

# Nonparametric regression estimation

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a.s.

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$h_n$  should be "small"

$nh_n^d$  should be "large"

$$\bar{m}_n(x) = \frac{\sum_{i=1}^n m(X_i) I_{\{\|X_i - x\| \leq h\}}}{\sum_{i=1}^n I_{\{\|X_i - x\| \leq h\}}}$$

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Error decomposition

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Variation

$$m_n(x) - \bar{m}_n(x) = \frac{\sum_{i=1}^n (Y_i - m(X_i)) I_{\{\|X_i - x\| \leq h\}}}{\sum_{i=1}^n I_{\{\|X_i - x\| \leq h\}}}$$

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Bias

$$\bar{m}_n(x) - m(x) \approx \frac{\sum_{i=1}^n (m(X_i) - m(x)) I_{\{\|X_i - x\| \leq h\}}}{\sum_{i=1}^n I_{\{\|X_i - x\| \leq h\}}}$$

$$\mathbf{E} \left\{ \left( \frac{\sum_{i=1}^n (Y_i - m(X_i)) I_{\{\|X_i - x\| \leq h\}}}{\sum_{i=1}^n I_{\{\|X_i - x\| \leq h\}}} \right)^2 \right\}$$

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if  $nh_n^d \rightarrow \infty$ .

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$$|m(x) - m(z)| \leq C\|x - z\|$$



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if  $h = h_n \rightarrow 0$ .

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Nonparametric features:

- construction of the estimate
- consistency

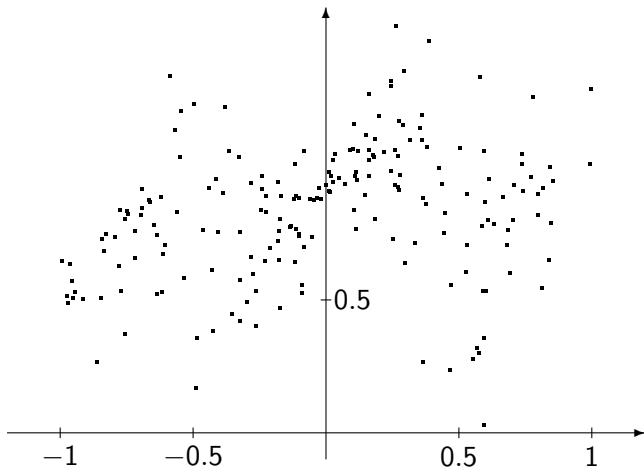
## Definition

The estimator  $m_n$  is called **weakly universally consistent** if

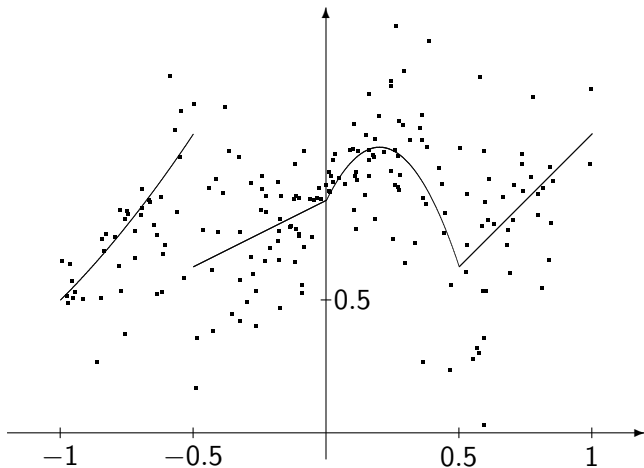
$$\mathbf{E} \{ (m(X) - m_n(X))^2 \} \rightarrow 0$$

for all distributions of  $(X, Y)$  with  $\mathbf{E}Y^2 < \infty$ .

# Simulated data points.



# Data points and regression function.





Stone (1977)

$$m_n(x) = \sum_{i=1}^n W_{ni}(x; X_1, \dots, X_n) Y_i.$$

## $k$ -nearest neighbor estimate

$W_{ni}$  is  $1/k$  if  $X_i$  is one of the  $k$  nearest neighbors of  $x$  among  $X_1, \dots, X_n$ , and  $W_{ni}$  is 0 otherwise.

