Anticipated and adaptive prediction in functional discriminant analysis

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The context

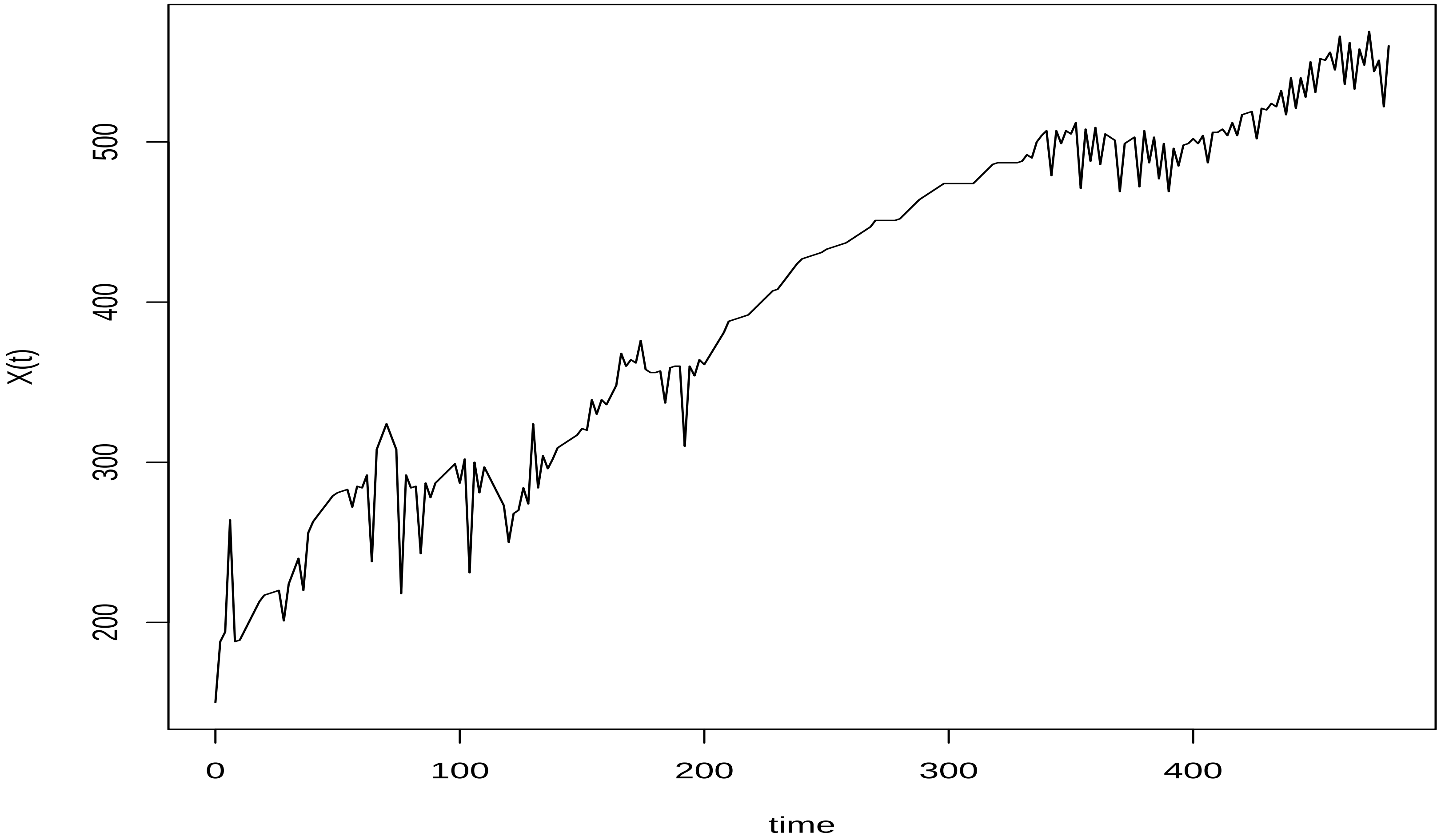
Cookie's quality at Danone and the kneading process

A cookie from Danone :

- choose a type of flour (components, density, etc)
- kneading process ($\approx$ 1h)
- **- Put the dough in form and cook it**
- Evaluate quality of the obtained cookies $\Big\}$ $>$ 2h.

