

# Least-Squares Regression for Non-stationary Designs

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<sup>1</sup>Joint work with E.Gobet (Polytechnique, CMAP) and G.Fort (Toulouse, IMT)

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All random variables are defined on  $(\Omega, \mathcal{A}, \mathbb{P})$ .



# The Question

Given a random vector  $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ , how to approximate a “regressor”  $f^*$  of  $Y$  given  $X$ ?

$$f^* \in \arg \min_{\{f: f \circ X \in L^2_{\mathbb{P}}\}} E[|f \circ X - Y|^2] \quad (1)$$

(so that  $f^* \circ X = E[Y|X]$  if  $Y \in L^2_{\mathbb{P}}$ ).

# Part I

## *A Theorem of Convergence for i.i.d. Samples*

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else  $(f^{*,k})_k$  with  $E[|f^{*,k} \circ X - Y|^2] \rightarrow_k \inf_{f \in \mathcal{F}} E[|f \circ X - Y|^2]$ .

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- **(I.i.d Design)**  $D_n := ((X_k, Y_k))_{k=1}^n$  an i.i.d. vector.  
 $(X_k, Y_k) \sim (X, Y)$ .
- **(LSR Strategy)** Given **data**  $D_n(\omega) = ((X_k(\omega), Y_k(\omega)))_{k=1}^n$

$$\hat{f}^*(\mathcal{F}, D_n(\omega)) \in \arg \min_{f \in \mathcal{F}} \frac{1}{n} \sum_{k=1}^n |f(X_k(\omega)) - Y_k(\omega)|^2. \quad (2)$$

# Heuristics



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- 1 By the Law of Large Numbers

$$\frac{1}{n} \sum_{k=1}^n |f(X_k(\omega)) - Y_k(\omega)|^2 \approx E[|f \circ X - Y|^2] \quad (3)$$

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- 2 Therefore, if  $N(f, \omega) = N$  is “uniform”

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{k=1}^n |f(X_k(\omega)) - Y_k(\omega)|^2 \approx \inf_{f \in \mathcal{F}} E|f \circ X - Y|^2. \quad (4)$$



*But are the “arg inf’s” close also?: the problem of generalization.*

# Remarks

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1. Within  $\mathcal{F}$ , one cannot do better than

$$\inf_{f \in \mathcal{F}} E|f \circ X - Y|^2 = \min_{\{f: f \circ X \in L^2_{\mathbb{P}}\}} E|f \circ X - Y|^2 =$$

$$\inf_{f \in \mathcal{F}} (E|f \circ X - Y|^2 - E|E[Y|X] - Y|^2) = \inf_{f \in \mathcal{F}} (E|f \circ X - E[Y|X]|^2) \quad (5)$$

(*approximation error*).

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- **Uniform concentration inequalities** (speed of convergence)

$$\mathbb{P}[\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{k=1}^n (|f \circ X_k - Y_k|^2 - E[|f \circ X_k - Y_k|^2]) \right| > \delta] \leq \epsilon(n, \delta). \quad (7)$$

$\epsilon(n, \delta) \rightarrow 0$  as  $n \rightarrow \infty$  for all  $\delta > 0$ .



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This leads to assumptions on the distribution of  $D_n$  and on  $\mathcal{F}$ .

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then

$$E \int |(\hat{f}^* I_{[\hat{f}^* \leq B]}(x)) - y|^2 d\mu_\infty(x, y) \leq C(\lambda) B^4 V_{\mathcal{F}} \frac{(1 + \log n)}{n} + \lambda \inf_{f \in \mathcal{F}} E |f \circ X - Y|^2. \quad (8)$$

$V_{\mathcal{F}} = VC$ - dimension associated to  $\mathcal{F}$ .

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$$\lim_n E|\hat{f}^* \circ X' - Y'|^2 = \inf_{f \in \mathcal{F}} E|f \circ X - Y|^2,$$

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(fix  $\lambda > 1$ , let  $n \rightarrow \infty$ , then let  $\lambda \rightarrow 1$ , then let  $B \rightarrow \infty$ ).

