \subset \mathcal{F}_{k+1}$ for all k.

白 と く ヨ と く ヨ と …

We wish to estimate a density f on \mathbb{R}^d that belongs to a parametric family, \mathcal{F}_k , where k is unknown, but $\mathcal{F}_k \subset \mathcal{F}_{k+1}$ for all k.

$$\mathcal{F} = \bigcup_{k \ge 1} \mathcal{F}_k.$$

白 と く ヨ と く ヨ と …

We wish to estimate a density f on \mathbb{R}^d that belongs to a parametric family, \mathcal{F}_k , where k is unknown, but $\mathcal{F}_k \subset \mathcal{F}_{k+1}$ for all k.

$$\mathcal{F} = \bigcup_{k \ge 1} \mathcal{F}_k.$$

the complexity associated with f is defined as

$$k^* = \min\{k \ge 1 : f \in \mathcal{F}_k\}.$$

伺 と く き と く き と

\mathcal{F}_k

is the set of mixtures of d dimensional normal densities, where the number of components is at most k

(4回) (1日) (日)

We wish to introduce an estimate k_n of the complexity k^* and

・ロト ・回ト ・ヨト ・ヨト

・日・ ・ヨ・ ・ヨ・

・ 回 と ・ ヨ と ・ ヨ と …

 k_n → k^{*} almost surely (i.e., k_n = k^{*} almost surely, for all n large enough)

・回 ・ ・ ヨ ・ ・ ヨ ・ ・

▲圖▶ ▲屋▶ ▲屋▶ ---

Biau, Devroye (2004)

回 と く ヨ と く ヨ と

Biau, Devroye (2004) k_n and \hat{f}_{k_n} via projection of the empirical measure with respect to the Yatracos class

回 と く ヨ と く ヨ と …

$$\mathbb{E}\left\{\left\|\hat{f}_{k_n}-f\right\|\right\}=O\left(\frac{1}{\sqrt{n}}\right).$$

Biau, Devroye (2004) k_n and \hat{f}_{k_n} via projection of the empirical measure with respect to the Yatracos class too complex

向下 イヨト イヨト

Testing homogeneity

回 と く ヨ と く ヨ と

Two mutually independent samples

$$X_1,\ldots,X_n$$
 and X'_1,\ldots,X'_n

distributed according to unknown probability distributions μ and μ' on \mathbb{R}^d .

白 と く ヨ と く ヨ と

Two mutually independent samples

$$X_1,\ldots,X_n$$
 and X'_1,\ldots,X'_n

distributed according to unknown probability distributions μ and μ' on \mathbb{R}^d .

We are interested in testing the null hypothesis that the two samples are homogeneous, that is

$$\mathcal{H}_0: \mu = \mu'.$$

向下 イヨト イヨト

Two mutually independent samples

$$X_1,\ldots,X_n$$
 and X'_1,\ldots,X'_n

distributed according to unknown probability distributions μ and μ' on $\mathbb{R}^d.$

We are interested in testing the null hypothesis that the two samples are homogeneous, that is

$$\mathcal{H}_0: \mu = \mu'.$$

empirical probability distributions μ_n and μ'_n

ヨット イヨット イヨッ

Based on a partition $\mathcal{P}_n = \{A_{n1}, \ldots, A_{nm_n}\}$ of \mathbb{R}^d , we let the test statistic be defined as

$$T_n = \sum_{j=1}^{m_n} |\mu_n(A_{nj}) - \mu'_n(A_{nj})|.$$

▲□→ ▲ □→ ▲ □→

Theorem. Under \mathcal{H}_0 , for all $0 < \varepsilon < 2$,

$$\mathbb{P}\{T_n > \varepsilon\} = e^{-n(g_T(\varepsilon) + o(1))},$$

as $n \to \infty$,

(1日) (日) (日)

