

Estimator selection  
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Cross-validation  
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CV for risk estimation  
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CV for estimator selection  
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Large  $\mathcal{M}$   
oooooooo  
Conclusion  
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## Cross-validation for estimator selection

Sylvain Arlot (joint works with Alain Celisse, Matthieu Lerasle,  
Nelo Magalhães)

<sup>1</sup>CNRS

<sup>2</sup>École Normale Supérieure (Paris), DI/ENS, Équipe SIERRA

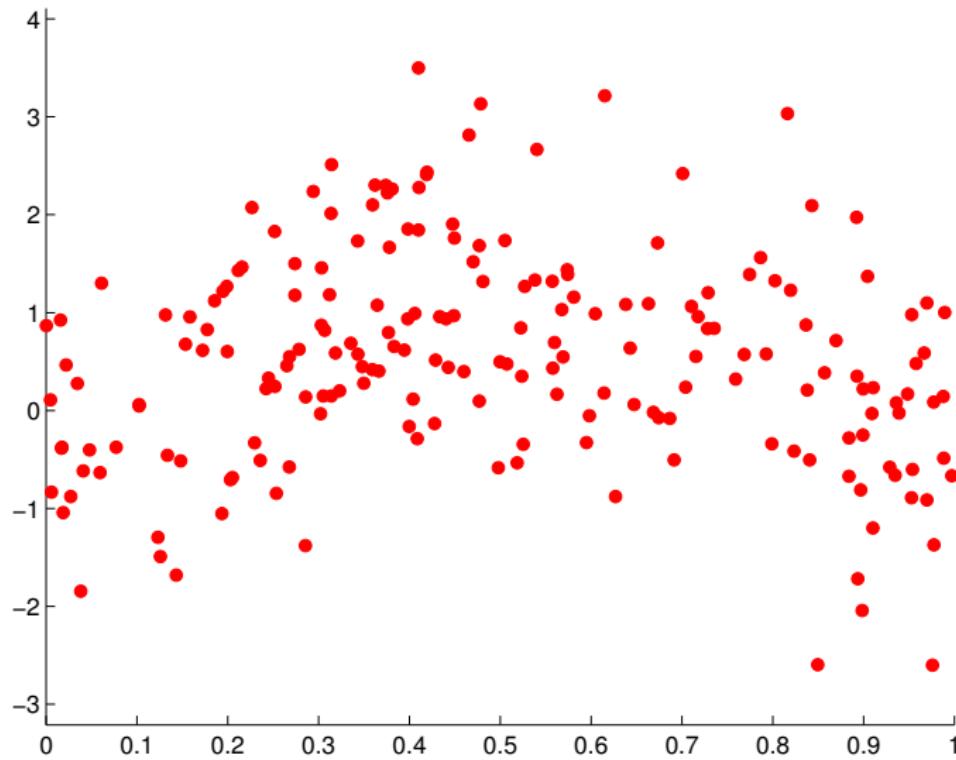
IHP, Paris  
April, 9th, 2015

Main reference (survey): arXiv:0907.4728

# Outline

- 1 Estimator selection
- 2 Cross-validation
- 3 Cross-validation for risk estimation
- 4 Cross-validation for estimator selection
- 5 Large  $\mathcal{M}$
- 6 Conclusion

## Regression: data $(X_1, Y_1), \dots, (X_n, Y_n)$



## Estimator selection

## Cross-validation

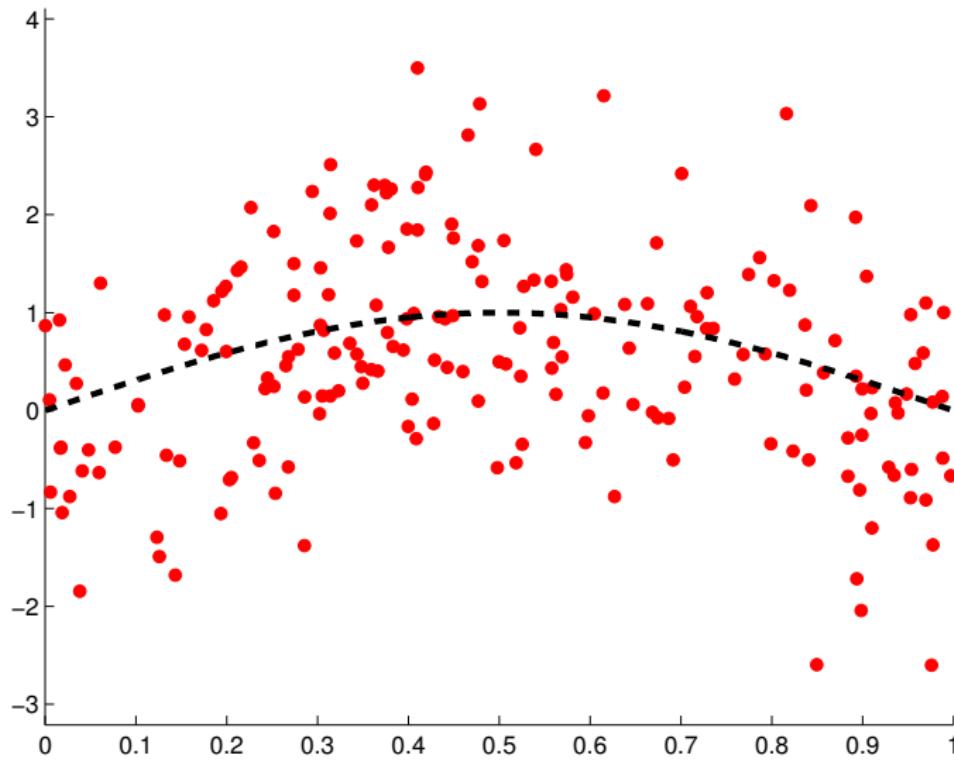
## CV for risk estimation

CV for estimator selection

Large  $M$

## Conclusion

Goal: predict  $Y$  given  $X$ , i.e., denoising



## Prediction problem / regression

- Data  $D_n$ :  $(X_1, Y_1), \dots, (X_n, Y_n) \in \mathcal{X} \times \mathcal{Y}$  (i.i.d.  $\sim P$ )
  - Contrast  $\gamma(t; (x, y))$  measures how well  $t(x)$  “predicts”  $y$
  - Goal: learn  $t \in \mathbb{S} = \{ \text{measurable functions } \mathcal{X} \rightarrow \mathcal{Y} \}$  s.t.  $\mathbb{E}_{(X, Y) \sim P} [\gamma(t; (X, Y))] =: P\gamma(t)$  is minimal.