- ② **(Speed of Convergence)** If the elements of  $\mathcal{F}$  are bounded by  $B$ , it gives a function  $N(\epsilon)$  such that

$$0 \leq E|\hat{f}^* \circ X' - Y'|^2 - \inf_{f \in \mathcal{F}} E|f \circ X - Y|^2 < \epsilon$$

if  $n \geq N(\epsilon)$ .

(Fix  $\epsilon > 0$  and  $\lambda = \lambda(\epsilon) > 1$  such that

$$(\lambda(\epsilon) - 1) \inf_{f \in \mathcal{F}} E|f \circ X - Y|^2 < \epsilon/2).$$

## Part II

*What happens if  $(X_k, Y_k)_k$  is **not** an i.i.d. sequence?*

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consider  $X \sim \tilde{X} | [\tilde{X} \in \tilde{A}]$ :

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**Problem:** how do we efficiently approximate

$$E[f(X, E[Y|X])]$$

supposing the knowledge of the *conditional* probability measures

$$Q(A, x) = \mathbb{P}(Y \in A | X = x) = \mathbb{P}(Y \in A | \tilde{X} = x)?$$

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- (*Regression Step*) Use the approximation (*why?*)

$$E[Y|X = \cdot] \approx \hat{h}_\omega(\cdot) := \arg \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{k=1}^n |X_k(\omega) - Y_k(\omega)|^2. \quad (9)$$

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- Use the approximation (**why?**)

$$Ef(X, E[Y|X]) \approx \frac{1}{n} \sum_{k=1}^n f(X_k(\omega), \hat{h}_\omega(X_k(\omega))). \quad (10)$$

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- For the *regression step*:

**(Contribution)** *Generalize [GKKM03], Theorem 11.5 using  $\beta$ -mixing coefficients associated to  $(X_k, Y_k)_k$ .*

**Definition ( $\beta$ -mixing Coefficients.)**

For sub sigma-algebras  $\mathcal{A}_1$  and  $\mathcal{A}_2$  of  $\mathcal{A}$ ,

$$BETA(\mathcal{A}_1, \mathcal{A}_2) = E\left[ \sup_{A_2 \in \mathcal{A}_2} |\mathbb{P}(A_2) - \mathbb{P}[A_2 | \mathcal{A}_1]| \right]. \quad (11)$$



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- $\rho_k$  the distribution of  $(X_k, Y_k)$ .  $\mu_n := (\rho_1 + \dots + \rho_n)/n$ .
- $I_1, \dots, I_L$  a fixed (arbitrary) **partition** of  $\{1, \dots, n\}$ ,  $|I_k| \leq |I_{k+1}|$ .

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- $\beta(k, j) := \text{BETA}(\sigma((X_{j'}, Y_{j'})_{j' \in I_k \cap \{1:j-1\}}), \sigma(X_j, Y_j))$ : the  $\beta$ -mixing coefficient between time  $j$  and its past **within**  $I_k$ .

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- $\mathcal{F}$  a family of functions with associated VC dimension  $V_{\mathcal{F}}$ .



## Theorem (A Rate of Convergence for LSR with bounded Response)

*In the setting of the previous slide, let*

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then

$$E \int |\hat{f}^* I_{[\hat{f}^* \leq B]}(x) - y|^2 d\mu_n(x, y) \leq C(\lambda) B^4 V_{\mathcal{F}} \frac{(1 + \log L + \log |I_1|)}{|I_1|} +$$

$$8B^2(\lambda + 1) \sum_{k=1}^L \sum_{j \in I_k} \beta(k, j) + \lambda \inf_{f \in \mathcal{F}} \int |f(x) - y|^2 d\mu_n.$$

