

# 1 Introduction and motivations

## Regression and classification from an infinite dimensional predictor

### Settings

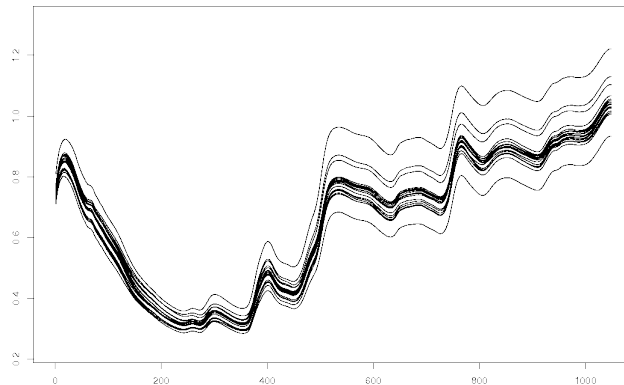
$(X, Y)$  is a random pair of variables where

- $Y \in \{-1, 1\}$  (binary classification problem) or  $Y \in \mathbb{R}$
- $X \in (X, \langle \cdot, \cdot \rangle_X)$ , an infinite dimensional Hilbert space.

We are given a **learning set**  $S_n = \{(X_i, Y_i)\}_{i=1}^n$  of  $n$  i.i.d. copies of  $(X, Y)$ .

**Purpose:** Find  $\phi_n : X \rightarrow \{-1, 1\}$  or  $\mathbb{R}$ , that is universally consistent: *Classification case:*  $\lim_{n \rightarrow +\infty} \mathbb{P}(\phi_n(X) \neq Y) = L^*$  where  $L^* = \inf_{\phi: X \rightarrow \{-1, 1\}} \mathbb{P}(\phi(X) \neq Y)$  is the **Bayes risk**. *Regression case:*  $\lim_{n \rightarrow +\infty} \mathbb{E}([\phi_n(X) - Y]^2) = L^*$  where  $L^* = \inf_{\phi: X \rightarrow \mathbb{R}} \mathbb{E}([\phi(X) - Y]^2)$  will also be called the Bayes risk.

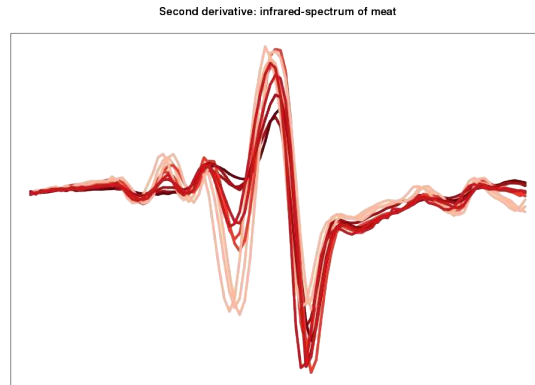
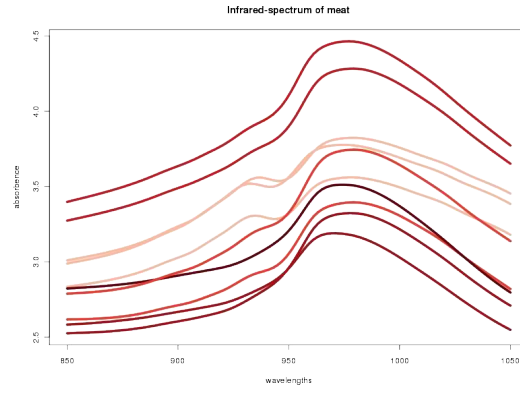
### An example



Predicting the **rate of yellow berry in durum wheat** from its **NIR spectrum**.

### Using derivatives

**Practically**,  $X^{(m)}$  is often more relevant than  $X$  for the prediction.



But  $X \rightarrow X^{(m)}$  induces **information loss** and

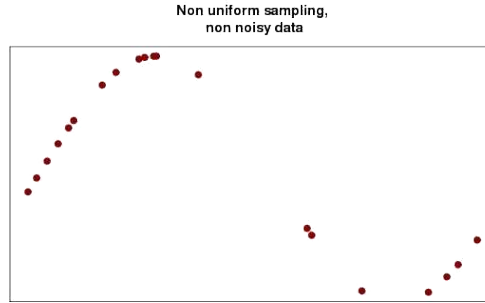
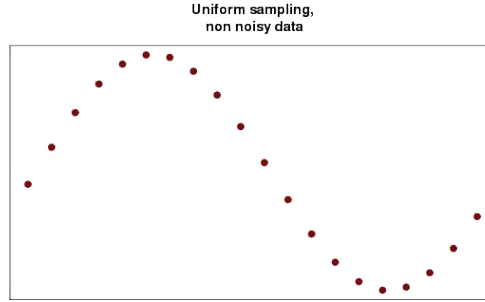
$$\inf_{\phi: D^m X \rightarrow \{-1,1\}} \mathbb{P}(\phi(X^{(m)}) \neq Y) \geq \inf_{\phi: X \rightarrow \{-1,1\}} \mathbb{P}(\phi(X) \neq Y) = L^*$$