Idea : predict the cookie's quality from elements derived from the kneading process : Danone gets time and money !

Dough resistance during the kneading process : $X = X(t)$**,** $t \in \{0, 2, 4, \ldots 480s\}$



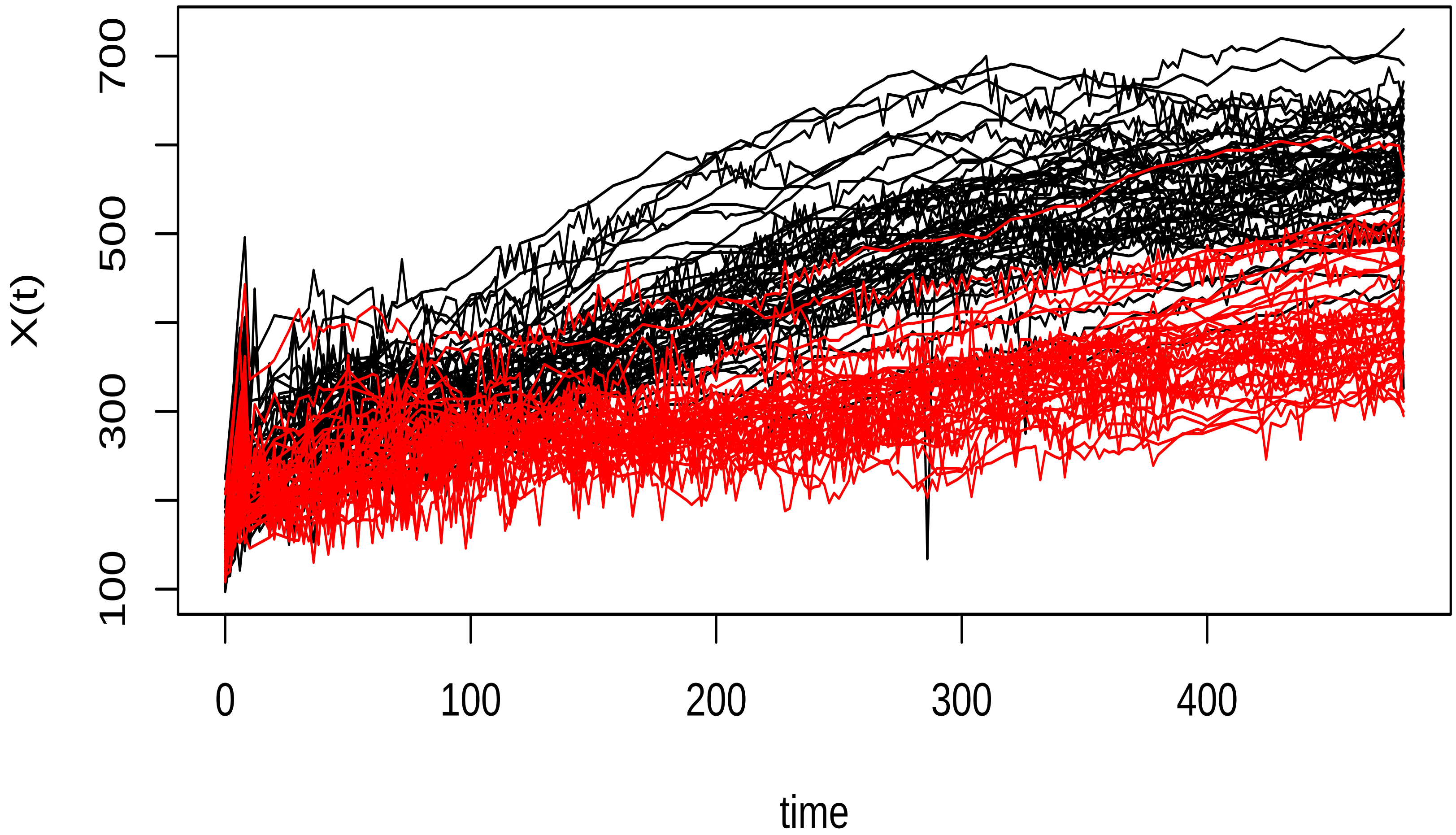
Flour evaluation

The quality of cookies obtained with some type of flour is given by experts.

