Model selection via penalization, resampling and cross-validation, with application to change-point detection

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- Model selection via penalization, with application to change-point detection
- Resampling methods for penalization, and robustness to heteroscedasticity in regression
- Cross-validation for model/estimator selection, with application to detecting changes in the mean of a signal



Learning	Model selection	Oracle inequality	Change-point detection	Conclusion

Part I

Model selection via penalization, with application to change-point detection

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2 Estimators

3 Model selection

- An oracle inequality for model selection: polynomial collection
- 5 Change-point detection via model selection

6 Conclusion

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Learning Estimators Model selection Oracle inequality Change-point detection Conclusion Regression: data $(x_1, Y_1), \ldots, (x_n, Y_n)$



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Goal: find the signal (denoising)



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General framework								

- Data: $\xi_1, \ldots, \xi_n \in \Xi$ i.i.d. $\sim P$
- Goal: estimate a feature $s^* \in \mathbb{S}$ of P
- Quality measure: loss function

$$orall t \in \mathbb{S} \;, \quad \mathcal{L}_{P}(t) = \mathbb{E}_{\xi \sim P}\left[\gamma(t;\xi)
ight] = P\gamma(t)$$

minimal at $t = s^{\star}$

Contrast function: $\gamma : \mathbb{S} \times \Xi \mapsto [0, +\infty)$

Excess loss

$$\ell(s^{\star},t) = P\gamma(t) - P\gamma(s^{\star})$$

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- Data: $(X_1, Y_1), \ldots, (X_n, Y_n) \in \Xi = \mathcal{X} \times \mathcal{Y}$
- Goal: predict Y given X with $(X, Y) = \xi \sim P$
- s^{*}(X) is the "best predictor" of Y given X, i.e., s^{*} minimizes the loss function

$$P\gamma(t)$$
 with $\gamma(t;(x,y)) = d(t(x),y)$

measuring some "distance" between y and the prediction t(x).

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Example: regression							

- prediction with $\mathcal{Y} = \mathbb{R}$
- Data: $(X_1, Y_1), \dots, (X_n, Y_n)$ i.i.d.

 $Y_i = \eta(X_i) + \varepsilon_i$ with $\mathbb{E}[\varepsilon_i \mid X_i] = 0$





- prediction with $\mathcal{Y} = \mathbb{R}$
- Data: $(X_1, Y_1), \dots, (X_n, Y_n)$ i.i.d.

 $Y_i = \eta(X_i) + \varepsilon_i$ with $\mathbb{E}[\varepsilon_i \mid X_i] = 0$

• least-squares contrast: $\gamma(t; (x, y)) = (t(x) - y)^2$

$$\Rightarrow \quad s^{\star} = \eta \quad \text{and} \quad \ell\left(s^{\star}, t\right) = \|t - \eta\|_{2}^{2} = \mathbb{E}\left[\left(t(X) - \eta(X)\right)^{2}\right]$$

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•
$$(X_1, \ldots, X_n) = (x_1, \ldots, x_n)$$
 deterministic

 $Y = F + \varepsilon \in \mathbb{R}^n$ with $F = (\eta(x_1), \dots, \eta(x_n)) \in \mathbb{R}^n$

and $\varepsilon_1, \ldots, \varepsilon_n$ centered and independent.

•
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• Homoscedastic case: $\varepsilon_1, \ldots, \varepsilon_n$ i.i.d.

•
$$(X_1, \ldots, X_n) = (x_1, \ldots, x_n)$$
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 $Y = F + \varepsilon \in \mathbb{R}^n$ with $F = (\eta(x_1), \dots, \eta(x_n)) \in \mathbb{R}^n$

and $\varepsilon_1, \ldots, \varepsilon_n$ centered and independent.