## Prediction problem / regression

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 $\mathbb{E}_{(X, Y) \sim P} [\gamma(t; (X, Y))] =: P\gamma(t)$  is minimal.
  - Example: regression  $\mathcal{Y} = \mathbb{R}$ ,  
least-squares contrast  $\gamma(t; (x, y)) = (t(x) - y)^2$   
 $s^* \in \operatorname{argmin}_{t \in \mathbb{S}} P\gamma(t)$  is the regression function:  
 $s^*(X) = \mathbb{E}[Y | X]$

⇒ excess loss

$$\ell(s^*, t) := P\gamma(t) - P\gamma(s^*) = \mathbb{E} \left[ (t(X) - s^*(X))^2 \right]$$

Estimator selection  
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Cross-validation  
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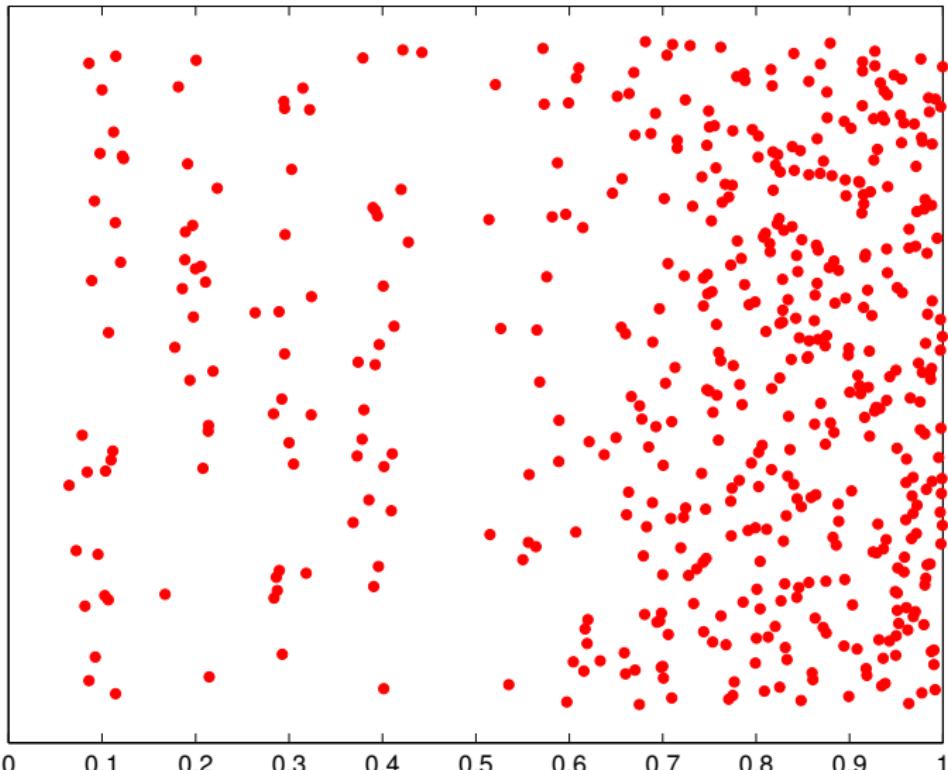
CV for risk estimation  
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CV for estimator selection  
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Large  $\mathcal{M}$   
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Conclusion  
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## Density estimation: data $\xi_1, \dots, \xi_n$



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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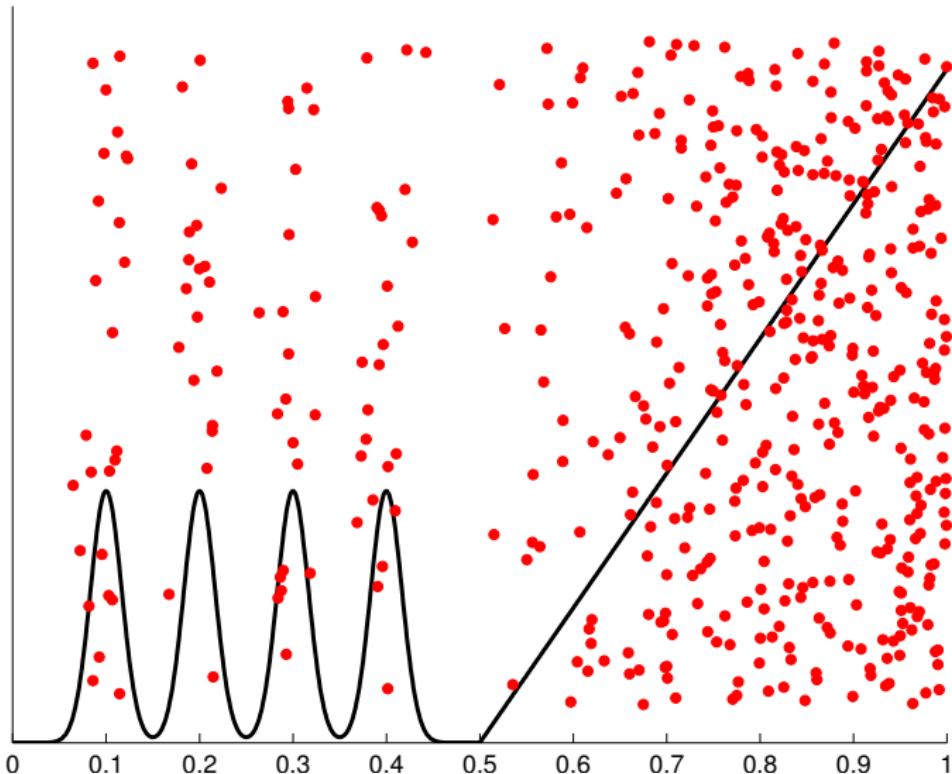
Large  $\mathcal{M}$ 

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Conclusion

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Goal: estimate the common density  $s^*$  of  $\xi_i$



# Problem: density estimation

- Data  $D_n$ :  $\xi_1, \dots, \xi_n \in \Xi$  (i.i.d.  $\sim P$ , density  $s^*$  w.r.t.  $\mu$ )
- Least-squares contrast  $\gamma(t, \xi) = \|t\|_{L^2(\mu)}^2 - 2t(\xi)$
- Goal: learn  $t \in \mathbb{S} = \{\text{measurable functions } \Xi \rightarrow \mathbb{R}\}$  s.t.  
 $\mathbb{E}_{\xi \sim P} [\gamma(t; \xi)] =: P\gamma(t)$  is minimal.