and

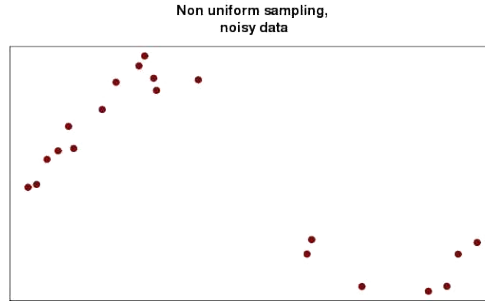
$$\inf_{\phi: D^m X \rightarrow \mathbb{R}} \mathbb{E}([ \phi(X^{(m)}) - Y ]^2) \geq \inf_{\phi: X \rightarrow \mathbb{R}} \mathbb{E}([ \phi(X) - Y ]^2) = L^*.$$

### Sampled functions

**Practically**,  $(X_i)_i$  are not perfectly known; only a discrete sampling is given:  $\mathbf{X}_i^{\tau_d} = (X_i(t))_{t \in \tau_d}$  where  $\tau_d = \{t_1^{\tau_d}, \dots, t_{|\tau_d|}^{\tau_d}\}$ .



The sampling can be non uniform...



... and the data can be corrupted by noise.  
**Then**,  $X_i^{(m)}$  is **estimated** from  $\mathbf{X}_i^{\tau_d}$ , by  $\widehat{X}_{\tau_d}^{(m)}$ , which also induces **information loss**:

$$\inf_{\phi: D^m \mathcal{X} \rightarrow \{-1, 1\}} \mathbb{P}(\phi(\widehat{X}_{\tau_d}^{(m)}) \neq Y) \geq \inf_{\phi: D^m \mathcal{X} \rightarrow \{-1, 1\}} \mathbb{P}(\phi(X^{(m)}) \neq Y) \geq L^*$$

and

$$\inf_{\phi: D^m \mathcal{X} \rightarrow \mathbb{R}} \mathbb{E}([ \phi(\widehat{X}_{\tau_d}^{(m)}) - Y ]^2) \geq \inf_{\phi: D^m \mathcal{X} \rightarrow \mathbb{R}} \mathbb{E}([ \phi(X^{(m)}) - Y ]^2) \geq L^*.$$

### Purpose of the presentation

Find a classifier or a regression function  $\phi_{n,\tau_d}$  built from  $\widehat{X}_{\tau_d}^{(m)}$  such that the risk of  $\phi_{n,\tau_d}$  **asymptotically reaches** the Bayes risk  $L^*$ :

$$\lim_{|\tau_d| \rightarrow +\infty} \lim_{n \rightarrow +\infty} \mathbb{P}(\phi_{n,\tau_d}(\widehat{X}_{\tau_d}^{(m)}) \neq Y) = L^*$$

or

$$\lim_{|\tau_d| \rightarrow +\infty} \lim_{n \rightarrow +\infty} \mathbb{E} \left( \left[ \phi_{n,\tau_d}(\widehat{X}_{\tau_d}^{(m)}) - Y \right]^2 \right) = L^*$$

**Main idea:** Use a relevant way to estimate  $X^{(m)}$  from  $\mathbf{X}^{\tau_d}$  (by smoothing splines) and combine the consistency of splines with the consistency of a  $\mathbb{R}^{|\tau_d|}$ -classifier or regression function.

## 2 A general consistency result

### Basics about smoothing splines I

Suppose that  $\mathcal{X}$  is the Sobolev space

$$\mathcal{H}^m = \left\{ h \in L^2_{[0,1]} \mid \forall j = 1, \dots, m, D^j h \text{ exists (weak sense) and } D^m h \in L^2 \right\}$$

equipped with the scalar product

$$\langle u, v \rangle_{\mathcal{H}^m} = \langle D^m u, D^m v \rangle_{L^2} + \sum_{j=1}^m B^j u B^j v$$

where  $B$  are  $m$  boundary conditions such that  $\text{Ker} B \cap \mathbb{P}^{m-1} = \{0\}$ .