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Here  $\beta(k, j) = 0$  for every  $k, j$ . We get, as before, the convergence (up to a exchange of limits)

$$E \int |\hat{f}^*(x) - y|^2 d\mu_n(x, y) - \inf_{f \in \mathcal{F}} \int |f(x) - y|^2 d\mu_n(x, y) \rightarrow_{n \rightarrow \infty} 0,$$

with speed  $(\sup_{(f, x) \in \mathcal{F} \times \mathbb{R}^d} |f(x)| \leq B)$

$$C(\lambda) V_{\mathcal{F}} B^4 \frac{(1 + \log n)}{n}.$$

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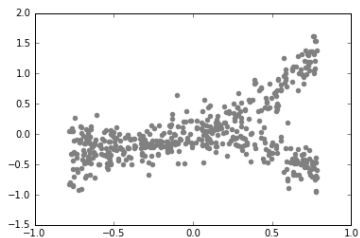
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$D_{n_k} = n_k$  independent copies of  $(X, Y^{(k)})$ .

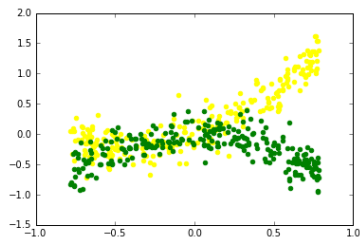


## Unclassified Data



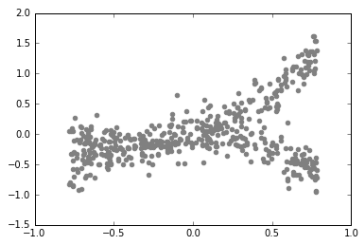
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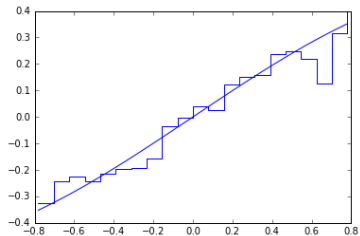


$$D_{n_1}, D_{n_2}$$

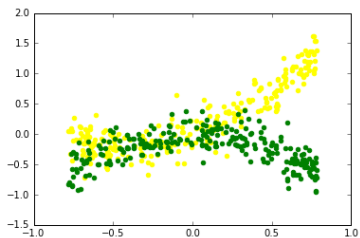
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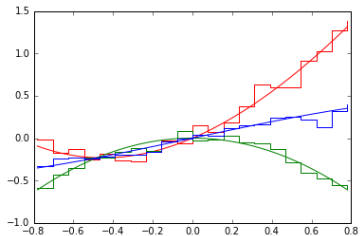
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## Classified Data



$$D_{n_1}, D_{n_2}$$



(The blue empirical approximation is at least “as good” as the other ones).

Note:



**Note:** Here  $n_1 = n_{-1}$ , and  $\hat{f}_B$  is an estimator of

$$E[Y|X] = \frac{1}{2}(E[Y^{(-1)}|X] + E[Y^{(1)}|X]).$$

where

- $Y := Y^{(-1)}I_{[R=-1]} + Y^{(1)}I_{[R=1]}$ .
- $R = \text{Rademacher}$  (independent from data).

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Indeed:

$$\inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{(X_k, Y_k) \in D_{n_{-1}} \cup D_{n_1}} E|f \circ X_k - Y_k|^2 =$$

$$\inf_{f \in \mathcal{F}} \frac{1}{2} (E|f \circ X - Y^{(-1)}|^2 + E|f \circ X - Y^{(1)}|^2) = \inf_{f \in \mathcal{F}} E|f \circ X - Y|^2.$$

# Exponentially Mixing Sequences

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**Recap:** Convergence of LSR for bounded  $Y$  with speed

$$C(\lambda)B^4V_{\mathcal{F}}\frac{(1 + \log L + \log |I_1|)}{|I_1|} + 8B^2(\lambda + 1)\sum_{k=1}^L\sum_{j \in I_k}\beta(k, j).$$