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$$(X_1, Y_1), \dots, (X_n, Y_n)$$

## $k$ -nearest neighbor estimate

$W_{ni}$  is  $1/k$  if  $X_i$  is one of the  $k$  nearest neighbors of  $x$  among  $X_1, \dots, X_n$ , and  $W_{ni}$  is 0 otherwise. Formally

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### Theorem

*If  $k_n \rightarrow \infty$ ,  $k_n/n \rightarrow 0$  then the  $k$ -nearest neighbor estimate is weakly universally consistent.*

# Nearest neighbor estimate

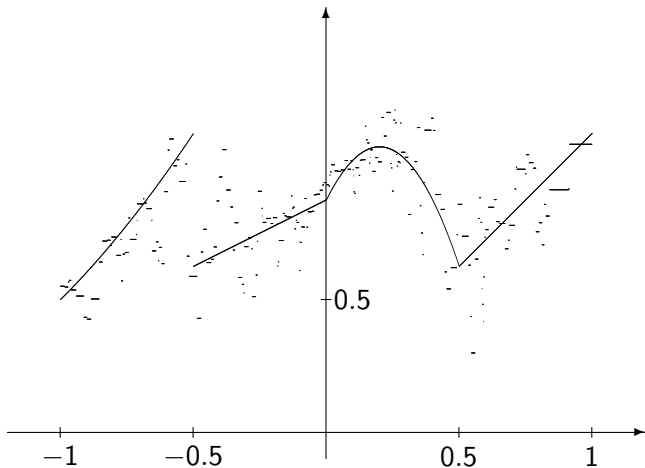


Figure: Undersmoothing:  $k_n = 3$ ,  $L_2$  error = 0.011703.



# Nearest neighbor estimate

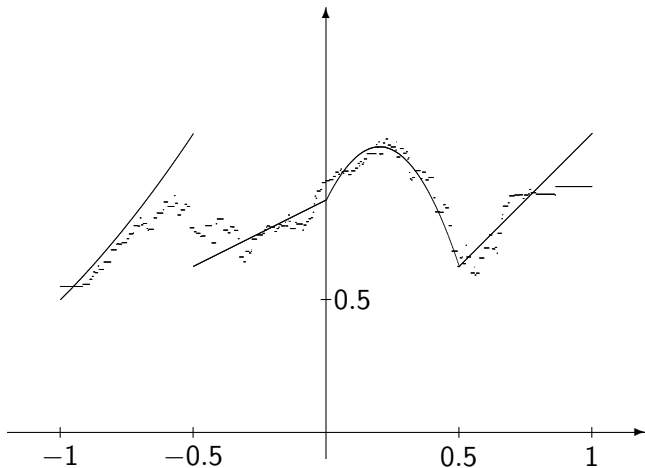


Figure: Good choice:  $k_n = 12$ ,  $L_2$  error = 0.004247.

# Nearest neighbor estimate

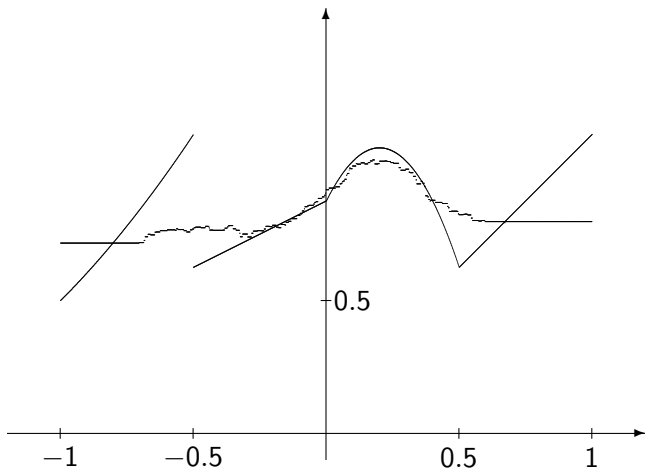


Figure: Oversmoothing:  $k_n = 50$ ,  $L_2$  error = 0.009931.