$(\mathcal{H}^m, \langle \cdot, \cdot \rangle_{\mathcal{H}^m})$  is a **RKHS**:  $\exists k_0 : \mathbb{P}^{m-1} \times \mathbb{P}^{m-1} \rightarrow \mathbb{R}$  and  $k_1 : \text{Ker} B \times \text{Ker} B \rightarrow \mathbb{R}$  such that

$$\forall u \in \mathbb{P}^{m-1}, t \in [0, 1], \langle u, k_0(t, \cdot) \rangle_{\mathcal{H}^m} = u(t)$$

and

$$\forall u \in \text{Ker} B, t \in [0, 1], \langle u, k_1(t, \cdot) \rangle_{\mathcal{H}^m} = u(t)$$

See **[Berlinet and Thomas-Agnan, 2004]** for further details.

## Basics about smoothing splines II

A simple example of boundary conditions:

$$h(0) = h^{(1)}(0) = \dots = h^{(m-1)}(0) = 0.$$

Then,

$$k_0(s, t) = \sum_{k=0}^{m-1} \frac{t^k s^k}{(k!)^2}$$

and

$$k_1(s, t) = \int_0^1 \frac{(t-w)_+^{m-1} (s-w)_+^{m-1}}{(m-1)!} dw.$$

## Estimating the predictors with smoothing splines I

**Assumption (A1)**

- $|\tau_d| \geq m - 1$
- sampling points are distinct in  $[0, 1]$
- $B^j$  are linearly independent from  $h \rightarrow h(t)$  for all  $t \in \tau_d$

**[Kimeldorf and Wahba, 1971]:** for  $\mathbf{x}^{\tau_d}$  in  $\mathbb{R}^{|\tau_d|}$ ,  $\exists ! \hat{x}_{\lambda, \tau_d} \in \mathcal{H}^m$  solution of

$$\arg \min_{h \in \mathcal{H}^m} \frac{1}{|\tau_d|} \sum_{l=1}^{|\tau_d|} (h(t_l) - \mathbf{x}^{\tau_d})^2 + \lambda \int_{[0,1]} (h^{(m)}(t))^2 dt.$$

and  $\hat{x}_{\lambda, \tau_d} = \mathcal{S}_{\lambda, \tau_d} \mathbf{x}^{\tau_d}$  where  $\mathcal{S}_{\lambda, \tau_d} : \mathbb{R}^{|\tau_d|} \rightarrow \mathcal{H}^m$ .

These assumptions are fulfilled by the previous simple example as long as  $0 \notin \tau_d$ .

## Estimating the predictors with smoothing splines II

$\mathcal{S}_{\lambda, \tau_d}$  is given by:

$$\begin{aligned} \mathcal{S}_{\lambda, \tau_d} &= \omega^T (U(K_1 + \lambda \mathbb{I}_{|\tau_d|}) U^T)^{-1} U (K_1 + \lambda \mathbb{I}_{|\tau_d|})^{-1} \\ &\quad + \eta^T (K_1 + \lambda \mathbb{I}_{|\tau_d|})^{-1} (\mathbb{I}_{|\tau_d|} - U^T (U(K_1 + \lambda \mathbb{I}_{|\tau_d|})^{-1} U (K_1 + \lambda \mathbb{I}_{|\tau_d|})^{-1}) \\ &= \omega^T M_0 + \eta^T M_1 \end{aligned}$$

with

- $\{\omega_1, \dots, \omega_m\}$  is a basis of  $\mathbb{P}^{m-1}$ ,  $\omega = (\omega_1, \dots, \omega_m)^T$  and  $U = (\omega_i(t))_{i=1, \dots, m}^T$   $t \in \tau_d$ ;
- $\eta = (k_1(t, \cdot))_{t \in \tau_d}^T$  and  $K_1 = (k_1(t, t'))_{t, t' \in \tau_d}$ .

The observations of the **predictor X (NIR spectra)** are then estimated from their sampling  $\mathbf{X}^{\tau_d}$  by  $\widehat{\mathbf{X}}_{\lambda, \tau_d}$ .