3

Theorem. Under \mathcal{H}_0 , for all $0 < \varepsilon < 2$,

$$\mathbb{P}\{T_n > \varepsilon\} = e^{-n(g_T(\varepsilon) + o(1))},$$

as $n \to \infty$, where

$$g_{\mathcal{T}}(\varepsilon) = (1 + \varepsilon/2) \ln(1 + \varepsilon/2) + (1 - \varepsilon/2) \ln(1 - \varepsilon/2) \approx \varepsilon^2/4.$$

(Biau, Györfi (2005))

回 と く ヨ と く ヨ と …

A strong consistent test

Corollary. Consider the test which rejects \mathcal{H}_0 when

$$T_n > 2\sqrt{\ln 2}\sqrt{\frac{m_n}{n}}.$$

白 と く ヨ と く ヨ と …

A strong consistent test

Corollary. Consider the test which rejects \mathcal{H}_0 when

$$T_n > 2\sqrt{\ln 2}\sqrt{\frac{m_n}{n}}.$$

Assume that

$$\lim_{n\to\infty}\frac{m_n}{n}=0 \quad \text{and} \quad \lim_{n\to\infty}\frac{m_n}{\ln n}=\infty.$$

回 と く ヨ と く ヨ と

A strong consistent test

Corollary. Consider the test which rejects \mathcal{H}_0 when

$$T_n > 2\sqrt{\ln 2}\sqrt{\frac{m_n}{n}}.$$

Assume that

$$\lim_{n \to \infty} \frac{m_n}{n} = 0 \quad \text{and} \quad \lim_{n \to \infty} \frac{m_n}{\ln n} = \infty.$$

Then, under \mathcal{H}_0 , after a random sample size the test makes a.s. no error.

白 と く ヨ と く ヨ と …

Corollary. Consider the test which rejects \mathcal{H}_0 when

$$T_n > 2\sqrt{\ln 2}\sqrt{\frac{m_n}{n}}.$$

Assume that

$$\lim_{n\to\infty}\frac{m_n}{n}=0 \quad \text{and} \quad \lim_{n\to\infty}\frac{m_n}{\ln n}=\infty.$$

Then, under \mathcal{H}_0 , after a random sample size the test makes a.s. no error.

Moreover, if $\mu \neq \mu'$, and for each sphere S centered at the origin

$$\lim_{n\to\infty}\max_{j:A_{n,j}\cap S\neq\emptyset}diam(A_{n,j})=0$$

通 とう ほう う ほうし

Corollary. Consider the test which rejects \mathcal{H}_0 when

$$T_n > 2\sqrt{\ln 2}\sqrt{\frac{m_n}{n}}.$$

Assume that

$$\lim_{n\to\infty}\frac{m_n}{n}=0 \quad \text{and} \quad \lim_{n\to\infty}\frac{m_n}{\ln n}=\infty.$$

Then, under \mathcal{H}_0 , after a random sample size the test makes a.s. no error.

Moreover, if $\mu \neq \mu'$, and for each sphere S centered at the origin

$$\lim_{n\to\infty}\max_{j:A_{n,j}\cap S\neq\emptyset}diam(A_{n,j})=0$$

then after a random sample size the test makes a.s. no error. (Biau, Györfi (2005))

通 とう ほう う ほうし

Split the sample into two subsamples:

 $\{X_1,\ldots,X_n\}$ and $\{X'_1,\ldots,X'_n\}=\{X_{n+1},\ldots,X_{2n}\}.$

(本部) (本語) (本語) (語)

Split the sample into two subsamples:

$$\{X_1,\ldots,X_n\}$$
 and $\{X'_1,\ldots,X'_n\}=\{X_{n+1},\ldots,X_{2n}\}.$

Let $\mathcal{P}_n = \{A_{nj} : j \ge 1\}$ be a cubic partition of \mathbb{R}^d with volume h_n^d .