The response (Y) is : this type of flour is **Good** or **Bad**.

90 flours were evaluated : 50 are good and 40 are bad.

90 flours : quality and dough resistance during 480s.



Good(black)   Bad(red)

Functional discriminant analysis

$$X = \{X_t\}_{t\in[0,T]}, \quad X_t : \mathbf{\Omega} \to \mathbb{R},$$

- $E(X_t^2) < \infty$,
- L_2–continuous,
- $\forall\omega \in \mathbf{\Omega} : (X_t(\omega))_{t\in[0,T]} \in L_2([0,T])$,
- $E(X_t) = 0, \forall t \in [0,T]$.

$$Y : \mathbf{\Omega} \to \{0,1\}.$$

Discriminant score :

$$d_T = \Phi(X)$$

Discriminant score estimation

$$\{(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n)\}$$

- Linear discriminant score :

$$\Phi(X) = \langle \beta, X \rangle_{L_2[0,T]}, \quad \beta \in L_2[0,T].$$

Criterion (Fisher):

$$\max_{\beta \in L_2[0,T]} \frac{\mathbb{V}(\mathbb{E}(\Phi(X)|Y))}{\mathbb{V}(\Phi(X))}$$

Estimation by functional linear regression model (PCR, PLS, etc).

- Nonparametric estimation

$$\hat{\Phi}(X) = \frac{\sum_{i=1}^{n} Y_i K(u(X, X_i)/h)}{\sum_{i=1}^{n} K(u(X, X_i)/h)}$$