# Problem: density estimation

- Data  $D_n$ :  $\xi_1, \dots, \xi_n \in \Xi$  (i.i.d.  $\sim P$ , density  $s^*$  w.r.t.  $\mu$ )
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- Goal: learn  $t \in \mathbb{S} = \{\text{measurable functions } \Xi \rightarrow \mathbb{R}\}$  s.t.  $\mathbb{E}_{\xi \sim P} [\gamma(t; \xi)] =: P\gamma(t)$  is minimal.

$$P\gamma(t) = \int t^2 d\mu - 2 \int ts^* d\mu = \int (t - s^*)^2 d\mu - \|s^*\|_{L^2(\mu)}^2$$

$\Rightarrow$  the true density  $s^* \in \operatorname{argmin}_{t \in \mathbb{S}} P\gamma(t)$  and the excess loss is

$$\ell(s^*, t) := P\gamma(t) - P\gamma(s^*) = \|t - s^*\|_{L^2(\mu)}^2$$

# General setting

- Data  $\xi_1, \dots, \xi_n \in \Xi$  i.i.d. with distribution  $P$   
prediction:  $\xi_i = (X_i, Y_i) \in \mathcal{X} \times \mathcal{Y}$
- Goal: Estimate some feature  $s^* \in \mathbb{S}$  of  $P$   
density, regression function, Bayes predictor...
- Contrast function  $\gamma : \mathbb{S} \times \Xi \rightarrow \mathbb{R}$  such that

$$s^* \in \operatorname{argmin}_{t \in \mathbb{S}} \{P\gamma(t)\} \quad \text{with} \quad P\gamma(t) := \mathbb{E}_{\xi \sim P} [\gamma(t; \xi)]$$

- Excess loss

$$\ell(s^*, t) := P\gamma(t) - P\gamma(s^*) \geq 0$$

# Examples

- **Prediction:**  $\xi_i = (X_i, Y_i)$   
 $X_{n+1} \rightsquigarrow$  “predict”  $Y_{n+1}$  with  $t(X_{n+1})$ ?  
 $\gamma(t; (x, y))$  quantifies the “distance” between  $t(x)$  and  $y$

- **Regression** ( $\mathcal{Y} = \mathbb{R}$ ), least squares:

$$\gamma(t; (x, y)) = (t(x) - y)^2 \quad s^*(X) = \mathbb{E}[Y|X]$$

- **Binary classification** ( $\mathcal{Y} = \{0, 1\}$ ), 0–1 contrast:

$$\gamma(t; (x, y)) = 1_{t(x) \neq y}$$

- **Density estimation** (reference measure  $\mu$ ):

least squares:  $\gamma(t; \xi) = \|t\|_{L^2(\mu)}^2 - 2t(\xi)$

log-likelihood:  $\gamma(t; \xi) = -\log(t(\xi))$

Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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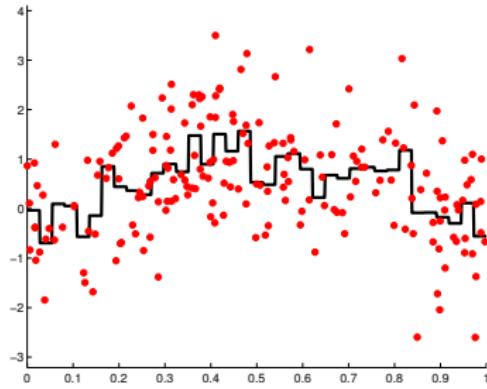
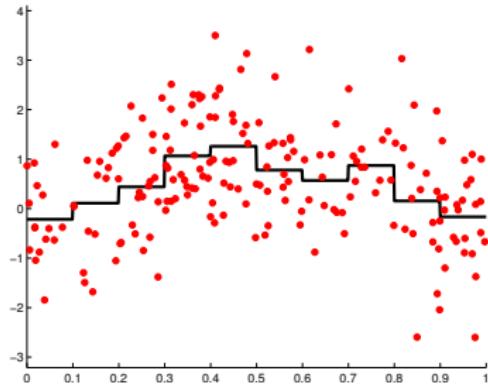
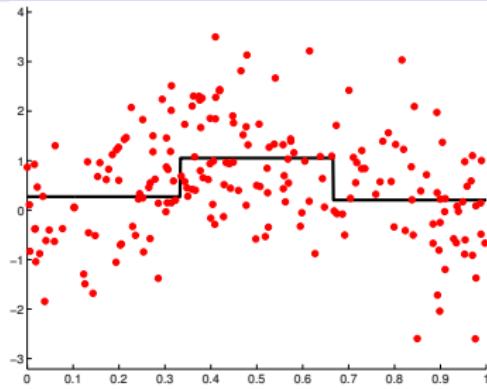
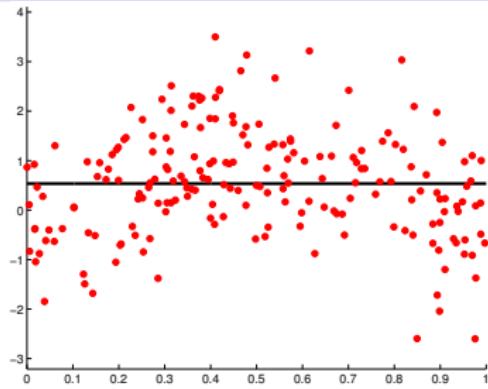
Large  $\mathcal{M}$ 

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Conclusion

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# Estimator selection (regression): regular regressograms