回 と く ヨ と く ヨ と

Split the sample into two subsamples:

$$\{X_1,\ldots,X_n\}$$
 and $\{X'_1,\ldots,X'_n\}=\{X_{n+1},\ldots,X_{2n}\}.$

Let $\mathcal{P}_n = \{A_{nj} : j \ge 1\}$ be a cubic partition of \mathbb{R}^d with volume h_n^d . Introduce the statistic

$$d_{n,k} = \inf_{g \in \mathcal{F}_k} \sum_{A \in \mathcal{P}_n} \left| \int_A g - \mu_{2n}(A) \right|.$$

白 と く ヨ と く ヨ と …

Split the sample into two subsamples:

$$\{X_1,\ldots,X_n\}$$
 and $\{X'_1,\ldots,X'_n\}=\{X_{n+1},\ldots,X_{2n}\}.$

Let $\mathcal{P}_n = \{A_{nj} : j \ge 1\}$ be a cubic partition of \mathbb{R}^d with volume h_n^d . Introduce the statistic

$$d_{n,k} = \inf_{g \in \mathcal{F}_k} \sum_{A \in \mathcal{P}_n} \left| \int_A g - \mu_{2n}(A) \right|.$$

Let the threshold be

$$T_n = \sum_{A \in \mathcal{P}_n} |\mu_n(A) - \mu'_n(A)|.$$

御 と く ぼ と く ほ と …

Split the sample into two subsamples:

$$\{X_1,\ldots,X_n\}$$
 and $\{X'_1,\ldots,X'_n\}=\{X_{n+1},\ldots,X_{2n}\}.$

Let $\mathcal{P}_n = \{A_{nj} : j \ge 1\}$ be a cubic partition of \mathbb{R}^d with volume h_n^d . Introduce the statistic

$$d_{n,k} = \inf_{g \in \mathcal{F}_k} \sum_{A \in \mathcal{P}_n} \left| \int_A g - \mu_{2n}(A) \right|.$$

Let the threshold be

$$T_n = \sum_{A \in \mathcal{P}_n} |\mu_n(A) - \mu'_n(A)|.$$

Estimate of k^* :

$$k_n = \min\{k \ge 1 : d_{n,k} \le T_n\}.$$

通 とう ほう う ほうし

Assume that, for each $k \ge 1$, \mathcal{F}_k is closed with respect to the weak convergence topology.

▲□→ ▲ □→ ▲ □→

Assume that, for each $k \ge 1$, \mathcal{F}_k is closed with respect to the weak convergence topology.

Then there exists a positive constant κ , depending on f, such that

$$\mathbb{P}\left\{k_n \neq k^*\right\} \leq \exp\left(-\kappa h_n^{-d}\right),$$

個 と く ヨ と く ヨ と …

Assume that, for each $k \ge 1$, \mathcal{F}_k is closed with respect to the weak convergence topology.

Then there exists a positive constant κ , depending on f, such that

$$\mathbb{P}\left\{k_n \neq k^*\right\} \leq \exp\left(-\kappa h_n^{-d}\right),\,$$

and consequently, for the choice $h_n = n^{-\delta}$ with $0 < \delta < 1/d$,

$$k_n = k^*$$

almost surely, for all *n* large enough. (Biau, Cadre, Devroye, Györfi (2008))

ヨット イヨット イヨッ

Fast density estimate

Fix $k \ge 1$ and introduce the (Yatracos) class of sets

$$\mathcal{A}_k = \{\{x: g_1(x) > g_2(x)\}: g_1, g_2 \in \mathcal{F}_k\}$$

白 と く ヨ と く ヨ と

Fast density estimate

Fix $k \ge 1$ and introduce the (Yatracos) class of sets

$$\mathcal{A}_k = \big\{ \{x: g_1(x) > g_2(x)\} : g_1, g_2 \in \mathcal{F}_k \big\}$$

and the goodness criterion for a density $g \in \mathcal{F}_k$:

$$\Delta_k(g) = \sup_{A \in \mathcal{A}_k} \bigg| \int_A g - \mu_{2n}(A) \bigg|.$$