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## Theorem

*For cubic partition, if*

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

*and*

$$\lim_{n \rightarrow \infty} n h_n^d \rightarrow \infty$$

*then the partitioning estimate is weakly universally consistent.*

# Partitioning estimate

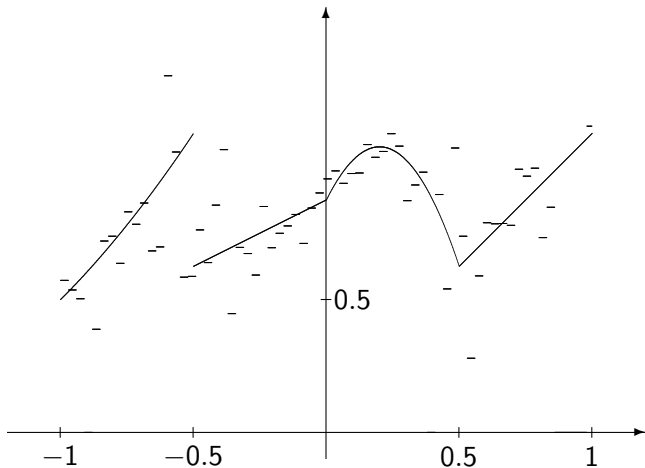


Figure: Undersmoothing:  $h = 0.03$ ,  $L_2$  error = 0.062433.



# Partitioning estimate

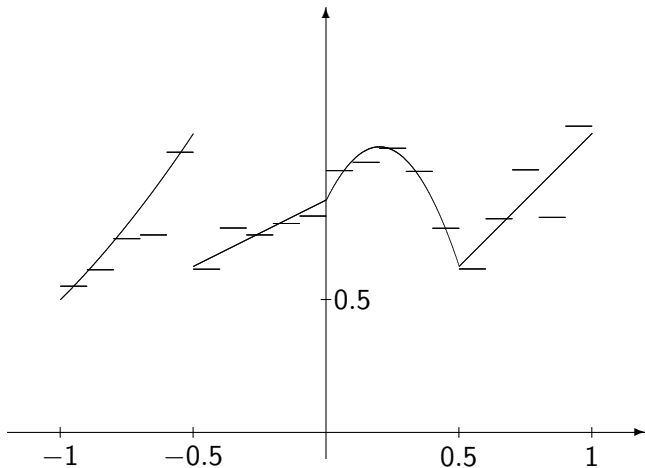


Figure: Good choice:  $h = 0.1$ ,  $L_2$  error = 0.003642.

# Partitioning estimate

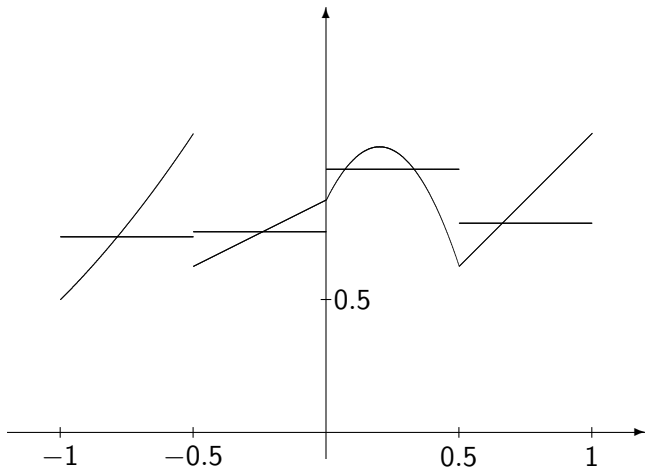


Figure: Oversmoothing:  $h = 0.5$ ,  $L_2$  error = 0.013208.

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## Theorem

*If  $h_n \rightarrow 0$ ,  $nh_n^d \rightarrow \infty$  then under some conditions on  $K$  the kernel estimate is weakly universally consistent.*

# Kernel estimate

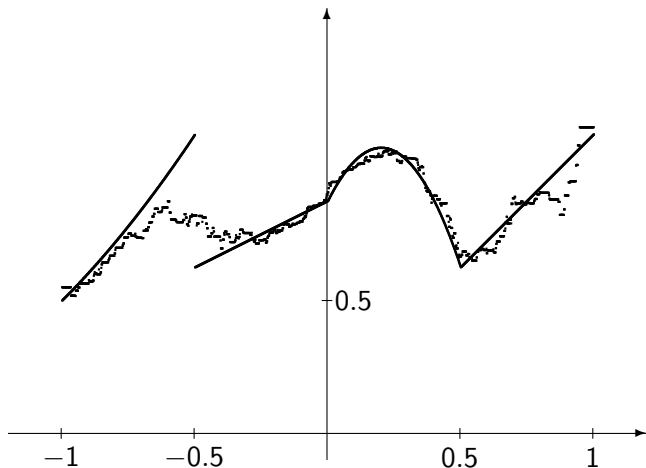


Figure: Kernel estimate for the naive kernel:  $h = 0.1$ ,  $L_2$  error = 0.004066.

