Classification and regression based on derivatives: a consistency result

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Outline

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 $Y \in \mathbb{R}$

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Purpose: Find $\phi_n : \mathcal{X} \rightarrow \{-1, 1\}$ or $\mathbb{R}$, that is universally consistent:
Classification case: $\lim_{n\rightarrow+\infty} \mathbb{P}\left(\phi_n(X) \neq Y\right) = L^*$ where $L^* = \inf_{\phi:\mathcal{X}\rightarrow\{-1,1\}} \mathbb{P}\left(\phi(X) \neq Y\right)$ is the **Bayes risk**.

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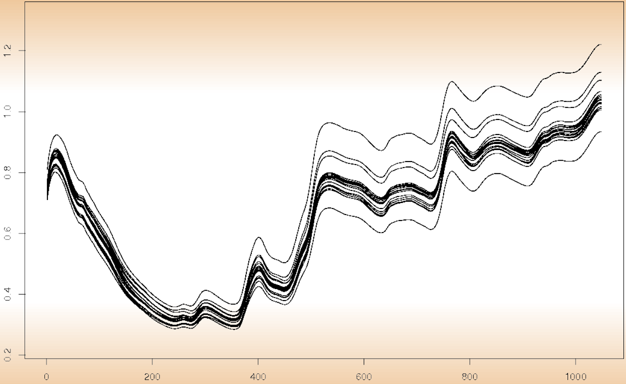
Regression case: $\lim_{n\rightarrow+\infty} \mathbb{E}\left([\phi_n(X) - Y]^2\right) = L^*$ where $L^* = \inf_{\phi:\mathcal{X}\rightarrow\mathbb{R}} \mathbb{E}\left([\phi(X) - Y]^2\right)$ will also be called the Bayes risk.

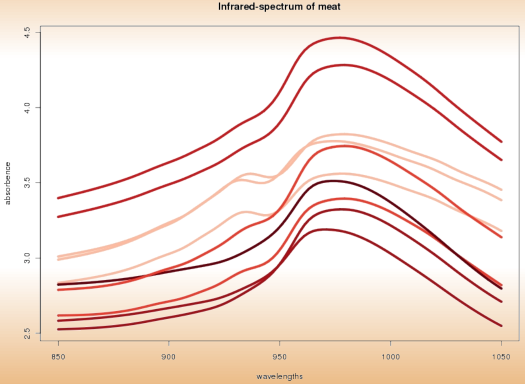
An example



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.



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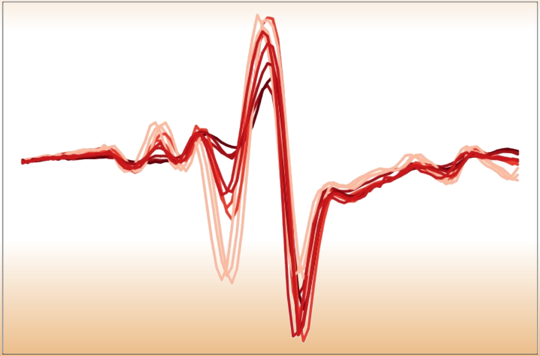
Second derivative: infrared-spectrum of meat



Using derivatives

Practically, $X^{(m)}$ is often more relevant than X for the prediction.
But $X \rightarrow X^{(m)}$ induces **information loss** and

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

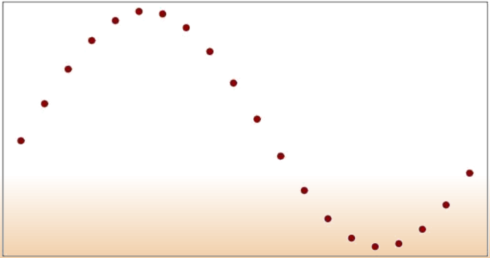
and

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

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 $\tau_d = \{t_1^{\tau_d}, \ldots, t_{|\tau_d|}^{\tau_d}\}$.

Uniform sampling,
non noisy data



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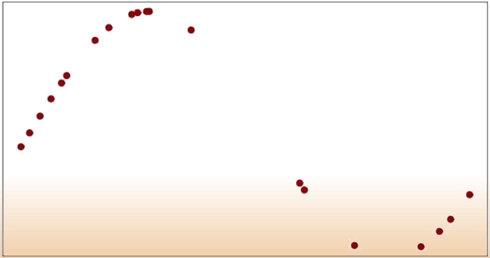

The sampling can be non uniform...