向下 イヨト イヨト

Fast density estimate

Fix $k \ge 1$ and introduce the (Yatracos) class of sets

$$\mathcal{A}_k = \big\{ \{x: g_1(x) > g_2(x)\} : g_1, g_2 \in \mathcal{F}_k \big\}$$

and the goodness criterion for a density $g \in \mathcal{F}_k$:

$$\Delta_k(g) = \sup_{A \in \mathcal{A}_k} \bigg| \int_A g - \mu_{2n}(A) \bigg|.$$

The minimum distance estimate \hat{f}_k minimizes the criterion $\Delta_k(g)$ over all g in \mathcal{F}_k .

伺下 イヨト イヨト

Fix $k \ge 1$ and introduce the (Yatracos) class of sets

$$\mathcal{A}_k = \big\{ \{x: g_1(x) > g_2(x)\} : g_1, g_2 \in \mathcal{F}_k \big\}$$

and the goodness criterion for a density $g \in \mathcal{F}_k$:

$$\Delta_k(g) = \sup_{A \in \mathcal{A}_k} \bigg| \int_A g - \mu_{2n}(A) \bigg|.$$

The minimum distance estimate \hat{f}_k minimizes the criterion $\Delta_k(g)$ over all g in \mathcal{F}_k . The density estimate is \hat{f}_{k_n} .

伺 と く き と く き と

If \mathcal{A}_{k^*} has finite Vapnik-Chervonenkis dimension

・ロン ・雪 と ・ ヨ と ・ ヨ と ・

If \mathcal{A}_{k^*} has finite Vapnik-Chervonenkis dimension then

$$\mathbb{E}\left\{\left\|\hat{f}_{k_n}-f\right\|\right\}=\mathsf{O}\left(\frac{1}{\sqrt{n}}\right).$$

If \mathcal{A}_{k^*} has finite Vapnik-Chervonenkis dimension then

$$\mathbb{E}\left\{\left\|\hat{f}_{k_n}-f\right\|\right\}=O\left(\frac{1}{\sqrt{n}}\right).$$

(Biau, Devroye (2004))

・ 回 ト ・ ヨ ト ・ ヨ ト

The projection with respect to the Yatracos class is too complex.

白 ト イヨト イヨト

The projection with respect to the Yatracos class is too complex. For a kernel function K and bandwidth r > 0, let f_{2n} be the kernel density estimate with sample size 2n:

$$f_{2n}(x) = \frac{1}{2nr^d} \sum_{i=1}^{2n} K\left(\frac{x-X_i}{r}\right).$$

回 と く ヨ と く ヨ と

The projection with respect to the Yatracos class is too complex. For a kernel function K and bandwidth r > 0, let f_{2n} be the kernel density estimate with sample size 2n:

$$f_{2n}(x) = \frac{1}{2nr^d} \sum_{i=1}^{2n} K\left(\frac{x - X_i}{r}\right)$$

let $K_r * g$ be the expectation of the kernel estimate with density g:

$$K_r * g(x) = \frac{1}{r^d} \int K\left(\frac{x-z}{r}\right) g(z) dz.$$

伺 とう きょう とう とう

The projection with respect to the Yatracos class is too complex. For a kernel function K and bandwidth r > 0, let f_{2n} be the kernel density estimate with sample size 2n:

$$f_{2n}(x) = \frac{1}{2nr^d} \sum_{i=1}^{2n} K\left(\frac{x - X_i}{r}\right)$$

let $K_r * g$ be the expectation of the kernel estimate with density g:

$$K_r * g(x) = \frac{1}{r^d} \int K\left(\frac{x-z}{r}\right) g(z) dz.$$

the estimate \overline{f}_n is defined as

$$\bar{f}_n = \operatorname*{arg\,min}_{g \in \mathcal{F}_{k_n}} \| K_r * g - f_{2n} \|,$$