## Two important consequences

### 1. No information loss

$$\inf_{\phi: \mathcal{H}^m \rightarrow \{-1,1\}} \mathbb{P}(\phi(\widehat{X}_{\lambda, \tau_d}) \neq Y) = \inf_{\phi: \mathbb{R}^{|\tau_d|} \rightarrow \{-1,1\}} \mathbb{P}(\phi(\mathbf{X}^{\tau_d}) \neq Y)$$

and

$$\inf_{\phi: \mathcal{H}^m \rightarrow \{-1,1\}} \mathbb{E} \left( [\phi(\widehat{X}_{\lambda, \tau_d}) - Y]^2 \right) = \inf_{\phi: \mathbb{R}^{|\tau_d|} \rightarrow \{-1,1\}} \mathbb{E} \left( [\phi(\mathbf{X}^{\tau_d}) - Y]^2 \right)$$

### 2. Easy way to use derivatives:

$$\begin{aligned} (\mathbf{Q}_{\lambda, \tau_d} \mathbf{u}^{\tau_d})^T (\mathbf{Q}_{\lambda, \tau_d} \mathbf{v}^{\tau_d}) (\mathbf{u}^{\tau_d})^T \mathbf{M}_{\lambda, \tau_d} \mathbf{v}^{\tau_d} (\mathbf{u}^{\tau_d})^T M_0^T W M_0 \mathbf{v}^{\tau_d} + (\mathbf{u}^{\tau_d})^T M_1^T K_1 M_1 \mathbf{v}^{\tau_d} \langle \mathbf{S}_{\lambda, \tau_d} \mathbf{u}^{\tau_d}, \mathbf{S}_{\lambda, \tau_d} \mathbf{v}^{\tau_d} \rangle_{\mathcal{H}^m} &= \langle \widehat{u}_{\lambda, \tau_d}, \widehat{v}_{\lambda, \tau_d} \rangle_{\mathcal{H}^m} \\ &\simeq \langle \widehat{u}_{\lambda, \tau_d}^{(m)}, \widehat{v}_{\lambda, \tau_d}^{(m)} \rangle_{\mathcal{H}^m} \end{aligned}$$

where  $K_1$ ,  $M_0$  and  $M_1$  have been previously defined and  $W = (\langle \omega_i, \omega_j \rangle_{\mathcal{H}^m})_{i,j=1,\dots,m}$ . where  $\mathbf{M}_{\lambda, \tau_d}$  is symmetric, definite positive. where  $\mathbf{Q}_{\lambda, \tau_d}$  is the Choleski triangle of  $\mathbf{M}_{\lambda, \tau_d}$ :  $\mathbf{Q}_{\lambda, \tau_d}^T \mathbf{Q}_{\lambda, \tau_d} = \mathbf{M}_{\lambda, \tau_d}$ . **Remark:**  $\mathbf{Q}_{\lambda, \tau_d}$  is calculated only from the RKHS,  $\lambda$  and  $\tau_d$ : it does not depend on the data set.

## Classification and regression based on derivatives

Suppose that we know a **consistent classifier or regression function in  $\mathbb{R}^{|\tau_d|}$**  that is based on  $\mathbb{R}^{|\tau_d|}$  scalar product or norm. The **corresponding derivative based classifier or regression function** is given by using the norm induced by  $\mathbf{Q}_{\lambda, \tau_d}$ :

**Example:** Nonparametric kernel regression

$$\Psi : u \in \mathbb{R}^{|\tau_d|} \rightarrow \frac{\sum_{i=1}^n T_i K \left( \frac{\|u - U_i\|_{\mathbb{R}^{|\tau_d|}}}{h_n} \right)}{\sum_{i=1}^n K \left( \frac{\|u - U_i\|_{\mathbb{R}^{|\tau_d|}}}{h_n} \right)}$$

where  $(U_i, T_i)_{i=1, \dots, n}$  is a learning set in  $\mathbb{R}^{|\tau_d|} \times \mathbb{R}$ .

$$\begin{aligned} \phi_{n,d} = \Psi \circ \mathbf{Q}_{\lambda, \tau_d} : x \in \mathcal{H}^m &\rightarrow \frac{\sum_{i=1}^n Y_i K \left( \frac{\|\mathbf{Q}_{\lambda, \tau_d} \mathbf{x}^{\tau_d} - \mathbf{Q}_{\lambda, \tau_d} \mathbf{X}_i^{\tau_d}\|_{\mathbb{R}^{|\tau_d|}}}{h_n} \right)}{\sum_{i=1}^n K \left( \frac{\|\mathbf{Q}_{\lambda, \tau_d} \mathbf{x}^{\tau_d} - \mathbf{Q}_{\lambda, \tau_d} \mathbf{X}_i^{\tau_d}\|_{\mathbb{R}^{|\tau_d|}}}{h_n} \right)} \\ &\xrightarrow{\simeq} \frac{\sum_{i=1}^n Y_i K \left( \frac{\|x^{(m)} - X_i^{(m)}\|_{L^2}}{h_n} \right)}{\sum_{i=1}^n K \left( \frac{\|x^{(m)} - X_i^{(m)}\|_{L^2}}{h_n} \right)} \end{aligned}$$

### Remark for consistency

**Classification case** (approximatively the same is true for regression):

$$\mathbb{P}(\phi_{n, \tau_d}(\widehat{X}_{\lambda, \tau_d}) \neq Y) - L^* = \mathbb{P}(\phi_{n, \tau_d}(\widehat{X}_{\lambda, \tau_d}) \neq Y) - L_d^* + L_d^* - L^*$$

where  $L_d^* = \inf_{\phi: \mathbb{R}^{|\tau_d|} \rightarrow \{-1, 1\}} \mathbb{P}(\phi(\mathbf{X}^{\tau_d}) \neq Y)$ .