- Homoscedastic case: $\varepsilon_1, \ldots, \varepsilon_n$ i.i.d.
- Quadratic loss of $t \in \mathbb{S} = \mathbb{R}^n$:

$$\mathcal{L}_{P}(t) = \mathbb{E}_{Y}\left[\frac{1}{n} \|Y - t\|^{2}\right] = \mathbb{E}_{Y}\left[\frac{1}{n}\sum_{i=1}^{n}(Y_{i} - t_{i})^{2}\right]$$

$$\Rightarrow \quad s^{*} = F \quad \text{and} \quad \ell(s^{*}, t) = \frac{1}{n}\|F - t\|^{2} = \frac{1}{n}\sum_{i=1}^{n}(\eta(x_{i}) - t_{i})^{2}$$



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Example: regression: fixed vs. random design

Learning

Random designFixed design
$$D_n$$
 $(X_i, Y_i)_{1 \le i \le n}$ i.i.d. $\sim P$ $Y = F + \varepsilon \in \mathbb{R}^n$ $(X_{n+1}, Y_{n+1}) \sim P$ $X_{n+1} \sim \mathcal{U}(x_1, \dots, x_n)$ \mathbb{S} $t : \mathcal{X} \to \mathbb{R}$ $t \in \mathbb{R}^n$ $P\gamma(t)$ $\mathbb{E}_{(X,Y)\sim P} \left[(Y - t(X))^2 \right]$ $E_Y \left[\frac{1}{n} ||Y - t||^2 \right]$ s^* $\eta : x \to \mathbb{E} \left[Y | | X = x \right]$ $F = (\eta(x_1), \dots, \eta(x_n))$ $\ell(s^*, t)$ $\mathbb{E}_{(X,Y)\sim P} \left[(t(X) - \eta(X))^2 \right]$ $\frac{1}{n} ||F - t||^2$ with $\forall x \in \mathbb{R}^n$ $||x||^2 = \sum_{i=1}^n x_i^2$

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Example: regression: fixed vs. random design

Learning

Random designFixed design
$$D_n$$
 $(X_i, Y_i)_{1 \le i \le n}$ i.i.d. $\sim P$ $Y = F + \varepsilon \in \mathbb{R}^n$ $(X_{n+1}, Y_{n+1}) \sim P$ $X_{n+1} \sim \mathcal{U}(x_1, \dots, x_n)$ \mathbb{S} $t : \mathcal{X} \to \mathbb{R}$ $t \in \mathbb{R}^n$ $P\gamma(t)$ $\mathbb{E}_{(X,Y)\sim P}\left[(Y - t(X))^2\right]$ $E_Y\left[\frac{1}{n} ||Y - t||^2\right]$ s^* $\eta : x \to \mathbb{E}\left[Y \mid X = x\right]$ $F = (\eta(x_1), \dots, \eta(x_n))$ $\ell(s^*, t)$ $\mathbb{E}_{(X,Y)\sim P}\left[(t(X) - \eta(X))^2\right]$ $\frac{1}{n} ||F - t||^2$ with $\forall x \in \mathbb{R}^n$ $||x||^2 = \sum_{i=1}^n x_i^2$

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Example: classification (prediction, $\mathcal{X} = \mathbb{R}$, $\mathcal{Y} = \{0, 1\}$)



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Estimators: example: regressogram



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• Natural idea: minimize an estimator of the risk $\frac{1}{n} ||F - t||^2$

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Least-squares estimators

Estimators

- Natural idea: minimize an estimator of the risk $\frac{1}{n} ||F t||^2$
- Least-squares criterion:

$$\frac{1}{n} \|t - Y\|^2 = \frac{1}{n} \sum_{i=1}^n (t_i - Y_i)^2$$
$$\forall t \in \mathbb{S} , \qquad \mathbb{E}\left[\frac{1}{n} \|t - Y\|^2\right] = \frac{1}{n} \|F - t\|^2 + \frac{1}{n} \mathbb{E}\left[\|\varepsilon\|^2\right]$$

Least-squares estimators

Estimators

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- Natural idea: minimize an estimator of the risk $\frac{1}{n} ||F t||^2$
- Least-squares criterion:

Model selection

$$\frac{1}{n} \|t - Y\|^2 = \frac{1}{n} \sum_{i=1}^n (t_i - Y_i)^2$$
$$\forall t \in \mathbb{S} , \qquad \mathbb{E}\left[\frac{1}{n} \|t - Y\|^2\right] = \frac{1}{n} \|F - t\|^2 + \frac{1}{n} \mathbb{E}\left[\|\varepsilon\|^2\right]$$

• Model: $S \subset \mathbb{S} \Rightarrow$ Least-squares estimator on S:

$$\widehat{F}_{\mathcal{S}} \in \arg\min_{t \in \mathcal{S}} \left\{ \frac{1}{n} \|t - Y\|^2 \right\} = \arg\min_{t \in \mathcal{S}} \left\{ \frac{1}{n} \sum_{i=1}^n (t_i - Y_i)^2 \right\}$$

so that

 $\widehat{F}_{S} = \prod_{S}(Y)$ (orthogonal projection)