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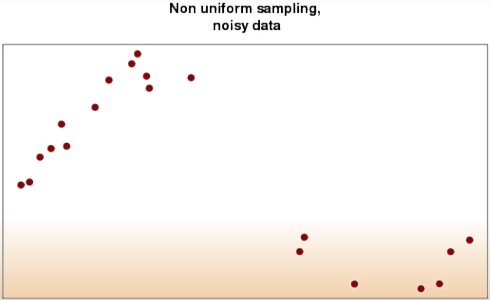

... and the data can be corrupted by noise.

Sampled functions

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Then, $X_i^{(m)}$ is **estimated** from $\mathbf{X}_i^{\tau_d}$, by $\widehat{X}_{\tau_d}^{(m)}$, which also induces **information loss**:

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

and

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

Purpose of the presentation

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

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

or

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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.

Outline

Basics about smoothing splines I

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

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

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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 $\mathrm{Ker} B \cap \mathbb{P}^{m-1} = \{0\}$.

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where B are m boundary conditions such that $\mathrm{Ker} B \cap \mathbb{P}^{m-1} = \{0\}$.
$(\mathcal{H}^m, \langle ., .\rangle_{\mathcal{H}^m})$ **is a RKHS**: $\exists\, k_0 : \mathbb{P}^{m-1} \times \mathbb{P}^{m-1} \rightarrow \mathbb{R}$ and $k_1 : \mathrm{Ker}B \times \mathrm{Ker}B \rightarrow \mathbb{R}$ such that

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

and

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

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

Basics about smoothing splines II

A simple example of boundary conditions:

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

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 $h \to h(t)$ for all $t \in \tau_d$

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[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 $\mathcal{S}_{\lambda,\tau_d} : \mathbb{R}^{|\tau_d|} \rightarrow \mathcal{H}^m$.

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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 fullfilled 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

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

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

Two important consequences

1. **No information loss**

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

and

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

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2. **Easy way to use derivatives**:

$$\langle \mathcal{S}_{\lambda,\tau_d}\mathbf{u}^{\tau_d}, \mathcal{S}_{\lambda,\tau_d}\mathbf{v}^{\tau_d}\rangle_{\mathcal{H}^m} = \langle \widehat{u}_{\lambda,\tau_d}, \widehat{v}_{\lambda,\tau_d}\rangle_{\mathcal{H}^m}$$

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2. **Easy way to use derivatives**:

$$(\mathbf{u}^{\tau_d})^T M_0^T W M_0 \mathbf{v}^{\tau_d} + (\mathbf{u}^{\tau_d})^T M_1^T K_1 M_1 \mathbf{v}^{\tau_d} \quad = \quad \langle \widehat{u}_{\lambda,\tau_d}, \widehat{v}_{\lambda,\tau_d}\rangle_{\mathcal{H}^m}$$

where K_1, M_0 and M_1 have been previously defined and $W = (\langle \omega_i, \omega_j\rangle_{\mathcal{H}^m})_{i,j=1,\ldots,m}$.

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$$(\mathbf{u}^{\tau_d})^T \mathbf{M}_{\lambda,\tau_d} \mathbf{v}^{\tau_d} \quad = \quad \langle \widehat{u}_{\lambda,\tau_d}, \widehat{v}_{\lambda,\tau_d} \rangle_{\mathcal{H}^m}$$

where $\mathbf{M}_{\lambda,\tau_d}$ is symmetric, definite positive.

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$$(\mathbf{Q}_{\lambda,\tau_d}\mathbf{u}^{\tau_d})^T(\mathbf{Q}_{\lambda,\tau_d}\mathbf{v}^{\tau_d}) \quad = \quad \langle \widehat{u}_{\lambda,\tau_d}, \widehat{v}_{\lambda,\tau_d}\rangle_{\mathcal{H}^m}$$

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, λ and τ_d: it does not depend on the data set.

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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.

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 $\mathbb{R}^{|\tau_d|} \times \mathbb{R}$.