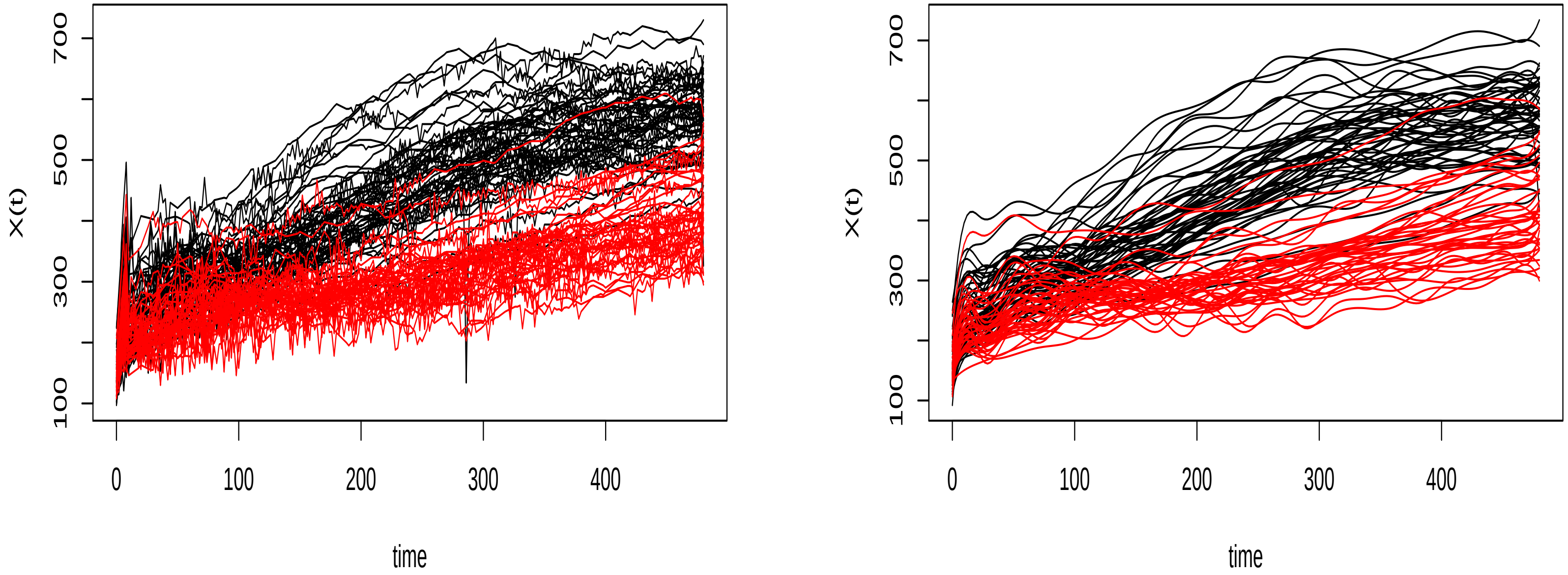
- RKHS approximation

$$\hat{\Phi}(X) = \sum_{i}^{n} \alpha_i K(X_i, X)$$

Criterion (logistic loss) :

$$L(x, y, \Phi) = -y\Phi(x) + \log(1 + e^{\Phi(x)})$$

Kneading data results



Good (black) and bad (red) flours. Left : original data. Right : smoothed data

Model	PLS_FLDA	NP	PC_FLDA	Gaussian(6)	LDA
Error rate	0.112	0.103	0.142	0.108	0.154

Error rate averaged over 100 test samples.

Anticipated prediction

X is observed on $[0, T]$

Problem : *find the smallest* T^*, $T^* < T$, *such that the prediction of* Y *by* X *observed on* $[0, T^*]$ *is "similar" to the prediction obtained with* X *observed on* $[0, T]$.

Discrimination power : ROC curve

– d : the discriminant score.

– threshold r : $Y = 1$ if $d > r$.

– "Sensitivity" : $P(d > r|Y = 1)$

– "Specificity" : $P(d > r|Y = 0)$.

Measure of discrimination : area under the ROC curve (AUC)

– Estimation of AUC

$\{Y=1\}: X_1 = d_{|Y=1}$, sample of size n_1

$\{Y=0\}: X_0 = d_{|Y=0}$, sample of size n_2

$$\widehat{AUC} = \frac{\#\{X_1 > X_0\}}{n_1 n_2}$$

$D = \{d_t\}_{0<t\leq T}, \ \ \{\widehat{AUC}(t)\}_{0<t\leq T}$

Criterion for T^* : compare $AUC(t)$ and $AUC(T)$ for $t < T$ and chose T^* as the largest t such that the test

$$H_0: \quad AUC(t) = AUC(T),$$

$$H_1: \quad AUC(t) < AUC(T)$$

is significant (p-value < 0.05).

Simulation

$$\text{Class } \{Y = 0\} : X_t = \begin{cases} W(1-t), & 0 \le t \le 1 \\ -2\sin(t-1) + W(t-1), & 1 < t \le 2 \end{cases}$$

$$\text{Class } \{Y = 1\} : X_t = \begin{cases} W(1-t), & 0 \le t \le 1 \\ 2\sin(t-1) + W(t-1), & 1 < t \le 2 \end{cases}$$