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 Model
 examples

- \bullet histograms on some partition Λ of ${\mathcal X}$
 - \Rightarrow the least-squares estimator (regressogram) can be written

$$\widehat{F}_{\Lambda}(x_i) = \sum_{\lambda \in \Lambda} \widehat{\beta}_{\lambda} \mathbb{1}_{x_i \in \lambda} \qquad \widehat{\beta}_{\lambda} = \frac{1}{\operatorname{Card} \left\{ x_i \in \lambda \right\}} \sum_{x_i \in \lambda} Y_i$$

- subspace generated by a subset of an orthogonal basis of $L^2(\mu)$ (Fourier, wavelets, and so on)
- variable selection: $x_i = (x_i^{(1)}, \dots, x_i^{(p)}) \in \mathbb{R}^p$ gathers p variables that can (linearly) explain Y_i

$$\forall m \subset \{1, \dots, p\}$$
, $S_m = \operatorname{vect}\left\{x^{(j)} \text{ s.t. } j \in m\right\}$

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Model selection: regular regressograms



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- Collection of candidate models: $(S_m)_{m \in \mathcal{M}}$
- Problem: choosing among $(\widehat{F}_m)_{m \in \mathcal{M}}$

with
$$\widehat{F}_m = \widehat{F}_{S_m} = \Pi_{S_m}(Y) = \Pi_m(Y)$$
.

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Model selection via penalization, resampling and cross-validation, with application to change-point detection

Learning Estimators Model selection Oracle inequality Cha cocococococo Goodo Cococo Cococo Cococo Goal: estimation or prediction

• Main goal: find \widehat{m} minimizing $\frac{1}{n} \left\| F - \widehat{F}_{\widehat{m}} \right\|^2$ • Oracle: $m^* \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| F - \widehat{F}_m \right\|^2 \right\}$

Goal: estimation or prediction

• Main goal: find \widehat{m} minimizing $\frac{1}{n} \left\| F - \widehat{F}_{\widehat{m}} \right\|^2$ • Oracle: $m^* \in \arg\min\left\{ \sum_{n=1}^{n} \int_{-\infty}^{1} \left\| F - \widehat{F}_{\widehat{m}} \right\|^2 \right\}$

Model selection

- Oracle: $m^* \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| F \widehat{F}_m \right\|^2 \right\}$
- Oracle inequality (in expectation or with high probability):

$$\frac{1}{n}\left\|F-\widehat{F}_{\widehat{m}}\right\|^{2} \leq C \inf_{m \in \mathcal{M}_{n}}\left\{\frac{1}{n}\left\|F-\widehat{F}_{m}\right\|^{2}\right\} + R_{n}$$

• Non-asymptotic: all parameters can vary with n, in particular the collection $\mathcal{M} = \mathcal{M}_n$

Goal: estimation or prediction

- Main goal: find \widehat{m} minimizing $\frac{1}{n} \left\| F \widehat{F}_{\widehat{m}} \right\|^2$
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- Non-asymptotic: all parameters can vary with n, in particular the collection $\mathcal{M} = \mathcal{M}_n$
- Adaptation (e.g., in the minimax sense) to the regularity of F, and so on (if (S_m)_{m∈M_n} is well chosen)

Model selection Oracle

Oracle inequality



- Additional assumption (model selection case): $F \in S_{m_0}$ for some $m_0 \in \mathcal{M}_n$
- Additional goal: select $\widehat{m} = m_0$ with a maximal probability
- Consistency:

$$\mathbb{P}\left(\,\widehat{m}=m_0\,\right) \xrightarrow[n\to\infty]{} 1$$



- Additional assumption (model selection case): $F \in S_{m_0}$ for some $m_0 \in \mathcal{M}_n$
- Additional goal: select $\widehat{m} = m_0$ with a maximal probability
- Consistency:

$$\mathbb{P}\left(\,\widehat{m}=m_0\,\right)\xrightarrow[n\to\infty]{}1$$

 Estimation and identification (AIC-BIC dilemma)? Contradictory goals in general (Yang, 2005) Sometimes possible to share the strengths of both approaches (e.g., Yang, 2005; van Erven et al., 2008)
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$$Y = F + \varepsilon$$
 with $\mathbb{E}\left[\varepsilon_i^2\right] = \sigma^2$

$$\widehat{F}_m = \Pi_m Y$$
 with $\Pi_m = \Pi_m^ op = \Pi_m^2$ and $\operatorname{tr}(\Pi_m) = \operatorname{dim}(S_m) = D_m$