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

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$$\overset{\simeq}{\rightarrow} \quad \frac{\sum_{i=1}^n Y_i K\left(\frac{\|x^{(m)} - X_i^{(m)}\|_{L^2}}{h_n}\right)}{\sum_{i=1}^n K\left(\frac{\|x^{(m)} - X_i^{(m)}\|_{L^2}}{h_n}\right)}$$

Remark for consistency

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

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

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

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

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

   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 $\widehat{X}_{\lambda,\tau_d}$.

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with consistency of spline estimate $\widehat{X}_{\lambda,\tau_d}$ and assumption on the regularity of $\mathbb{E}(Y|X = .)$, consistency would be proved.

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

Spline consistency

Let λ depends on d and denote $(\lambda_d)_d$ the series of regularization parameters. Also introduce

$\overline{\Delta}_{\tau_d} := \max\{t_1, t_2 - t_1, \ldots, 1 - t_{|\tau_d|}\}$, $\underline{\Delta}_{\tau_d} := \min_{1 \leq i < |\tau_d|}\{t_{i+1} - t_i\}$

Assumption (A2)

- $\exists\, R$ such that $\overline{\Delta}_{\tau_d} / \underline{\Delta}_{\tau_d} \leq R$ for all d;
- $\lim_{d \to +\infty} |\tau_d| = +\infty$;
- $\lim_{d \to +\infty} \lambda_d = 0$.

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[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 $\lambda_d > 0$,

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

Bayes risk consistency

Assumption (A3a)

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

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

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

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

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

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

- 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 Gyorfi's Theorem.

Then the result follows.

Proof under assumption (A3b)

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$\tau_d \subset \tau_{d+1}$ 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),

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

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 $(U_i, T_i)_{i=1,\ldots,n}$ in $\mathbb{R}^p \times \{-1, 1\}$, gaussian SVM is the classifier

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

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

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

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

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

A practical application to SVM II

Additional assumptions related to SVM: Assumptions (A4)

- For all d, the regularization parameter depends on n such that $\lim_{n\rightarrow+\infty} nC_n^d = +\infty$ and $C_n^d = \mathcal{O}_n\left(n^{\beta_d - 1}\right)$ 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 $\mathcal{B}_d$.

A practical application to SVM II

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- 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 $\phi_{n,d} : x \in \mathcal{H}^m \to$

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

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

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

Under suitable (and usual) regularity assumptions on $\mathbb{E}(Y|X = .)$ 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 ν is either equal to m or to a Lipchitz constant related to $\mathbb{E}(Y|X = .)$.

Outline

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 $\mathbb{R}^p \times \mathbb{R}$.

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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.

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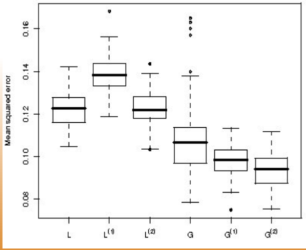
Methodology for comparison:

- **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.

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

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)
Gaussian on second derivatives ($G^{(2)}$)	**0.094** (8.35)

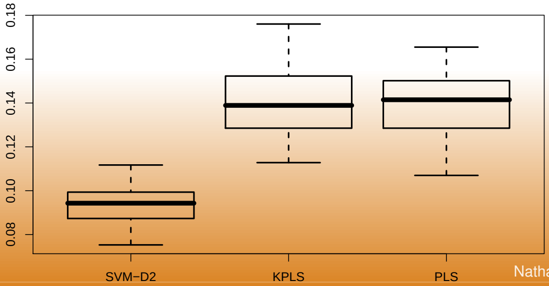


The differences are significant between $G^{(2)}$ / $G^{(1)}$ and between $G^{(1)}$ / G.

Comparison with PLS...