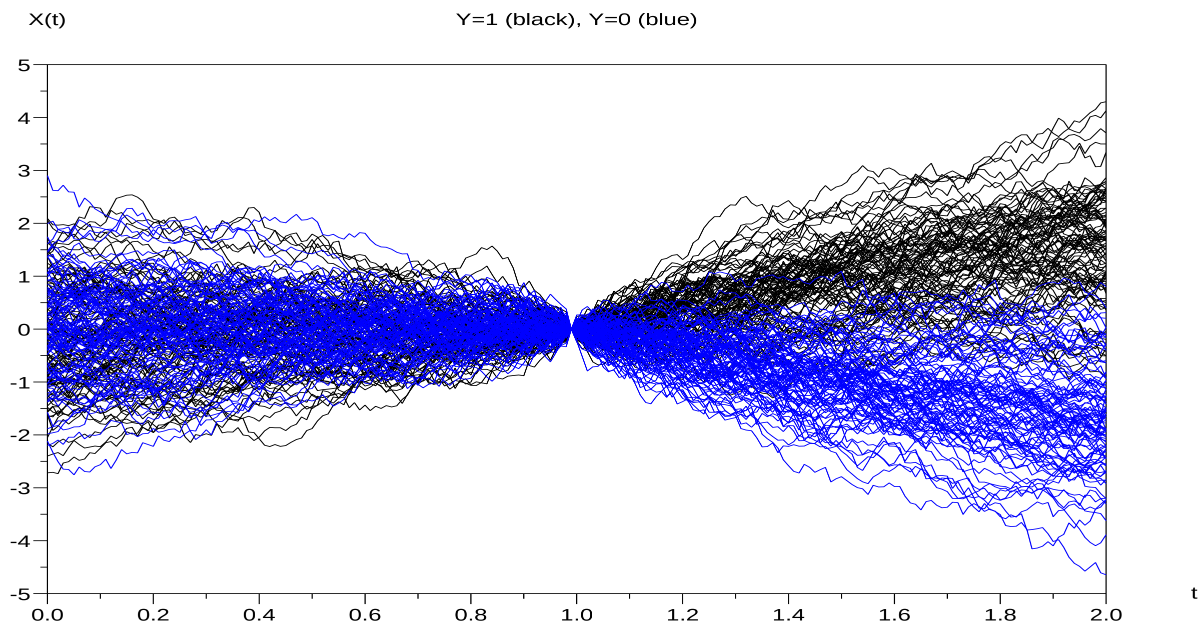


Figure : Sample of size $n = 100$ for each class of Y.

$M = 50$ learning and test samples of size 100.

For each $t \in \{0, 2.00, 1.98, \ldots, 0\}$: sample of size $M = 50$ of $\widehat{AUC}(t)$.

– $T^* = 1.46$.

– test statistic : $S = 1.663$

$\overline{\widehat{AUC}(t^*)} = 0.856$, $\overline{\widehat{AUC}(T)} = 0.872$

Kneading data

$Y \in \{Bad, Good\}$. The sample of 90 flours is randomly divided into a learning sample of size 60 and a test sample of size 30.

Error test rate (PLS estimation) $T = 480 : 0.112$,
– $\overline{\widehat{AUC}}(T) = 0.746$.

Anticipated prediction : $T^* = 186$.
Error test rate (PLS estimation) $T^* = 186 : 0.121$,
– $\overline{\widehat{AUC}}(T^*) = 0.778$.

Conclusion : *the predictive power of the dough curves for the cookies quality is resumed by the first* 186 *seconds of the kneading process.*