 \Rightarrow Bias-variance decomposition of the risk

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$$\widehat{F}_m = \Pi_m Y$$
 with $\Pi_m = \Pi_m^ op = \Pi_m^2$ and $\operatorname{tr}(\Pi_m) = \dim(S_m) = D_m$

 \Rightarrow Bias-variance decomposition of the risk

$$F_m := \arg\min_{t \in S_m} \left\{ \frac{1}{n} \|F - t\|^2 \right\} = \Pi_m F$$
$$\mathbb{E}\left[\frac{1}{n} \|\widehat{F}_m - F\|^2 \right] = \frac{1}{n} \|(\Pi_m - I)F\|^2 + \frac{\sigma^2 D_m}{n}$$
$$= \text{Bias} + \text{Variance}$$

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Model selection: bias and variance

$$\mathbb{E}\left[\frac{1}{n}\left\|F-\widehat{F}_{m}\right\|^{2}\right] = \text{Bias} + \text{Variance}$$

Bias or Approximation error

$$\frac{1}{n} \left\| F - F_m \right\|^2 := \inf_{t \in S_m} \left\{ \frac{1}{n} \left\| F - t \right\|^2 \right\}$$

Variance or Estimation error

$$\frac{\sigma^2 D_m}{n}$$





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Model selection: bias and variance

$$\mathbb{E}\left[\frac{1}{n}\left\|F-\widehat{F}_{m}\right\|^{2}\right] = \text{Bias} + \text{Variance}$$

Bias or Approximation error

$$\frac{1}{n} \left\| F - F_m \right\|^2 := \inf_{t \in S_m} \left\{ \frac{1}{n} \left\| F - t \right\|^2 \right\}$$

Variance or Estimation error

$$\frac{\sigma^2 D_m}{n}$$



Bias-variance trade-off \Rightarrow avoid over-fitting and under-fitting

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Model selection

Unbiased risk estimation principle

$$\widehat{m} \in \arg \min_{m \in \mathcal{M}_n} \{\operatorname{crit}(m)\}$$
$$\operatorname{crit}_{\operatorname{id}}(m) = \frac{1}{n} \left\| F - \widehat{F}_m \right\|^2$$
$$\operatorname{rit}(m) \approx \mathbb{E} \left[\frac{1}{n} \left\| F - \widehat{F}_m \right\|^2 \right]$$

$$\Rightarrow$$
 valid if Card(\mathcal{M}_n) is not too large (+ concentration inequalities)

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Penalization

• Penalization: crit
$$(m) = \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \operatorname{pen}(m)$$

$$\widehat{m} \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \operatorname{pen}(m) \right\}$$

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Penalization

• Penalization: crit
$$(m) = \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \operatorname{pen}(m)$$

$$\widehat{m} \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \operatorname{pen}(m) \right\}$$

Ideal penalty:

$$\mathsf{pen}_{\mathrm{id}}(m) = rac{1}{n} \left\| F - \widehat{F}_m \right\|^2 - rac{1}{n} \left\| \widehat{F}_m - Y \right\|^2$$

• Mallows' heuristics: $pen(m) \approx \mathbb{E}[pen_{id}(m)] \Rightarrow oracle inequality$

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 Computation of the ideal penalty and its expectation
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Recall that

$$Y = F + \varepsilon \quad \text{with} \quad \mathbb{E}\left[\varepsilon_i^2\right] = \sigma^2$$
$$\widehat{F}_m = \Pi_m Y \quad \text{with} \quad \Pi_m = \Pi_m^\top = \Pi_m^2 \quad \text{and} \quad \operatorname{tr}(\Pi_m) = D_m$$
$$\mathbb{E}\left[\frac{1}{n} \left\|\widehat{F}_m - F\right\|^2\right] = \frac{1}{n} \left\|(\Pi_m - I)F\right\|^2 + \frac{\sigma^2 D_m}{n}$$

 \Rightarrow Empirical risk? Ideal penalty? Expectations?