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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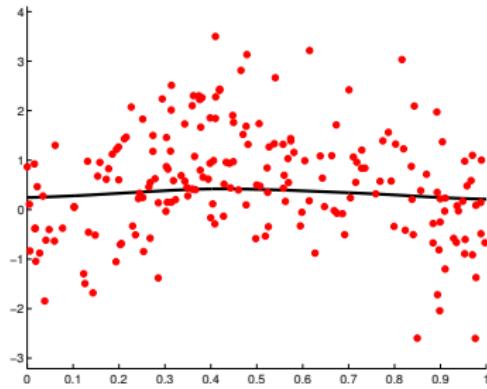
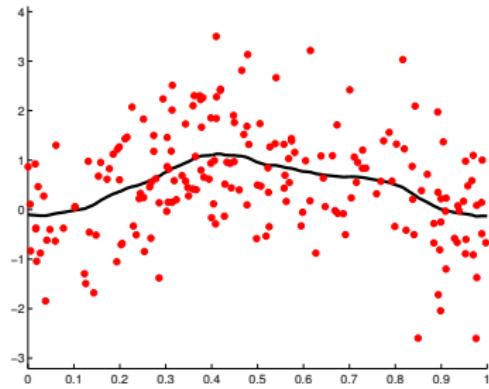
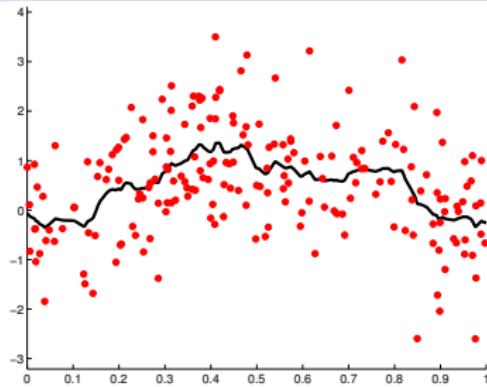
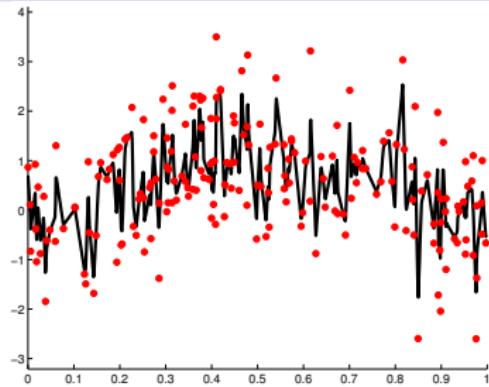
Large  $M$ 

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Conclusion

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# Estimator selection (regression): kernel ridge



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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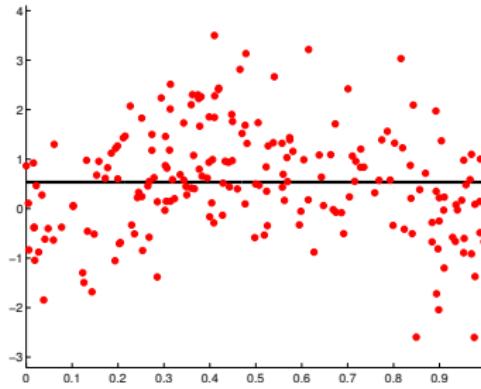
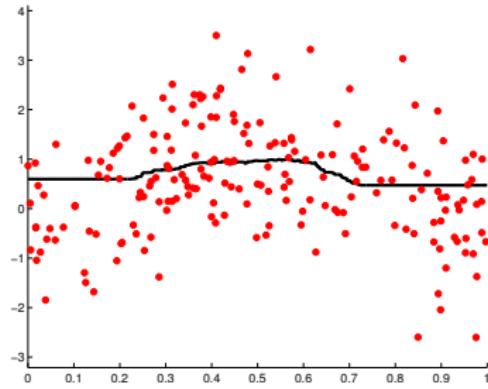
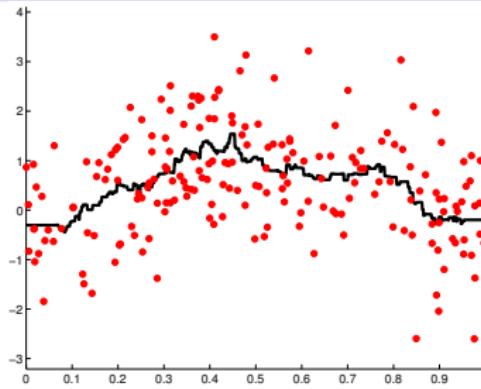
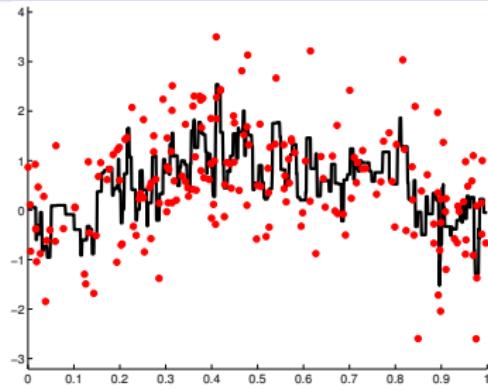
Large  $\mathcal{M}$ 

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Conclusion

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# Estimator selection (regression): $k$ nearest neighbours