Adaptive prediction

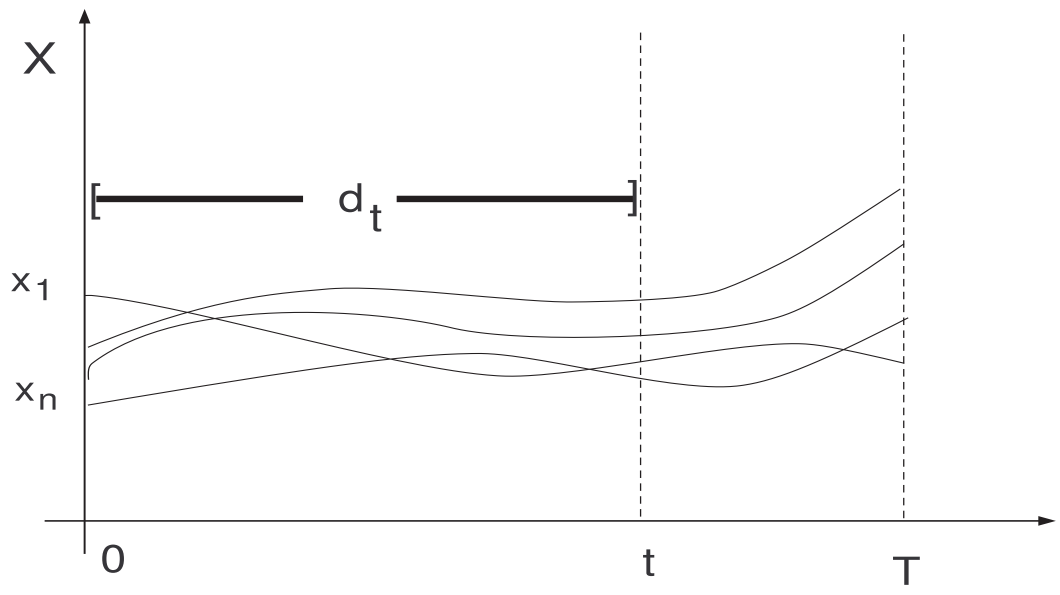
Remark : in anticipated prediction T^* is a constant.

Let $\omega \in \Omega$ be a new observation for which one wants to predict Y from X. Suppose that X is observed in a sequential way. The problem addressed by the adaptive prediction is :

Problem : *find the smallest* $T^*(\omega)$, $T^*(\omega) < T$, *such that* X *observed on* $[0, T^*(\omega)]$ *provides similar prediction as it is observed on* $[0, T]$.

Remark :
- here T^* is a random variable.
- to observe $X(\omega)$ on $[T^*, T]$ will not change the prediction for $Y(\omega)$ obtained with X on $[0, T^*(\omega)]$.

Conservative index for prediction :

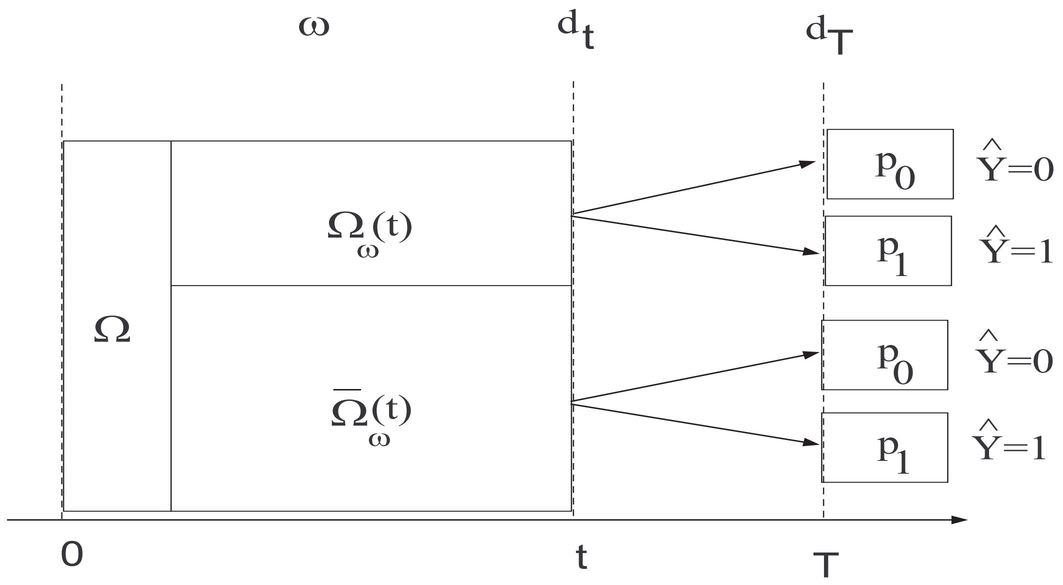


The discriminant score d_t.