# Least squares estimates

Regression problem

$$\min_f \mathbf{E}\{(Y - f(X))^2\}$$



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the class  $\mathcal{F}_n$  grows slowly as  $n$  grows

# Least squares estimates

Examples for  $\mathcal{F}_n$ :

- polynomials
- splines
- neural networks
- radial basis functions

*Springer Series in Statistics*

László Györfi Michael Kohler  
Adam Krzyżak Harro Walk

# A Distribution- Free Theory of Nonparametric Regression



Springer



# Prediction of time series: squared loss

László (Laci) Györfi<sup>1</sup>

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August 27, 2012

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[www.cs.bme.hu/~gyorfi](http://www.cs.bme.hu/~gyorfi)

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After  $n$  time instant the empirical squared error

$$L_n(g) = \frac{1}{n} \sum_{i=1}^n (g_i(X_1^i, Y_1^{i-1}) - Y_i)^2.$$



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$$L^* = \mathbf{E}\{(Y_0 - \mathbf{E}\{Y_0 \mid X_{-\infty}^0, Y_{-\infty}^{-1}\})^2\}$$

is the minimal mean squared error of any prediction for the value of  $Y_0$  based on the infinite past  $X_{-\infty}^0, Y_{-\infty}^{-1}$ .

there are universally consistent prediction sequence  $g_n$ :

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Such prediction sequence is called **universally consistent**.



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Then the local averaging prediction of the expert  $(k, \ell)$  is the average of  $y_i$ 's if  $i \in J_n^{(k, \ell)}$ :

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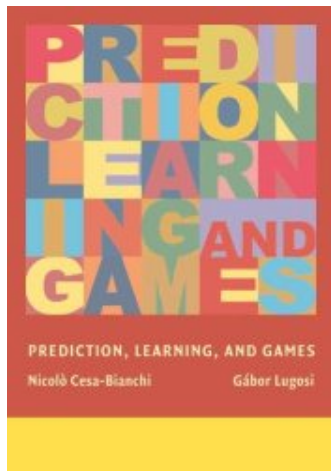
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The problem is how to choose  $k$ ,  $r_{k, \ell} > 0$  and  $r'_{k, \ell} > 0$  in a data dependent way.



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Then the combined prediction

$$g_t(x_1^t, y_1^{t-1}) = \sum_{k,\ell=1}^{\infty} p_{t,k,\ell} h^{(k,\ell)}(x_1^t, y_1^{t-1}) .$$

**Theorem.** (Györfi, Lugosi (2001)) If  $|Y_0| \leq B$ , then the combined predictor  $g$  is universally consistent.

# Expert Lemma

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with  $c \geq 8B^2$ , and

$$v_{t,k} = \frac{w_{t,k}}{\sum_{i=1}^{\infty} w_{t,i}}.$$



# Expert Lemma

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then for every  $n \geq 1$ ,

$$L_n(\tilde{g}) \leq \inf_k \left( L_n(\tilde{h}_k) - \frac{c \ln q_k}{n} \right).$$

Introduce

$$W_1 = 1$$

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$$W_{t+1} = \sum_{k=1}^{\infty} w_{t,k} e^{-(y_t - \tilde{h}_k(x_1^t, y_1^{t-1}))^2 / c} = W_t \sum_{k=1}^{\infty} v_{t,k} e^{-(y_t - \tilde{h}_k(x_1^t, y_1^{t-1}))^2 / c},$$

so that

$$-c \ln \frac{W_{t+1}}{W_t} = -c \ln \left( \sum_{k=1}^{\infty} v_{t,k} e^{-(y_t - \tilde{h}_k(x_1^t, y_1^{t-1}))^2 / c} \right).$$

so that

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Introduce the function

$$F_t(z) = e^{-(y_t - z)^2 / c}$$

so that

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Because of  $c \geq 8B^2$ , the function  $F_t$  is concave on  $[-B, B]$ , therefore Jensen's inequality implies that

$$\left[ \sum_{k=1}^{\infty} v_{t,k} \left( y_t - \tilde{h}_k(x_1^t, y_1^{t-1}) \right) \right]^2 \leq -c \ln \frac{W_{t+1}}{W_t}$$