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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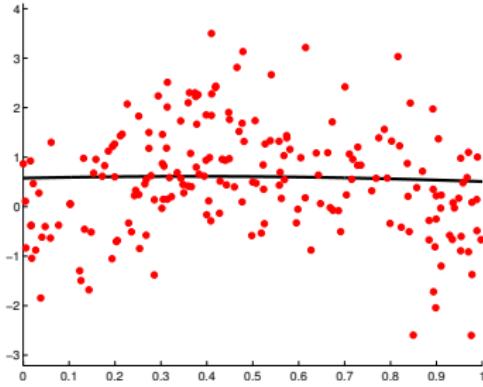
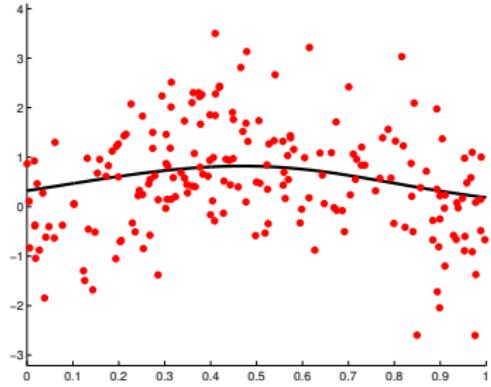
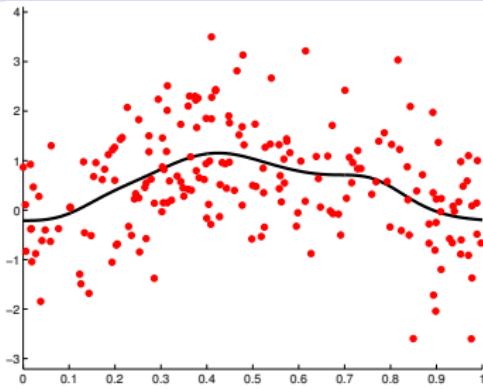
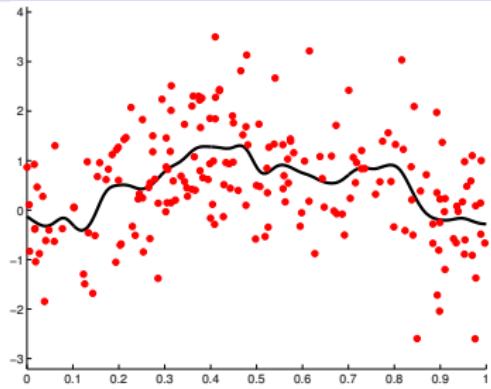
Large  $\mathcal{M}$ 

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Conclusion

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# Estimator selection (regression): Nadaraya-Watson



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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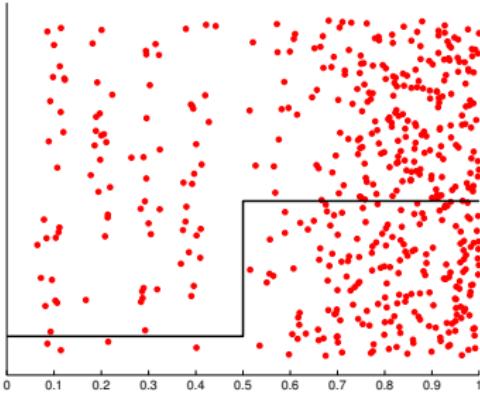
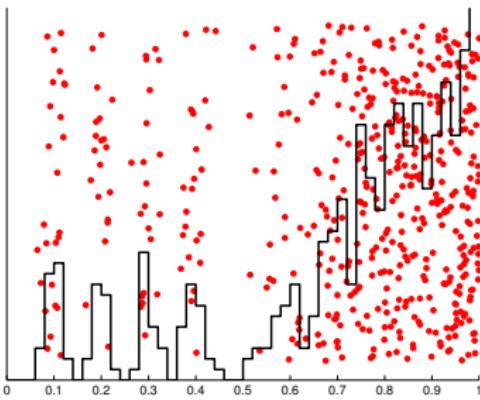
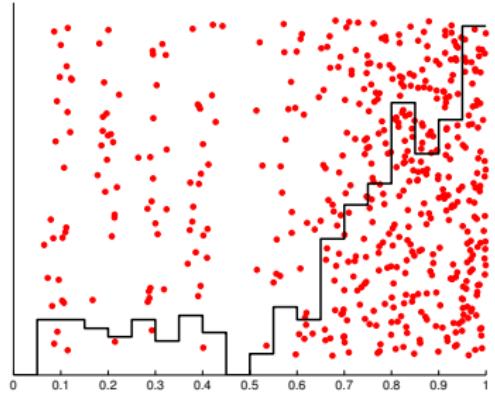
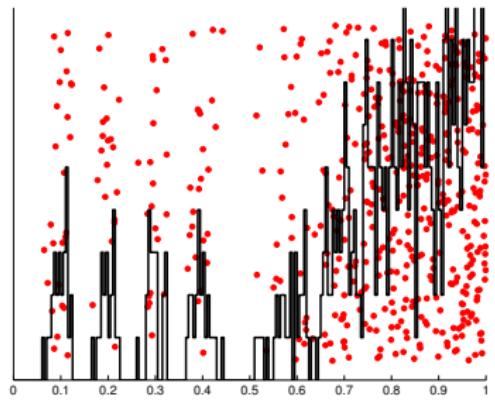
Large  $M$ 

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Conclusion

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## Estimator selection (density): regular histograms



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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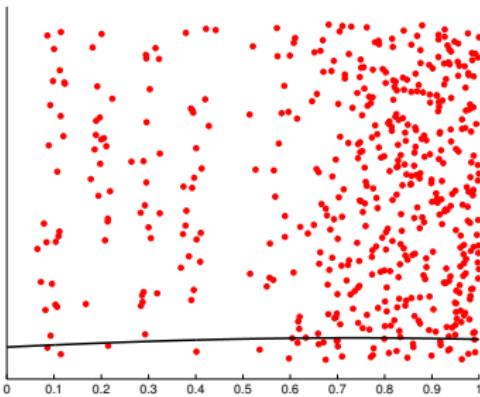
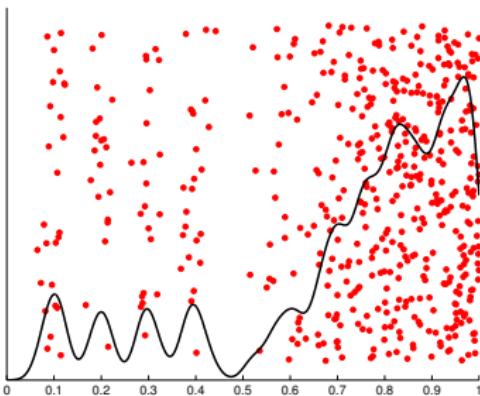
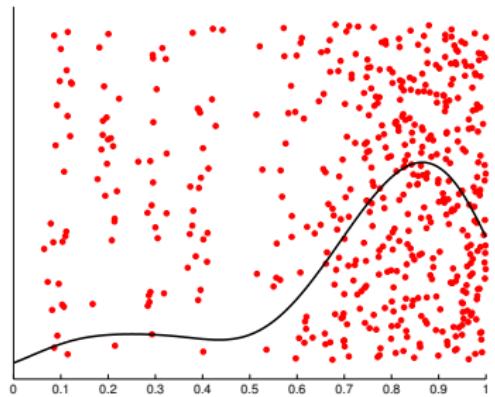
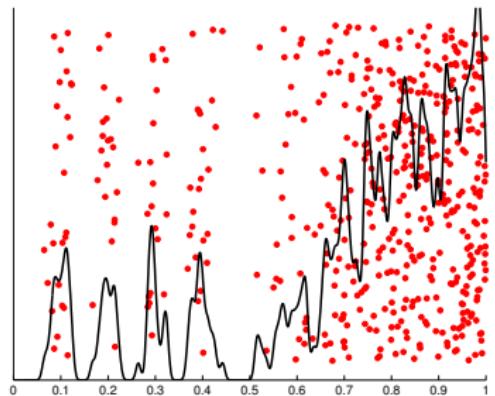
Large  $\mathcal{M}$ 