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Recall that

$$Y = F + \varepsilon \quad \text{with} \quad \mathbb{E}\left[\varepsilon_{i}^{2}\right] = \sigma^{2}$$
$$\widehat{F}_{m} = \Pi_{m}Y \quad \text{with} \quad \Pi_{m} = \Pi_{m}^{\top} = \Pi_{m}^{2} \quad \text{and} \quad \operatorname{tr}(\Pi_{m}) = D_{m}$$
$$= \begin{bmatrix} 1 & \|\widehat{\omega}\|_{\infty} & \|u\|_{\infty}^{2} \end{bmatrix} \quad \frac{1}{2} \|u\|_{\infty} = \|u\|_{\infty}^{2} \quad \sigma^{2}D_{m}$$

$$\mathbb{E}\left[\frac{1}{n}\left\|\widehat{F}_m - F\right\|^2\right] = \frac{1}{n}\left\|(\Pi_m - I)F\right\|^2 + \frac{\sigma^2 D_m}{n}$$

 \Rightarrow Empirical risk? Ideal penalty? Expectations?

$$pen_{id}(m) = \frac{2}{n} \langle \Pi_m \varepsilon, \varepsilon \rangle + \frac{2}{n} \langle (\Pi_m - I_n) F, \varepsilon \rangle$$
$$\mathbb{E}[pen_{id}(m)] = \frac{2\sigma^2 D_m}{n} \qquad \Rightarrow \quad C_p \text{ (Mallows, 1973)}$$

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• C_p (Mallows, 1973; regression, least-squares estimator):

 $2\sigma^2 D_m/n$

• C_L (Mallows, 1973; regression, linear estimator $\hat{F}_m = A_m Y$):

 $2\sigma^2 \operatorname{tr}(A_m)/n$

• AIC (Akaike, 1973; log-likelihood, p degrees of freedom):

2**p**/n

• BIC (Schwarz, 1978; log-likelihood, identification goal):

 $\ln(n)p/n$

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Unbiased risk estimation principle

Heuristics:

$$\mathbb{E}[\operatorname{crit}(m)] \approx \mathbb{E}\left[\frac{1}{n} \left\|F - \widehat{F}_{m}\right\|^{2}\right] \quad \Leftrightarrow \quad \mathbb{E}[\operatorname{pen}(m)] \approx \mathbb{E}[\operatorname{pen}_{\operatorname{id}}(m)]$$

Examples:

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- FPE (Akaike, 1970), SURE (Stein, 1981)
- some kinds of cross-validation (e.g., leave-p-out, $p \ll n$)
- log-likelihood: AIC (Akaike, 1973), AICc (Sugiura, 1978; Hurvich & Tsai, 1989)
- least-squares: C_p, C_L (Mallows, 1973), GCV (Craven & Wahba, 1979)
- covariance penalties (Efron, 2004)
- bootstrap penalty (Efron, 1983), resampling (A., 2009)

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A key lemma					

Lemma

Let pen : $\mathcal{M}_n \mapsto \mathbb{R}$ some penalty (possibly data-dependent). On the event Ω on which for every $m, m' \in \mathcal{M}_n$,

$$egin{aligned} (\operatorname{\mathsf{pen}}(m) - \operatorname{\mathsf{pen}}_{\operatorname{id}}(m)) - ig(\operatorname{\mathsf{pen}}(m') - \operatorname{\mathsf{pen}}_{\operatorname{id}}(m')ig) \ &\leq \mathcal{A}(m) + \mathcal{B}(m') \end{aligned}$$

we have
$$\forall \widehat{m} \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \operatorname{pen}(m) \right\}$$

 $\frac{1}{n} \left\| \widehat{F}_{\widehat{m}} - F \right\|^2 - B(\widehat{m}) \leq \inf_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 + A(m) \right\}$

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Assumptions:

- Fixed design regression, least-squares contrast
- Gaussian homoscedastic noise: $\varepsilon \sim \mathcal{N}(0, \sigma^2)$
- Model collection of polynomial complexity: $Card(\mathcal{M}_n) \leq Cn^{\alpha}$
- For all $m \in \mathcal{M}_n$, $\widehat{F}_m = \prod_m Y$ (least-squares estimator)

Penalty

$$\mathsf{pen}(m) = rac{K\sigma^2 D_m}{n}$$
 with $K>1$

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$$-B(m) \le \operatorname{pen}(m) - \operatorname{pen}_{\operatorname{id}}(m) \le A(m)$$

$$\Rightarrow \qquad \frac{1}{n} \left\| \widehat{F}_{\widehat{m}} - F \right\|^2 - B(\widehat{m}) \le \inf_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 + A(m) \right\}$$

$$\mathsf{pen}_{\mathrm{id}}(m) = rac{2}{n} \langle \Pi_m \varepsilon, \, \varepsilon \rangle + rac{2}{n} \langle (\Pi_m - I_n) F, \, \varepsilon \rangle$$

First term has expectation $\frac{2\sigma^2 D_m}{n}$, the second term is centered.