Denote by

$$\Omega_\omega(t) = \{\omega_i \in \Omega | \hat{Y}_t(\omega) = \hat{Y}_{t,i}\} \text{ and } \overline{\Omega}_\omega(t) = \Omega - \Omega_\omega(t)$$

the class of elements having the same prediction as ω, respectively its complement with respect to Ω.



Conservation rate of the prediction for ω and t.

Let

$$p_{0|\Omega_\omega(t)} = \frac{\left|\{\omega' \in \Omega | \hat{Y}_T(\omega') = 0\} \cap \Omega_\omega(t)\}\right|}{|\Omega_\omega(t)|}.$$

be the observed rate of elements in $\Omega_\omega(t)$ predicted in the class $Y = 0$ at the time T using the score d_T. Similarly, let $p_{1|\Omega_\omega(t)}$, $p_{0|\overline{\Omega}_\omega(t)}$and $p_{1|\overline{\Omega}_\omega(t)}$
Let define by $C_{\Omega_\omega(t)} = \max\{p_{0|\Omega_\omega(t)}, p_{1|\Omega_\omega(t)}\}$, respectively by $C_{\overline{\Omega}_\omega(t)} = \max\{p_{0|\overline{\Omega_\omega}(t)}, p_{1|\overline{\Omega}_\omega(t)}\}$ the *conservation* rate of the prediction at the time t with respect to the time T for the elements of $\Omega_\omega(t)$, respectively of $\overline{\Omega}_\omega(t)$.
As a global measure of conservation we consider

$$C_\Omega(\omega, t) = \min\{C_{\Omega_\omega(t)}, C_{\overline{\Omega}_\omega(t)}\}.$$

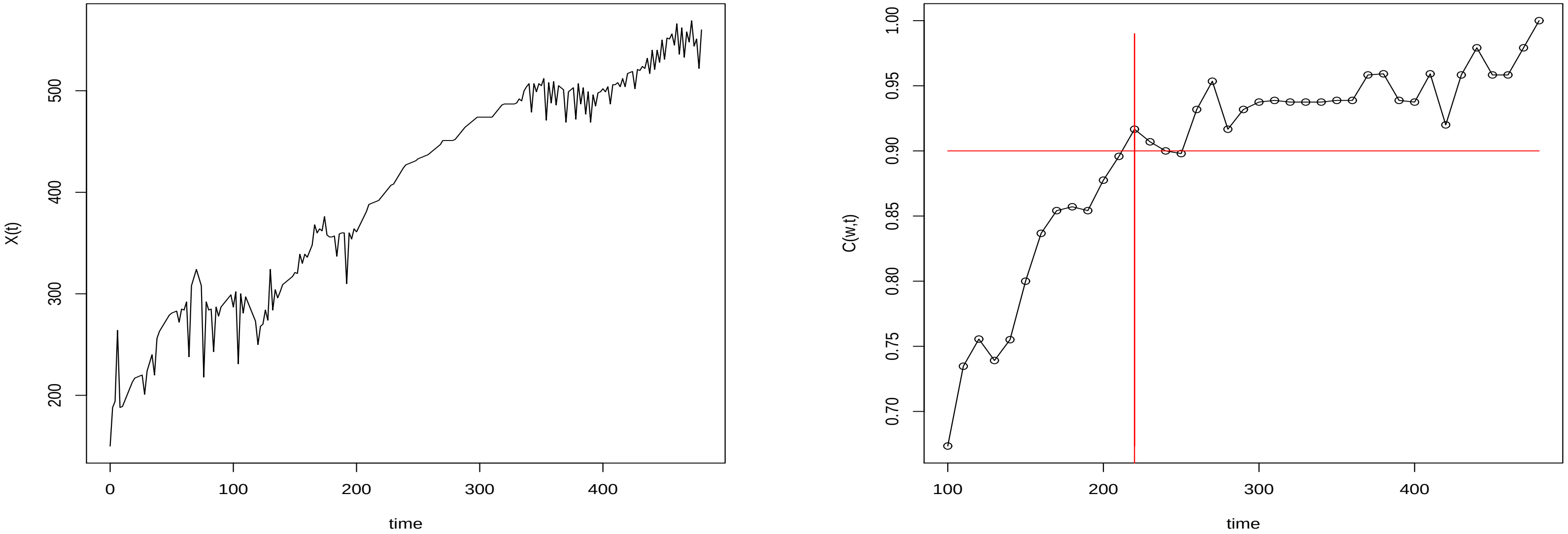
Remark : For each $t \in [0, T]$, $C_\Omega(\omega, t)$ is such that $0.5 \leq C_\Omega(\omega, t) \leq 1$ and $C_\Omega(\omega, T) \ = \ 1.$