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**Exercise:** Assume the *(sub)exponential mixing condition*

$$\beta(\sigma((X_{j'}, Y_{j'})_{j' \leq j}), \sigma((X_{j+k}, Y_{j+k}))) \leq ae^{-ck}, \quad (a, c) \in [0, \infty) \times (0, \infty) \quad (12)$$

and consider the partition  $I_1, \dots, I_L$  of  $\{1, \dots, n\}$  where

$$L = \left\lceil \left(1 + \frac{1}{c}\right) \log n \right\rceil, \quad I_k := \{jL + k\}_{j=0}^{m-1}$$

for  $0 \leq k < L$  (adjust the necessary details) to prove the following:

## Theorem (Rate of convergence of LSR for Exponential Mixing Sequences)

Under (12) (and the rest of our working hypotheses):

$$E \int |\hat{f}^* I_{[\hat{f}^* \leq B]}(x) - y|^2 d\mu_n(x, y) \leq C(\lambda) B^4 V_{\mathcal{F}} \left(1 + \frac{1}{c}\right)^2 \log n \times$$

$$\left( \frac{(1 + \log n)}{n} + a \left(1 + \frac{\log n}{n}\right) n^{-c} \right) + \lambda \inf_{f \in \mathcal{F}} \int |f(x) - y|^2 d\mu_n(x, y).$$

for  $n \geq 2$  such that  $e^n \geq n^{1+\frac{1}{c}}$ .

# First Conclusion (convergence of Averages)

*Under mixing conditions (exponential, polynomial) on the data sequence  $(X_k, Y_k)_k$ , and for the LSR estimator  $\hat{f}^*$  (constructed from  $D_n = (X_k, Y_k)_{k=1}^n$ ), one has the convergence (if  $\mathcal{F}$  is a VC class and  $\|Y_k\|_{\mathbb{P}, \infty} \leq B$ )*

$$\lim_{n \rightarrow \infty} \left( E \int |\hat{f}^*(x) - y|^2 d\mu_n(x, y) - \inf_{f \in \mathcal{F}} \int |f(x) - y|^2 d\mu_n(x, y) \right) = 0. \quad (13)$$

*with an explicit rate (depending on  $\lambda > 1$ ) in the bounded case for an error less than*

$$(\lambda - 1) \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{k=0}^n E |f \circ X_k - Y_k|^2.$$

## Part III

### Convergence in Distribution of Least-Squares Regression



## An Interpretation of the Previous Results

For (not necessarily i.i.d.) mixing data  $D_n := \{(X_k, Y_k)\}_{k=1}^n$  with uniformly bounded response ( $\|Y_k\|_{\mathbb{P}, \infty} \leq B$ ), the LSR

$$\hat{f}_{n,B} = \hat{f}^*(T_B \mathcal{F}, D_n)$$

is a  $L^2$ -**universally consistent** estimator of the **best  $L^2$  approximation** of  $Y$  as a function of  $X$  taken from  $T_B \mathcal{F}$ :

$$\hat{f}_{n,B} \approx f^*(T_B \mathcal{F}, D_n) \in \arg \min_{f \in T_B \mathcal{F}} \frac{1}{n} \sum_{k=1}^n E|f \circ X_k - Y_k|^2 =$$

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$$\arg \min_{f \in T_B \mathcal{F}} \int_{\mathbb{R}^d \times \mathbb{R}} |f(x) - y|^2 d\mu_n(x, y). \quad (14)$$

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**Note:** if  $(X_k, Y_k) \sim (X, Y)$  (thus  $\mu_n = \mu_\infty$ ), the r.h.s of (14) reduces to

$$\arg \min_{f \in T_B \mathcal{F}} E[|f \circ X - Y|^2].$$

# Questions on Convergence

(When) is there a limit, as  $n \rightarrow \infty$ , to

$$\inf_{T_{B\mathcal{F}}} \int_{\mathbb{R}^d \times \mathbb{R}} |f(x) - y|^2 d\mu_n(x, y)?$$

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*If such limit exists, is there a speed of convergence?*