1. For all fixed  $d$ ,

$$\lim_{n \rightarrow +\infty} \mathbb{P}(\phi_{n, \tau_d}(\widehat{X}_{\lambda, \tau_d}) \neq Y) = L_d^*$$

as long as the  $\mathbb{R}^{|\tau_d|}$ -classifier is consistent because there is a one-to-one mapping between  $\mathbf{X}^{\tau_d}$  and  $\widehat{X}_{\lambda, \tau_d}$ .

2.  $L_d^* - L^* \leq \mathbb{E} \left( \left| \mathbb{E}(Y | \widehat{X}_{\lambda, \tau_d}) - \mathbb{E}(Y | X) \right| \right)$  with consistency of spline estimate  $\widehat{X}_{\lambda, \tau_d}$  and assumption on the regularity of  $\mathbb{E}(Y | X = \cdot)$ , consistency would be proved. **But** continuity of  $\mathbb{E}(Y | X = \cdot)$  is a strong assumption in infinite dimensional case, and is not easy to check.

### Spline consistency

Let  $\lambda$  depends on  $d$  and denote  $(\lambda_d)_d$  the series of regularization parameters. Also introduce  $\bar{\Delta}_{\tau_d} := \max\{t_1, t_2 - t_1, \dots, 1 - t_{|\tau_d|}\}$ ,  $\underline{\Delta}_{\tau_d} := \min_{1 \leq i < |\tau_d|} \{t_{i+1} - t_i\}$

**Assumption (A2)**  $\bar{\Delta}_{\tau_d} / \underline{\Delta}_{\tau_d} \leq R$  for all  $d$ ;

- $\lim_{d \rightarrow +\infty} |\tau_d| = +\infty$ ;
- $\lim_{d \rightarrow +\infty} \lambda_d = 0$ .

**[Ragozin, 1983]:** Under (A1) and (A2),  $\exists A_{R,m}$  and  $B_{R,m}$  such that for any  $x \in \mathcal{H}^m$  and any  $\lambda_d > 0$ ,

$$\|\hat{x}_{\lambda_d, \tau_d} - x\|_{L^2}^2 \leq \left( A_{R,m} \lambda_d + B_{R,m} \frac{1}{|\tau_d|^{2m}} \right) \|D^m x\|_{L^2}^2 \xrightarrow{d \rightarrow +\infty} 0$$

### Bayes risk consistency

#### Assumption (A3a)

$\mathbb{E}(\|D^m X\|_{L^2}^2)$  is finite and  $Y \in \{-1, 1\}$ .

or

#### Assumption (A3b)

$\tau_d \subset \tau_{d+1}$  for all  $d$  and  $\mathbb{E}(Y^2)$  is finite.

Under (A1)-(A3),  $\lim_{d \rightarrow +\infty} L_d^* = L^*$ .

### Proof under assumption (A3a)

#### Assumption (A3a)

$\mathbb{E}(\|D^m X\|_{L^2}^2)$  is finite and  $Y \in \{-1, 1\}$ .

The proof is based on a result of **[Faragó and Györfi, 1975]**:

*For a pair of random variables  $(X, Y)$  taking their values in  $X \times \{-1, 1\}$  where  $X$  is an arbitrary metric space and for a series of functions  $T_d : X \rightarrow X$  such that*

$$\mathbb{E}(\delta(T_d(X), X)) \xrightarrow{d \rightarrow +\infty} 0$$

*then  $\lim_{d \rightarrow +\infty} \inf_{\phi: X \rightarrow \{-1, 1\}} \mathbb{P}(\phi(T_d(X)) \neq Y) = L^*$ .*

- $T_d$  is the spline estimate based on the sampling;
- the inequality of **[Ragozin, 1983]** about this estimate is exactly the assumption of Farago and Györfi's Theorem.

Then the result follows.

### Proof under assumption (A3b)

#### Assumption (A3b)

$\tau_d \subset \tau_{d+1}$  for all  $d$  and  $\mathbb{E}(Y^2)$  is finite.