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Conclusion

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# Estimator selection (density): Parzen, Gaussian kernel



# Estimator selection

- Estimator/Learning algorithm:  $\hat{s} : D_n \mapsto \hat{s}(D_n) \in \mathbb{S}$
- Example: least-squares estimator on some model  $S_m \subset \mathbb{S}$

$$\hat{s}_m \in \operatorname{argmin}_{t \in S_m} \{P_n \gamma(t)\} \quad \text{where} \quad P_n \gamma(t) := \frac{1}{n} \sum_{\xi \in D_n} \gamma(t; \xi)$$

Examples of models: histograms,  $\operatorname{span}\{\varphi_1, \dots, \varphi_D\}$

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- Estimator collection  $(\hat{s}_m)_{m \in \mathcal{M}} \Rightarrow$  choose  $\hat{m} = \hat{m}(D_n)?$

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- Estimator collection  $(\hat{s}_m)_{m \in \mathcal{M}} \Rightarrow$  choose  $\hat{m} = \hat{m}(D_n)?$
- Examples:
  - model selection
  - calibration of tuning parameters (choosing  $k$  or the distance for  $k$ -NN, choice of a regularization parameter, choice of a kernel, etc.)
  - choice between different methods  
ex.:  $k$ -NN vs. smoothing splines?

## Estimator selection: two possible goals

- **Estimation goal:** minimize the risk of the final estimator, i.e., **Oracle inequality** (in expectation or with a large probability):

$$\ell(s^*, \hat{s}_{\hat{m}}) \leq C \inf_{m \in \mathcal{M}} \{\ell(s^*, \hat{s}_m)\} + R_n$$

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- **Identification goal:** select the (asymptotically) best model/estimator, assuming it is well-defined, i.e., Selection consistency:

$$\mathbb{P}(\hat{m}(D_n) = m^*) \xrightarrow{n \rightarrow \infty} 1.$$

Equivalent to estimation in the **parametric** setting.

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Equivalent to estimation in the **parametric** setting.

- Both goals with the same procedure (AIC-BIC dilemma)? **No** in general (Yang, 2005). Sometimes possible.

# Estimation goal: Bias-variance trade-off

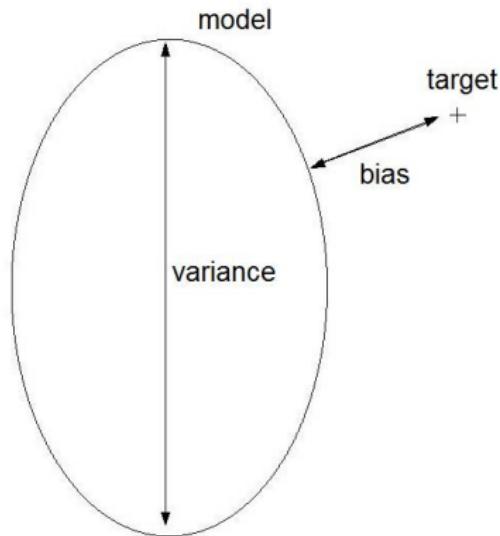
$$\mathbb{E} [\ell(s^*, \hat{s}_m)] = \text{Bias} + \text{Variance}$$

**Bias** or Approximation error

$$\ell(s^*, s_m^*) = \inf_{t \in S_m} \ell(s^*, t)$$

**Variance** or Estimation error

OLS in regression:  $\frac{\sigma^2 \dim(S_m)}{n}$



# Estimation goal: Bias-variance trade-off

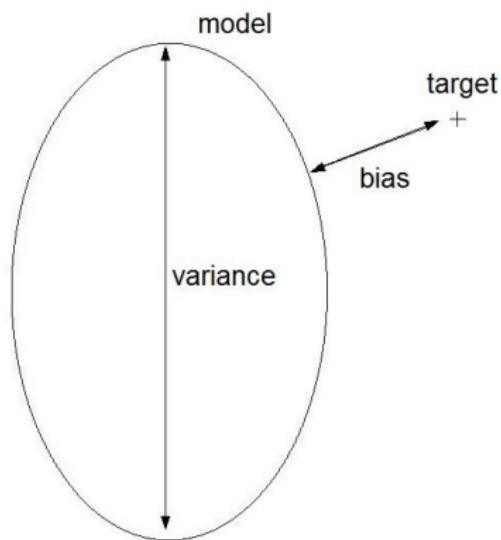
$$\mathbb{E} [\ell(s^*, \hat{s}_m)] = \text{Bias} + \text{Variance}$$