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We have seen: under mixing conditions

$$0 = \lim_n (E \int |\hat{f}_{n,B}(x) - y|^2 d\mu_n(x, y) - \inf_{f \in T_{B,F}} \int |f(x) - y|^2 d\mu_n(x, y)).$$

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Let  $\mu$  be a measure. Assuming the “diagonal” convergence

$$0 = \lim_n (E \int |\hat{f}_{n,B}(x) - y|^2 d\mu_n(x, y) - E \int |\hat{f}_{n,B}(x) - y|^2 d\mu(x, y)), \quad (15)$$

we get  $0 = \lim_n (E[\int |\hat{f}_{n,B}(x) - y|^2 d\mu] - \inf_{f \in T_{B,F}} \int |f(x) - y|^2 d\mu_n(x, y)).$



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we get  $0 = \lim_n (E[\int |\hat{f}_{n,B}(x) - y|^2 d\mu] - \inf_{f \in T_{B\mathcal{F}}} \int |f(x) - y|^2 d\mu_n(x, y))$ .

If in addition “ $\lim_n \inf_{T_{B\mathcal{F}}} = \inf_{f \in T_{B\mathcal{F}}} \lim_n$ ” we arrive at

$$\lim_n E[\int |\hat{f}_{n,B}(x) - y|^2 d\mu(x, y)] = \inf_{f \in T_{B\mathcal{F}}} \int |f(x) - y|^2 d\mu(x, y). \quad (16)$$

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Assume that  $(X_k, Y_k)_k$ ,  $\hat{f}_{n,B}$  is as above ( $(X_k, Y_k)$   $\beta$ -mixing,  $\|Y_k\|_{\mathbb{P},\infty} \leq B$ , etc.) and let

$$\mu_n := \frac{1}{n} \sum_{k=1}^n \mu(X_k, Y_k)$$

be the average measure at time  $n$ .

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be the average measure at time  $n$ . **If  $\mu_n$  converges to  $\mu$  in total variation distance, then**

$$\lim_n E \int |\hat{f}_{n,B}(x) - y|^2 d\mu(x, y) = \inf_{f \in T_{B,\mathcal{F}}} \int |f(x) - y|^2 d\mu(x, y).$$

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**Proof:** Convergence in TVD implies

$$\lim_n \sup_{f \in T_{B,\mathcal{F}}} \left| \int |f(x) - y|^2 d\mu_n(x, y) - \int |f(x) - y|^2 d\mu(x, y) \right| = 0.$$

This implies the exchange of “lim” and “inf”.

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$$L_{Q^m} := \sup_{x_1 \neq x_2} \|Q^m(x_1, \cdot) - Q^m(x_2, \cdot)\|_{TV} < \delta.$$



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Under the Doeblin condition, there exists a unique probability measure  $\pi$  with  $Q\pi = \pi$  and for every probability measure  $\pi'$

$$\|\pi' Q^n - \pi\|_{TV} \leq \|\pi' - \pi\|_{TV} \delta^{\lfloor n/m \rfloor}.$$

## Theorem (LSR under the Doeblin Condition)

Assume that  $(X_k, Y_k)_k$  is an homogeneous (perhaps non-stationary) Markov chain satisfying the Doeblin Condition. Then if  $\pi$  is the unique stationary distribution of  $(X_k, Y_k)_k$ , there exists  $(a, c) \in [0, \infty) \times (0, \infty)$  such that for all  $\lambda > 1$



$$E \int |\hat{f}_{n,B}(x) - y|^2 d\pi(x, y) \leq$$

$$C(\lambda)B^4 V_{\mathcal{F}} \left(1 + \frac{1}{c}\right)^2 \log n \times \left(\frac{(1 + \log n)}{n} + a\left(1 + \frac{\log n}{n}\right)n^{-c}\right) +$$

$$\lambda \inf_{f \in T_{B\mathcal{F}}} \int |f(x) - y|^2 d\pi(x, y).$$

# Thank you!

# References

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