Under (A3b),  $(\mathbb{E}(Y|\widehat{X}_{\lambda_d, \tau_d}))_d$  is a uniformly bounded martingale and thus converges for the  $L^1$ -norm. Using the consistency of  $(\widehat{X}_{\lambda_d, \tau_d})_d$  to  $X$  ends the proof.



### Concluding result (consistency)

#### Theorem

Under assumptions (A1)-(A3),

$$\lim_{|\tau_d| \rightarrow +\infty} \lim_{n \rightarrow +\infty} \mathbb{P}(\phi_{n,\tau_d}(\widehat{X}_{\lambda_d,\tau_d}) \neq Y) = L^*$$

and

$$\lim_{|\tau_d| \rightarrow +\infty} \lim_{n \rightarrow +\infty} \mathbb{E} \left( \left[ \phi_{n,\tau_d}(\widehat{X}_{\lambda_d,\tau_d}) - Y \right]^2 \right) = L^*$$

**Proof:** For a  $\epsilon > 0$ , fix  $d_0$  such that, for all  $d \geq d_0$ ,  $L_d^* - L^* \leq \epsilon/2$ .

Then, by consistency of the  $\mathbb{R}^{|\tau_d|}$ -classifier or regression function, conclude.

### A practical application to SVM I

**Recall** that, for a learning set  $(U_i, T_i)_{i=1,\dots,n}$  in  $\mathbb{R}^p \times \{-1, 1\}$ , gaussian SVM is the classifier

$$u \in \mathbb{R}^p \rightarrow \text{Sign} \left( \sum_{i=1}^n \alpha_i T_i e^{-\gamma \|u - U_i\|_{\mathbb{R}^p}^2} \right)$$

where  $(\alpha_i)_i$  satisfy the following quadratic optimization problem:

$$\arg \min_w \sum_{i=1}^n |1 - T_i w(U_i)|_+ + C \|w\|_{\mathcal{S}}^2$$

where  $w(u) = \sum_{i=1}^n \alpha_i e^{-\gamma \|u - U_i\|_{\mathbb{R}^p}^2}$  and  $\mathcal{S}$  is the RKHS associated with the gaussian kernel and  $C$  is a **regularization parameter**.

Under suitable assumptions, [Steinwart, 2002] proves the consistency of SVM classifiers.

### A practical application to SVM II

**Additional assumptions related to SVM:** Assumptions (A4) such that  $\lim_{n \rightarrow +\infty} n C_n^d = +\infty$  and  $C_n^d = O_n(n^{\beta_d - 1})$  for a  $0 < \beta_d < 1/d$ .

- For all  $d$ , there is a bounded subset of  $\mathbb{R}^{|\tau_d|}$ ,  $\mathcal{B}_d$ , such that  $\mathbf{X}^{\tau_d}$  belongs to  $\mathcal{B}_d$ .

**Result:** Under assumptions (A1)-(A4), the SVM  $\phi_{n,d} : x \in \mathcal{H}^m \rightarrow$

$$\text{Sign} \left( \sum_{i=1}^n \alpha_i Y_i e^{-\gamma \|\mathbf{Q}_{\lambda_d,\tau_d} \mathbf{x}^{\tau_d} - \mathbf{Q}_{\lambda_d,\tau_d} \mathbf{X}_i^{\tau_d}\|_{\mathbb{R}^d}^2} \right) \simeq \text{Sign} \left( \sum_{i=1}^n \alpha_i Y_i e^{-\gamma \|x^{(m)} - X_i^{(m)}\|_{L^2}^2} \right)$$

is consistent:  $\lim_{|\tau_d| \rightarrow +\infty} \lim_{n \rightarrow +\infty} \mathbb{P}(\phi_{n,\tau_d}(\widehat{X}_{\lambda_d,\tau_d}) \neq Y) = L^*$ .

### Additional remark about the link between $n$ and $|\tau_d|$

Under suitable (and usual) regularity assumptions on  $\mathbb{E}(Y|X = \cdot)$  and if  $n \sim \nu^{|\tau_d| \log |\tau_d|}$ , the **rate of convergence** of this method is of order  $d^{-\frac{2\nu}{2\nu+1}}$  where  $\nu$  is either equal to  $m$  or to a Lipchitz constant related to  $\mathbb{E}(Y|X = \cdot)$ .

### 3 Examples

#### Chosen regression method: Regression with kernel ridge regression

Recall that **kernel ridge regression** in  $\mathbb{R}^p$  is given by solving

$$\arg \min_w \sum_{i=1}^n (T_i - w(U_i))^2 + C \|w\|_{\mathcal{S}}^2$$

where  $\mathcal{S}$  is a RKHS induced by a given kernel (such as the Gaussian kernel) and  $(U_i, T_i)_i$  is a training sample in  $\mathbb{R}^p \times \mathbb{R}$ .