Bias or Approximation error

$$\ell(s^*, s_m^*) = \inf_{t \in S_m} \ell(s^*, t)$$

Variance or Estimation error

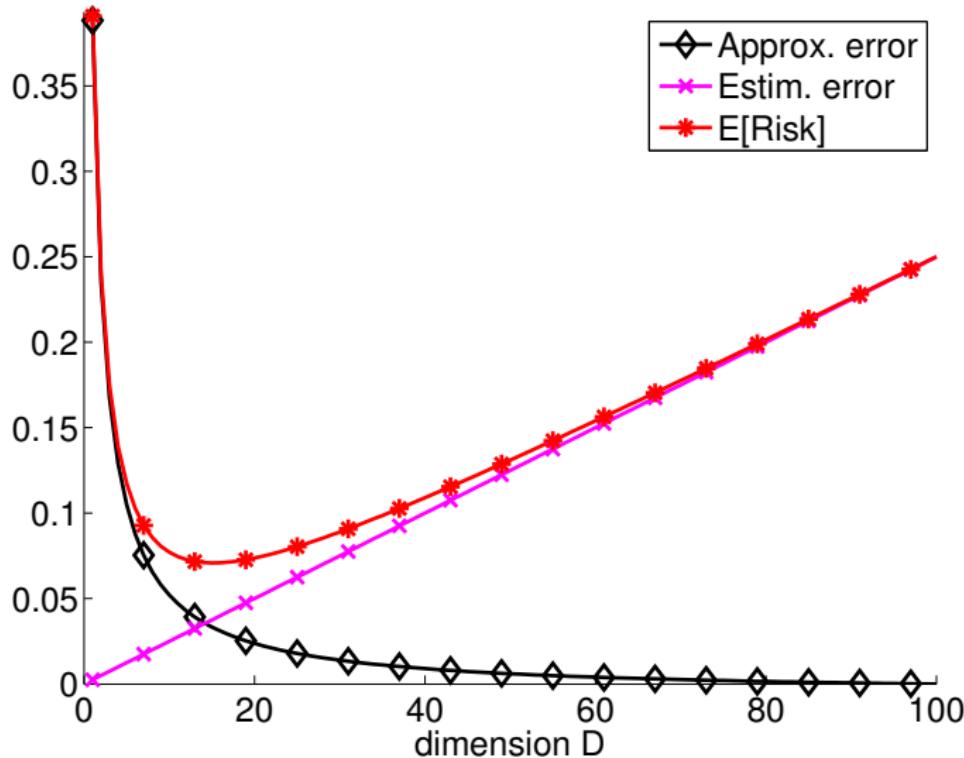
OLS in regression:  $\frac{\sigma^2 \dim(S_m)}{n}$



**Bias-variance trade-off**

↔ avoid **overfitting** and **underfitting**

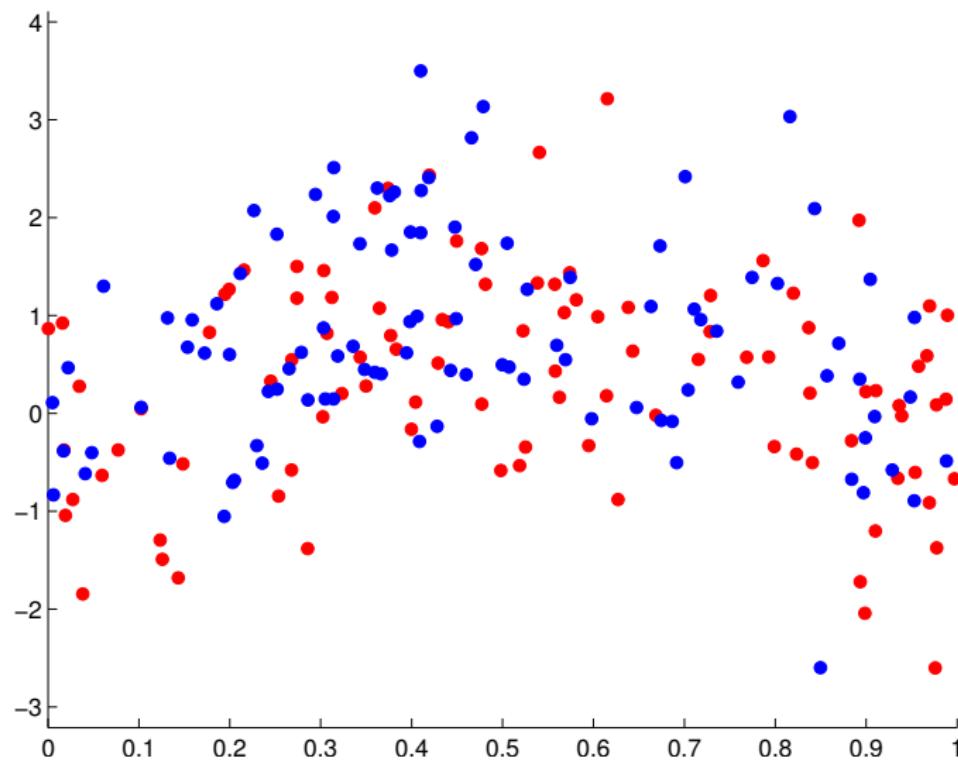
## Estimation goal: Bias-variance trade-off



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# Validation principle



Estimator selection  
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Cross-validation  
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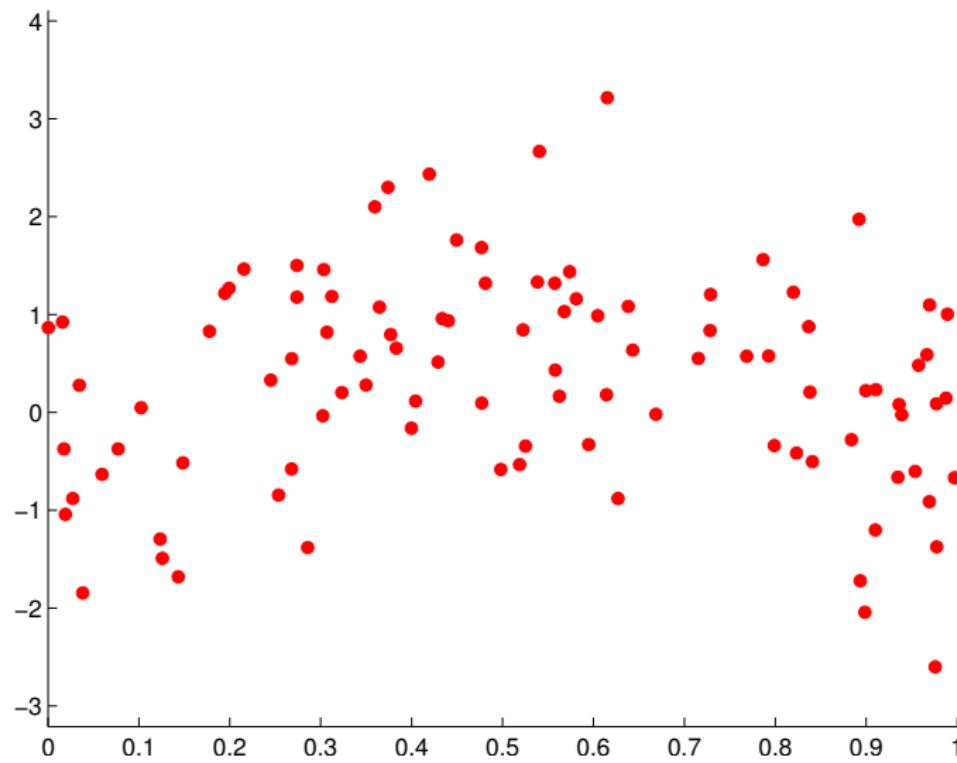
CV for risk estimation  
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CV for estimator selection  
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Large  $\mathcal{M}$   
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Conclusion  
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## Validation principle: learning sample