Model selection via penalization, resampling and cross-validation, with application to change-point detection

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Two Gaussian concentration results (see Massart 2007):

Proposition

Let ξ be some standard Gaussian vector in \mathbb{R}^n , $\alpha \in \mathbb{R}^n$, $M \in \mathcal{M}_n(\mathbb{R})$. Then, for every $x \ge 0$,

$$\mathbb{P}\left(\left|\langle \xi, \alpha \rangle\right| \le \sqrt{2x} \left\|\alpha\right\|_{2}\right) \ge 1 - 2e^{-x}$$
$$\mathbb{P}\left(\left|\langle \xi, M\xi \rangle - \operatorname{tr}(M)\right| \le 2\sqrt{x \operatorname{tr}(M^{\top}M)} + 2\left\|\|M\|\|x\right) \ge 1 - 2e^{-x}$$

Model selection via penalization, resampling and cross-validation, with application to change-point detection



Sketch of the proof:

- For all $m \in \mathcal{M}_n$, concentrate $\langle \Pi_m \varepsilon, \varepsilon \rangle$ around $\sigma^2 D_m$ and $\langle (\Pi_m - I_n)F, \varepsilon \rangle$ around 0
- Apply the Lemma on the intersection of these Card(\mathcal{M}_n) events
- Control the remainder terms



Theorem (Birgé & Massart, 2001–2007)

For every $x \ge 0$, with probability at least $1 - 4 \operatorname{Card}(\mathcal{M}_n)e^{-x}$, for every

$$\widehat{m} \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| Y - \widehat{F}_m \right\|^2 + \frac{K \sigma^2 D_m}{n} \right\}$$

we get the oracle inequality $\forall \delta > 0$,

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}} - F \right\|^{2} \leq \left(\frac{1 + (K - 2)_{+}}{1 - (2 - K)_{+}} + \delta \right) \inf_{m \in \mathcal{M}_{n}} \left\{ \frac{1}{n} \left\| \widehat{F}_{m} - F \right\|^{2} \right\} + \frac{C(K) \times \sigma^{2}}{\delta n}$$

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Change-point detection: data



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Change-point detection: target function



Model selection via penalization, resampling and cross-validation, with application to change-point detection

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$$Y_i = \eta(t_i) + \varepsilon_i$$
 with $\mathbb{E}[\varepsilon_i] = 0$ $\mathbb{E}[\varepsilon_i^2] = \sigma^2 > 0$

- Goal: detect the change-points of the mean η of the signal Y
- ⇒ Model selection, collection of regressograms with $M_n = \mathfrak{P}_{interv}(\{t_1, \ldots, t_n\})$ (partitions into intervals)

with
$$F_i = \eta(t_i)$$

Model selection via penalization, resampling and cross-validation, with application to change-point detection

The previous oracle inequality is not sufficient

Problem :
$$Card(\mathcal{M}_n) = 2^{n-1}$$

Theorem (Birgé & Massart, 2001–2007)

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Model selection via penalization, resampling and cross-validation, with application to change-point detection

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Theorem (Birgé & Massart, 2001)

Let K > 1 and $(L_m)_{m \in M_n}$ be nonnegative weights such that $\sum_{m \in M_n} e^{-L_m D_m} = \Sigma < +\infty$. For every

$$\widehat{m} \in \arg\min_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| Y - \widehat{F}_m \right\|^2 + \frac{K\sigma^2 D_m}{n} \left(1 + \sqrt{2L_m} \right)^2 \right\}$$

we get the oracle inequality

$$\mathbb{E}\left[\frac{1}{n}\left\|F-\widehat{F}_{\widehat{m}}\right\|^{2}\right] \leq C(K)\inf_{m\in\mathcal{M}_{n}}\left\{\frac{1}{n}\left\|F-F_{m}\right\|^{2}+\operatorname{pen}(m)\right\} + \frac{C'(K)\Sigma\sigma^{2}}{n}$$