In the following examples,  $U_i$  is either:

- the original (sampled) functions  $\mathbf{X}_i$  (viewed as  $\mathbb{R}^{|\tau_d|}$  vectors);
- $\mathbf{Q}_{\lambda, \tau_d} \mathbf{X}_i^{\tau_d}$  for derivatives of order 1 or 2.

#### Example 1: Predicting yellow berry in durum wheat from NIR spectra

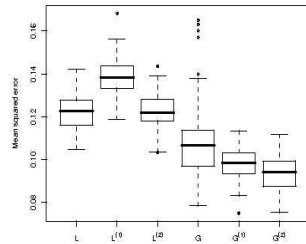
953 wheat samples were analyzed:

- **NIR spectrometry**: 1049 wavelengths regularly ranged from 400 to 2498 nm;
- **Yellow berry**: manual count (%) of affected grains.

#### Methodology for comparison:

- **Split the data** into train/test sets (50 times);
- **Train** 50 regression functions for the 50 train sets (hyper-parameters were tuned by CV);
- **Evaluate** these regression functions by calculating the **MSE** for the 50 corresponding test sets.

Kernel (SVM)	MSE on test (and sd $\times 10^{-3}$ )
Linear ( $L$ )	0.122 (8.77)
Linear on derivatives ( $L^{(1)}$ )	0.138 (9.53)
Linear on second derivatives ( $L^{(2)}$ )	0.122 (1.71)
Gaussian ( $G$ )	0.110 (20.2)
Gaussian on derivatives ( $G^{(1)}$ )	0.098 (7.92)
<b>Gaussian on second derivatives (<math>G^{(2)}</math>)</b>	<b>0.094</b> (8.35)



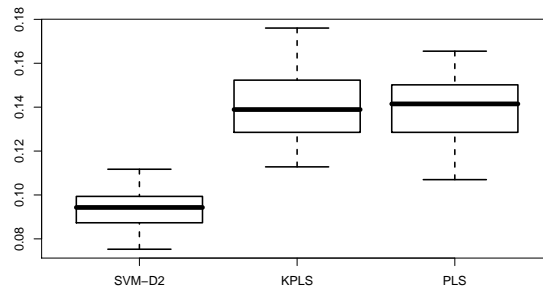
The differences are significant between  $G^{(2)}$  /  $G^{(1)}$  and between  $G^{(1)}$  /  $G$ .

### Comparison with PLS...

	MSE (mean)	MSE (sd)
PLS	0.154	0.012
Kernel PLS	0.154	0.013
KRR splines (reg. $D^2$ )	0.094	0.008

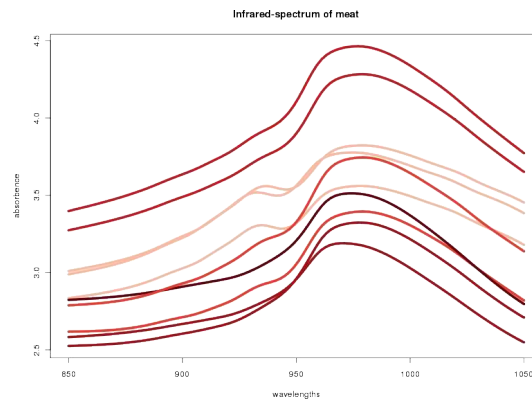
**Error decrease: almost**

**40 %**

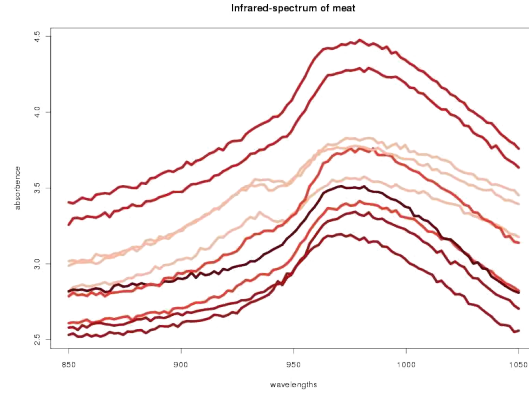


### Example 2: Simulated noisy spectra

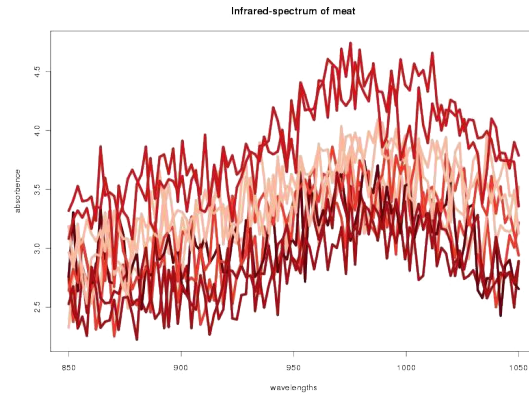
Original data:



**Variable to predict:** Fat content of pieces of meat. Noisy data:  $X_i^b(t) = X_i(t) + \epsilon_{it}$ ,  $\epsilon_{it} \sim \mathcal{N}(0, 0.01)$ , i.i.d.:



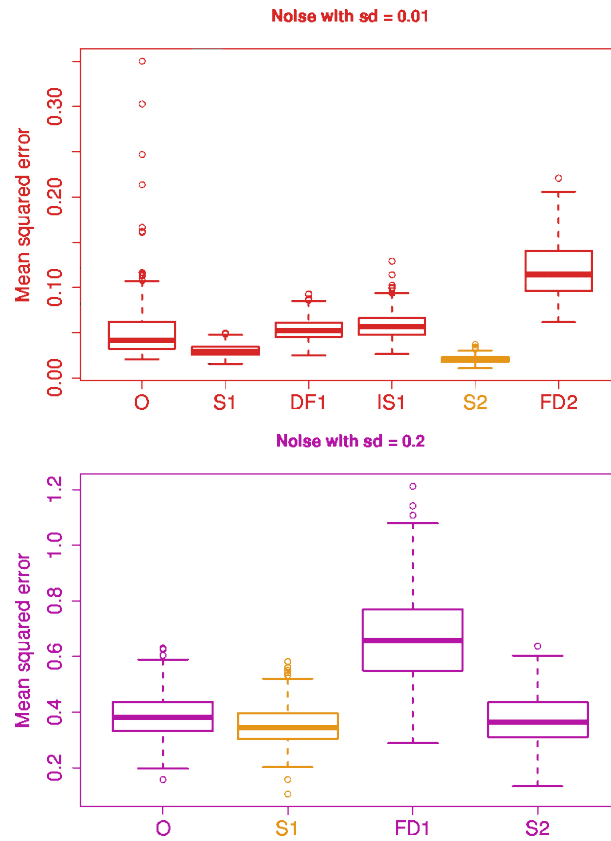
Worse noisy data:  $X_i^b(t) = X_i(t) + \epsilon_{it}$ ,  $\epsilon_{it} \sim \mathcal{N}(0, 0.2)$ , i.i.d.:



### Methodology for comparison

- **Split the data** into train/test sets (250 times);
- **Train** 250 regression functions for the 250 train sets (hyper-parameters were tuned by CV) with the predictors being
  - the original (sampled) functions  $\mathbf{X}_i$  (viewed as  $\mathbb{R}^{|\tau_d|}$  vectors);
  - $\mathbf{Q}_{\lambda, \tau_d} \mathbf{X}_i^{\tau_d}$  for derivatives of order 1 or 2: **smoothing splines derivatives**;
  - $\mathbf{Q}_{0, \tau_d} \mathbf{X}_i^{\tau_d}$  for derivatives of order 1 or 2: **interpolating splines derivatives**;
  - derivatives of order 1 or 2 evaluated by  $\frac{X_i(t_{j+1}) - X_i(t_j)}{t_{j+1} - t_j}$ : **finite differences derivatives**;
- **Evaluate** these regression functions by calculating the **MSE** for the 50 corresponding test sets.

## Performances



## References

## References

- [Berlinet and Thomas-Agnan, 2004] Berlinet, A. and Thomas-Agnan, C. (2004). *Reproducing Kernel Hilbert Spaces in Probability and Statistics*. Kluwer Academic Publisher.
- [Faragó and Györfi, 1975] Faragó, T. and Györfi, L. (1975). On the continuity of the error distortion function for multiple-hypothesis decisions. *IEEE Transactions on Information Theory*, 21(4):458–460.
- [Kimeldorf and Wahba, 1971] Kimeldorf, G. and Wahba, G. (1971). Some results on Tchebycheffian spline functions. *Journal of Mathematical Analysis and Applications*, 33(1):82–95.

- [Ragozin, 1983] Ragozin, D. (1983). Error bounds for derivative estimation based on spline smoothing of exact or noisy data. *Journal of Approximation Theory*, 37:335–355.
- [Steinwart, 2002] Steinwart, I. (2002). Support vector machines are universally consistent. *Journal of Complexity*, 18:768–791.

**Any question?**