Thus,

$$nL_n(\tilde{g}) = \sum_{t=1}^n (y_t - \tilde{g}(x_1^t, y_1^{t-1}))^2$$



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# Sketch of the proof of the Theorem

Because of the fundamental limit

$$\liminf_{n \rightarrow \infty} L_n(\mathbf{g}) \geq \lim_{n \rightarrow \infty} L_n(\mathbf{g}^*) = L^* \quad \text{a.s.}$$



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Because of the fundamental limit

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it is enough to show that

$$\limsup_{n \rightarrow \infty} L_n(\mathbf{g}) \leq L^* \quad \text{a.s.}$$

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$$L_n(g) \leq \inf_{k,\ell} \left( L_n(h^{(k,\ell)}) - \frac{c \ln q_{k,\ell}}{n} \right),$$

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# Pattern recognition

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# Decision problem

$Y \in \{1, 2, \dots, M\}$  valued

$X$  feature vector

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Probability of error:

$$P(g(X) \neq Y).$$

Problem: find

$$\min_g P(g(X) \neq Y).$$

# Bayes decision

a posteriori probability

$$P_i(x) = \mathbf{P}\{Y = i|X = x\}.$$

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$L^*$  Bayes error

## Lemma

For any decision  $g$ ,

$$L^* := \mathbf{P}\{g^*(X) \leq Y\} \leq \mathbf{P}\{g(X) \neq Y\}.$$

$$\mathbf{P}\{g(X) \neq Y\} = \mathbf{E}\{\mathbf{P}\{g(X) \neq Y \mid X\}\}$$

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$\tilde{P}_i(x)$  approximations of  $P_i(x)$



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Lemma

$$\mathbf{P}\{g(X) \neq Y\} - L^* \leq \sum_{j=1}^M \mathbf{E}\{|P_j(X) - \tilde{P}_j(X)|\}.$$

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If  $g^*(X) = g(X)$  then

$$\mathbf{P}\{g(X) \neq Y \mid X\} - \mathbf{P}\{g^*(X) \neq Y \mid X\} = 0$$

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Data:  $(X_1, Y_1), \dots, (X_n, Y_n)$

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$$g_n(x) = g_n((X_1, Y_1), \dots, (X_n, Y_n), x).$$

## Definition

The classifier  $g_n$  is called **weakly universally consistent** if

$$P(g_n(X) \neq Y) \rightarrow L^*$$

for all distributions of  $(X, Y)$ .



# Local majority voting

the a posteriori probabilities

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$$\begin{aligned} \mathbf{P}\{g(X) \neq Y\} - L^* &\leq \sum_{j=1}^M \mathbf{E}\{|P_j(X) - \tilde{P}_{n,j}(X)|\} \\ &\leq \sum_{j=1}^M \sqrt{\mathbf{E}\{|P_j(X) - \tilde{P}_{n,j}(X)|^2\}}. \end{aligned}$$

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## Theorem

*The *k*-NN rule and the partitioning rule and the kernel rule are strongly universally consistent.*



# Empirical error minimization

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Examples for  $\mathcal{G}_n$ :

- polynomial classifiers
- tree classifiers
- neural networks classifiers
- radial basis functions classifiers

**Applications of Mathematics**  
Stochastic Modelling and Applied Probability

31

Luc Devroye  
László Györfi  
Gábor Lugosi

A Probabilistic Theory  
of Pattern Recognition



Springer

# Prediction of time series: 0 – 1 loss

László (Laci) Györfi<sup>1</sup>

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August 27, 2012

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After  $n$  round the empirical 0 – 1 error for  $X_1^n, Y_1^n$  is

$$R_n(f) = \frac{1}{n} \sum_{i=1}^n I_{\{f(X_1^i, Y_1^{i-1}) \neq Y_i\}},$$

i.e., the loss is the 0 – 1 loss, and  $R_n(f)$  is the relative frequency of errors.

# Dependent data: time series

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$$f_t^*(X_1^t, Y_1^{t-1}) = \begin{cases} 1 & \text{if } \mathbf{P}\{Y_t = 1 \mid X_1^t, Y_1^{t-1}\} > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

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Fundamental limit: for any classification strategy  $f$  and stationary ergodic process  $\{(X_n, Y_n)\}_{n=-\infty}^{\infty}$ ,

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there are universally consistent classifier sequence  $f_n$ :

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Such classifier sequence is called **universally consistent**.