向下 イヨト イヨト

The projection with respect to the Yatracos class is too complex. For a kernel function K and bandwidth r > 0, let f_{2n} be the kernel density estimate with sample size 2n:

$$f_{2n}(x) = \frac{1}{2nr^d} \sum_{i=1}^{2n} K\left(\frac{x - X_i}{r}\right)$$

let $K_r * g$ be the expectation of the kernel estimate with density g:

$$K_r * g(x) = \frac{1}{r^d} \int K\left(\frac{x-z}{r}\right) g(z) dz.$$

the estimate \overline{f}_n is defined as

$$\bar{f}_n = \operatorname*{arg\,min}_{g \in \mathcal{F}_{k_n}} \| K_r * g - f_{2n} \|,$$

 \overline{f}_n is an L_1 -projection of the kernel density estimate f_{2n} with fixed bandwidth r.

< 注→

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k\geq 1.$

・ロン ・聞と ・ほと ・ほと

3

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k \ge 1$. Choose k_n as before

・ 回 ト ・ ヨ ト ・ ヨ ト

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k \geq 1$. Choose k_n as before such that the bandwidth is $h = h_n = (\ln n)^{-(1+\delta)/d}$ with $\delta > 0$

▲圖▶ ▲屋▶ ▲屋▶ ---

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k \ge 1$. Choose k_n as before such that the bandwidth is $h = h_n = (\ln n)^{-(1+\delta)/d}$ with $\delta > 0$ Choose the kernel function K such that it is a density function and its characteristic function is everywhere non-zero.

向下 イヨト イヨト

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k \ge 1$. Choose k_n as before such that the bandwidth is $h = h_n = (\ln n)^{-(1+\delta)/d}$ with $\delta > 0$ Choose the kernel function K such that it is a density function and its characteristic function is everywhere non-zero. Suppose that

$$\sup_{g\in\mathcal{F}_{k^*}}\frac{\|g-f\|}{\|K_r*g-K_r*f\|}<\infty,$$

į

向下 イヨト イヨト

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k \ge 1$. Choose k_n as before such that the bandwidth is $h = h_n = (\ln n)^{-(1+\delta)/d}$ with $\delta > 0$ Choose the kernel function K such that it is a density function and its characteristic function is everywhere non-zero. Suppose that

$$\sup_{g \in \mathcal{F}_{k^*}} \frac{\|g - f\|}{\|K_r * g - K_r * f\|} < \infty,$$
$$\int \sqrt{f} < \infty$$

and

伺 とう ヨン うちょう

Assume that \mathcal{F}_k is closed in the weak convergence topology for every $k \ge 1$. Choose k_n as before such that the bandwidth is $h = h_n = (\ln n)^{-(1+\delta)/d}$ with $\delta > 0$ Choose the kernel function K such that it is a density function and its characteristic function is everywhere non-zero. Suppose that

$$\sup_{g\in\mathcal{F}_{k^*}}\frac{\|g-f\|}{\|K_r*g-K_r*f\|}<\infty,$$

and

$$\int \sqrt{f} < \infty.$$

Then

$$\mathbf{E}\left\{\left\|\bar{f}_n-f\right\|\right\} \leq O\left(\frac{1}{\sqrt{n}}\right).$$

向下 イヨト イヨト

Let f be the density of a multidimensional normal distribution.

・ 回 と ・ ヨ と ・ ヨ と

Let f be the density of a multidimensional normal distribution. Find the optimal density estimate in L_1 .

個 と く ヨ と く ヨ と …

Let f be the density of a multidimensional normal distribution. Find the optimal density estimate in L_1 .

$$\min_{f_n} \mathbf{E} \| f_n - f \|$$

個 と く ヨ と く ヨ と …

Let f be the density of a multidimensional normal distribution. Find the optimal density estimate in L_1 .

$$\min_{f_n} \mathbf{E} \| f_n - f \|$$

The plug-in estimate is not optimal.

向下 イヨト イヨト