Given a confidence conservation threshold $\gamma \in (0, 1)$, e.g. $\gamma = 0.90$, we define the following *adaptive prediction rule* for ω and t :

(1) if $C_\Omega(\omega, t) \geq \gamma$ then the observation of X for ω on the time interval $[0, t]$ is sufficient for the prediction of $Y(\omega)$. $\hat{Y}(\omega)$ is then the same as the prediction at time T of the subgroup of $\Omega_\omega(t)$ corresponding to $C_{\Omega_\omega(t)}$.

(2) if $C_\Omega(\omega, t) < \gamma$ then the observation process of X for ω should continue after t. Put $t = t + h$ and repeat the adaptive prediction procedure.

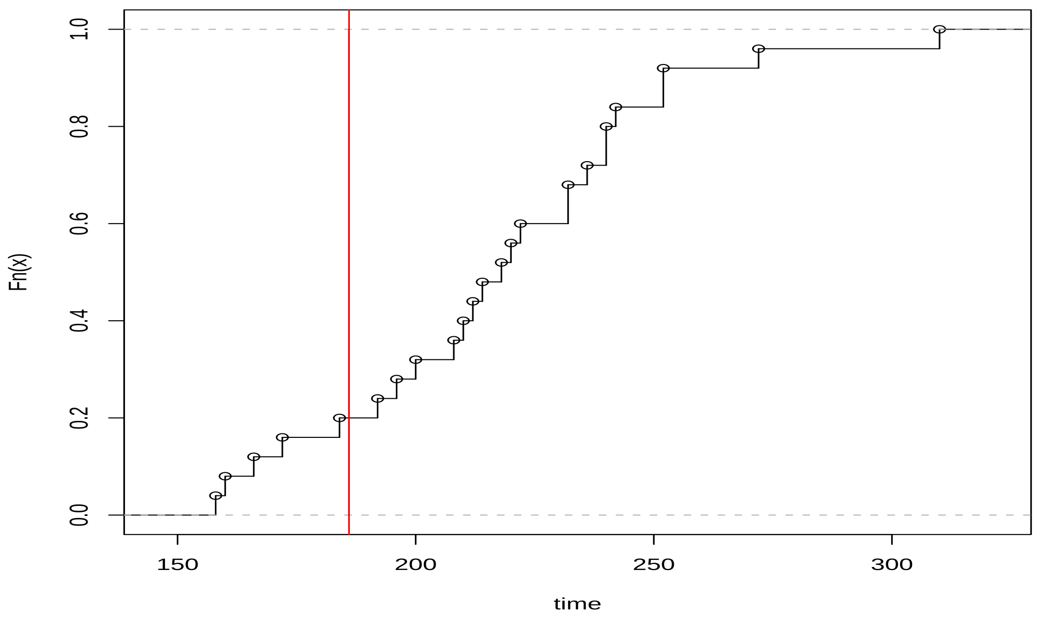
Then, $T^*(\omega)$ is the smallest t such that the condition (1) of the adaptive prediction rule is satisfied.



Left : new flour ω.   Right : $C_{\Omega}(\omega, t)$, $t \in [100, 480]$, $\gamma = 0.90$.

$$T^*(\omega) = 220.$$

For 25 new flours, the adaptive procedure is applied.



Empirical cumulative distribution function of T^* (in red, the time point t=186).