## Theorem

Let  $g_t(X_1^t, Y_1^{t-1})$  be a universally consistent prediction scheme, for bounded  $Y$ , estimating the conditional probability

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Then  $f_t$  is a universally consistent classifier (Györfi, Lugosi (2001)).

# Martingale difference sequences

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## Definition

there are two sequences of random variables:

$$\{Z_n\} \quad \{X_n\}$$

- $Z_n$  is a function of  $X_1, \dots, X_n$ ,
- $\mathbf{E}\{Z_n \mid X_1, \dots, X_{n-1}\} = 0$  almost surely.

Then  $\{Z_n\}$  is called martingale difference sequence with respect to  $\{X_n\}$ .

## Chow Theorem:

# A strong law of large numbers

**Chow Theorem:** If  $\{Z_n\}$  is a martingale difference sequence with respect to  $\{X_n\}$  and

$$\sum_{n=1}^{\infty} \frac{\mathbf{E}\{Z_n^2\}}{n^2} < \infty$$

then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n Z_i = 0 \text{ a.s.}$$



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if, for example,  $\mathbf{E}\{Z_i^2\}$  is a bounded sequence.

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almost surely.

# Sketch of the proof of the Theorem

Because of the fundamental limit, we have to show that

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By the Plug-in Lemma,

$$\begin{aligned} |\bar{R}_n(f^*) - \bar{R}_n(f)| &\leq \frac{1}{n} \sum_{i=1}^n |g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\}| \\ &\leq \sqrt{\frac{1}{n} \sum_{i=1}^n |g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\}|^2} \end{aligned}$$



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Need

$$\frac{1}{n} \sum_{i=1}^n |g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\}|^2 \rightarrow 0 \quad \text{a.s.}$$

# Corollary

Let  $\{g_n\}$  be a sequence of universally consistent predictors for the class of stationary, ergodic processes with  $|Y| < B$ ,

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$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n (g_i(X_1^i, Y_1^{i-1}) - Y_i)^2 = L^*$$

a.s. for the class of stationary and ergodic sequences with  $|Y| < B$ .

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a.s. for the class of stationary and ergodic sequences with  $|Y| < B$ . Then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n (g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})^2 = 0$$

a.s.

## Decomposition

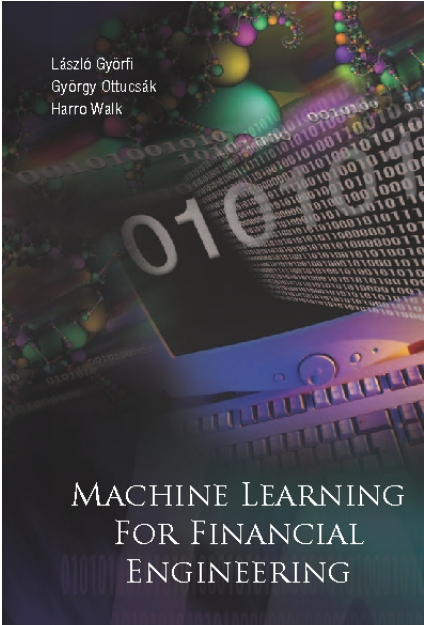
$$\begin{aligned} & (g_i(X_1^i, Y_1^{i-1}) - Y_i)^2 \\ = & (g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})^2 \\ & + 2(g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})(\mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\} - Y_i) \\ & + (\mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\} - Y_i)^2 \end{aligned}$$

## Decomposition

$$\begin{aligned}
 & (g_i(X_1^i, Y_1^{i-1}) - Y_i)^2 \\
 = & (g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})^2 \\
 & + 2(g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})(\mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\} - Y_i) \\
 & + (\mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\} - Y_i)^2
 \end{aligned}$$

Thus

$$\begin{aligned}
 & (g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})^2 \\
 = & (g_i(X_1^i, Y_1^{i-1}) - Y_i)^2 \\
 & - 2(g_i(X_1^i, Y_1^{i-1}) - \mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\})(\mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\} - Y_i) \\
 & - (\mathbf{E}\{Y_i \mid X_{-\infty}^i, Y_{-\infty}^{i-1}\} - Y_i)^2
 \end{aligned}$$



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