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Weights for change-point detection

If $L_m = L(D_m)$,

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Weights for change-point detection

If $L_m = L(D_m)$,

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$$\sum_{m \in \mathcal{M}_n} e^{-L_m D_m} = \sum_{D \ge 1} \operatorname{Card} \left\{ m \in \mathcal{M}_n \text{ s.t. } D_m = D \right\} e^{-DL(D)}$$
$$= \sum_{D \ge 1} \exp\left[-DL(D) + \ln\operatorname{Card} \left\{ m \in \mathcal{M}_n \text{ s.t. } D_m = D \right\} \right]$$

is finite by taking (for instance)

 $L(D) = \ln (\operatorname{Card} \{ m \in \mathcal{M}_n \text{ s.t. } D_m = D \}) + \alpha D \text{ with } \alpha > 0$,

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Weights for change-point detection

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and for change-point detection

$$\ln\left(\operatorname{Card}\left\{m\in\mathcal{M}_n \text{ s.t. } D_m=D\right\}\right) = \ln\binom{n-1}{D-1} \leq \frac{D}{\ln\left(\frac{en}{D}\right)}$$

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• Birgé-Massart theory + simulation experiments for optimizing the constants (Lebarbier, 2005):

$$\widehat{m} \in \operatorname{argmin}_{m \in \mathcal{M}_n} \left\{ \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \frac{C\sigma^2 D_m}{n} \left(5 + 2\ln\left(\frac{n}{D_m}\right) \right) \right\}$$

• Equivalent to aggregating models of the same dimension:

$$\widetilde{S}_{D} := \bigcup_{m \in \mathcal{M}_{n}, D_{m} = D} S_{m}$$

$$\widehat{F}_{D} \in \operatorname{argmin}_{t \in \widetilde{S}_{D}} \left\{ \frac{1}{n} \| t - Y \|^{2} \right\}$$

$$\widehat{D} \in \operatorname{argmin}_{1 \le D \le n} \left\{ \frac{1}{n} \| \widehat{F}_{D} - Y \|^{2} + \frac{C\sigma^{2}D}{n} \left(5 + 2\ln\left(\frac{n}{D}\right) \right) \right\}_{\frac{50}{50}}$$

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Computational complexity

- Dynamic programming algorithm (Bellman & Dreyfus, 1962)
- Key remark: $\widehat{F}_D = \widehat{F}_{\widehat{m}(D)}$ with

$$\widehat{m}(D) \in \operatorname*{argmin}_{m \in \mathcal{M}_n, D_m = D} \left\{ \sum_{\lambda \in m} f(\lambda) \right\} \quad \text{with} \quad f(\lambda) = \operatorname{var}\left((Y_i)_{i \in \lambda} \right)$$

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- Algorithm:
 - Compute f(λ) for all possible λ (n(n+1)/2 possible segments):

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 - **2** For $1 \le i \le k \le n$, let $\hat{m}_k(i)$ be a minimizer of the empirical risk over segmentations of $\{1, \ldots, k\}$ into *i* segments, and $R_k(i)$ the corresponding empirical risk. Then, $\{\hat{m}_k(1), \ldots, \hat{m}_k(k)\}$ and $\{R_k(1), \ldots, R_k(k)\}$ can be computed sequentially from k = 1 to k = n.

Computational complexity

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- Algorithm:
 - Compute f(λ) for all possible λ (n(n + 1)/2 possible segments):

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- \Rightarrow complexity $\mathcal{O}(n^2)$
 - Remark: can be done faster with pruning (Rigaill, 2011)

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- penalization:
 - Baraud, Giraud & Huet 2009: multiplicative penalty, Gaussian noise
 - Zhang & Siegmund, 2007: modified BIC
 - see also Lavielle, 2005
- cross-validation (third lecture; A. & Celisse, 2010)
- Picard *et al.*, 2005: penalized maximum likelihood, looks for change-points of (η, σ) , assuming a Gaussian model

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Conclus	sion				

- bias-variance trade-off for model selection (overfitting vs. underfitting)
- model selection via penalization: E [pen_{id}(m)] leads to an oracle inequality for polynomial collection of models
- possible extension to exponential collections, with larger penalties example: change-point detection
- related problem: data-driven calibration of constants in the penalty (σ^2): slope heuristics

http://www.di.ens.fr/~arlot/2012cergy.htm