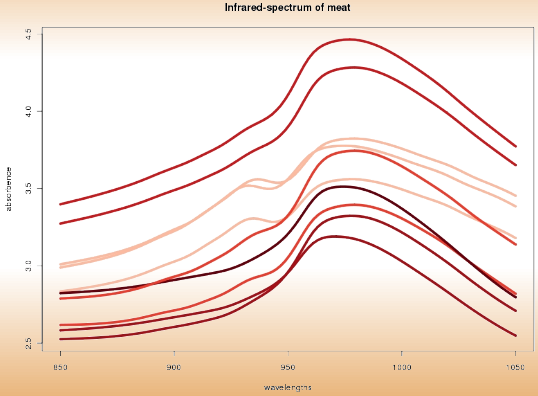
	MSE (mean)	MSE (sd)
PLS	0.154	0.012
Kernel PLS	0.154	0.013
KRR splines (reg. D^2)	0.094	0.008

Error decrease: almost 40 %



Example 2: Simulated noisy spectra

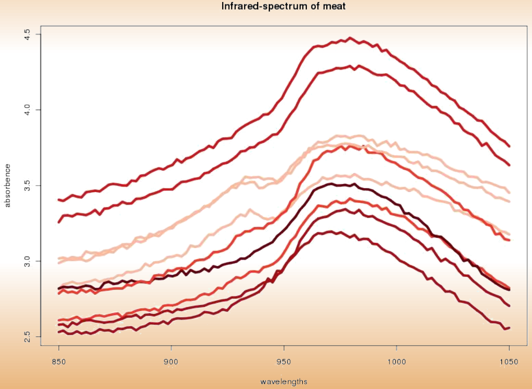
Original data:



Variable to predict: Fat content of pieces of meat.

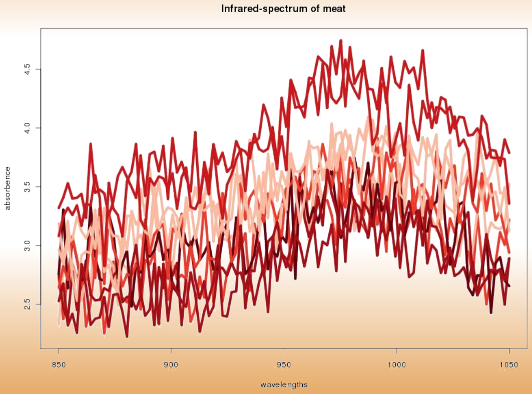
Example 2: Simulated noisy spectra

Noisy data: $X_i^b(t) = X_i(t) + \epsilon_{it}$, $\epsilon_{it} \sim \mathcal{N}(0, 0.01)$, i.i.d.:



Example 2: Simulated noisy spectra

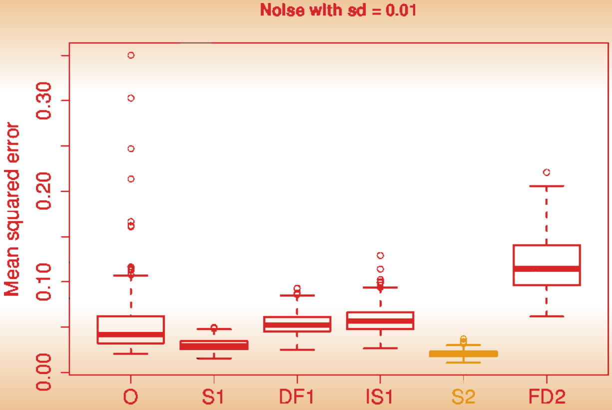
Worse noisy data: $X_i^b(t) = X_i(t) + \epsilon_{it}$, $\epsilon_{it} \sim \mathcal{N}(0, 0.2)$, i.i.d.:



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



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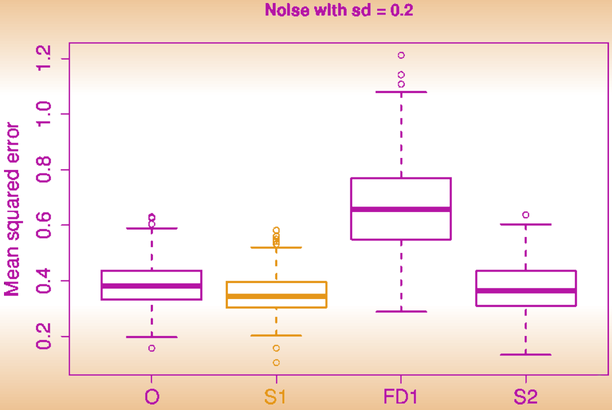

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Any question?