Estimator selection  
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Cross-validation  
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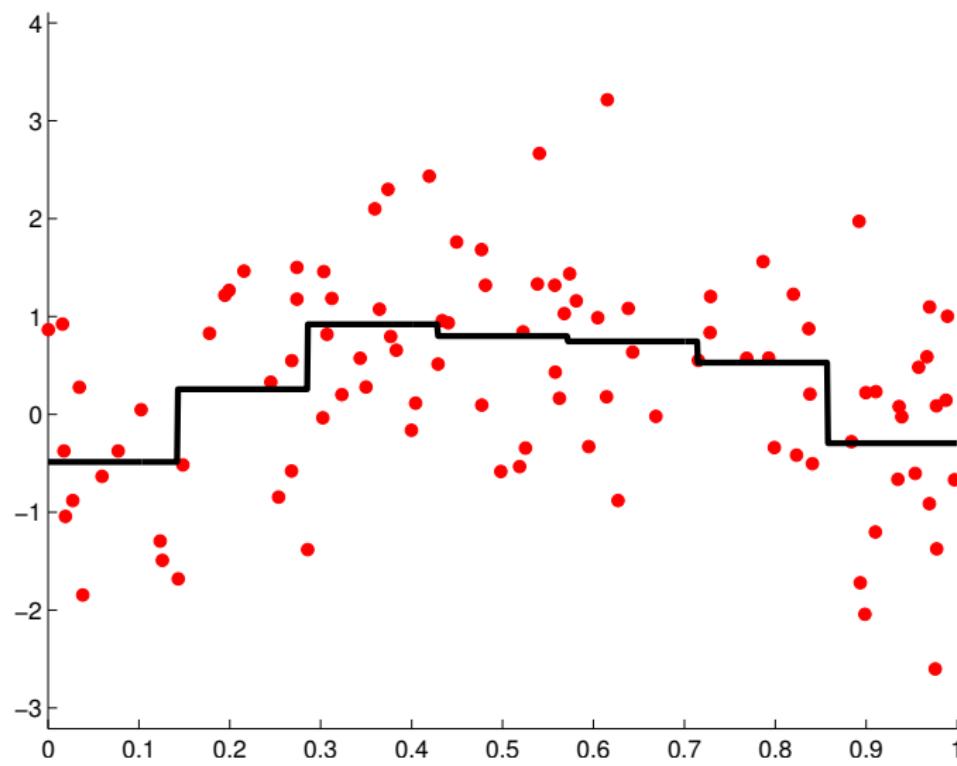
CV for risk estimation  
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CV for estimator selection  
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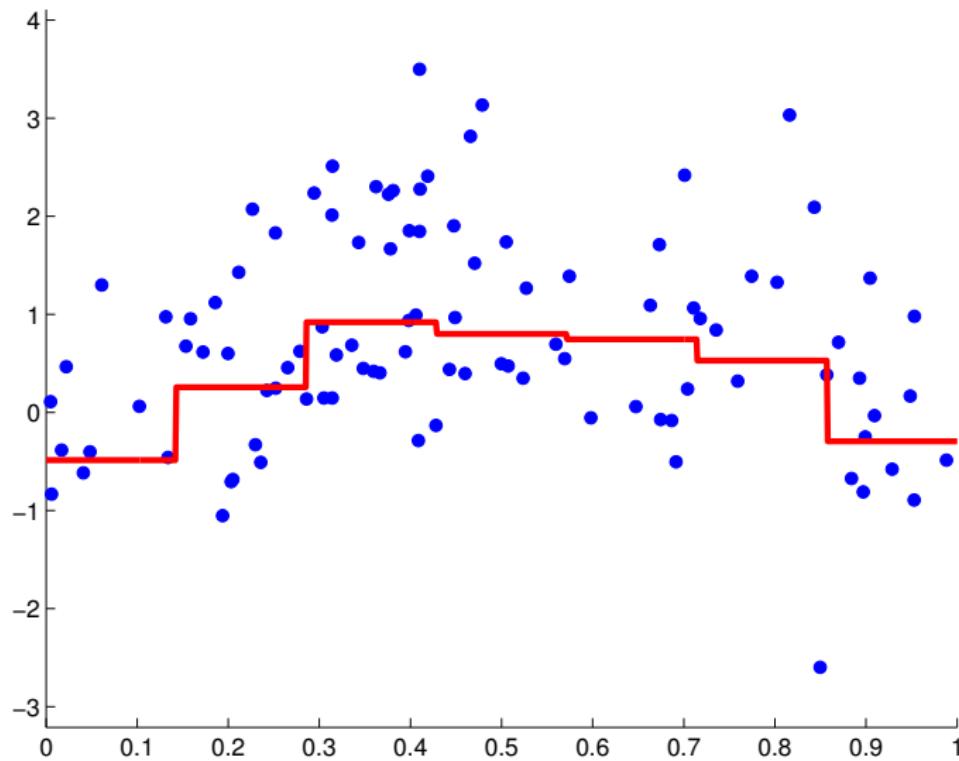
Large  $\mathcal{M}$   
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Conclusion  
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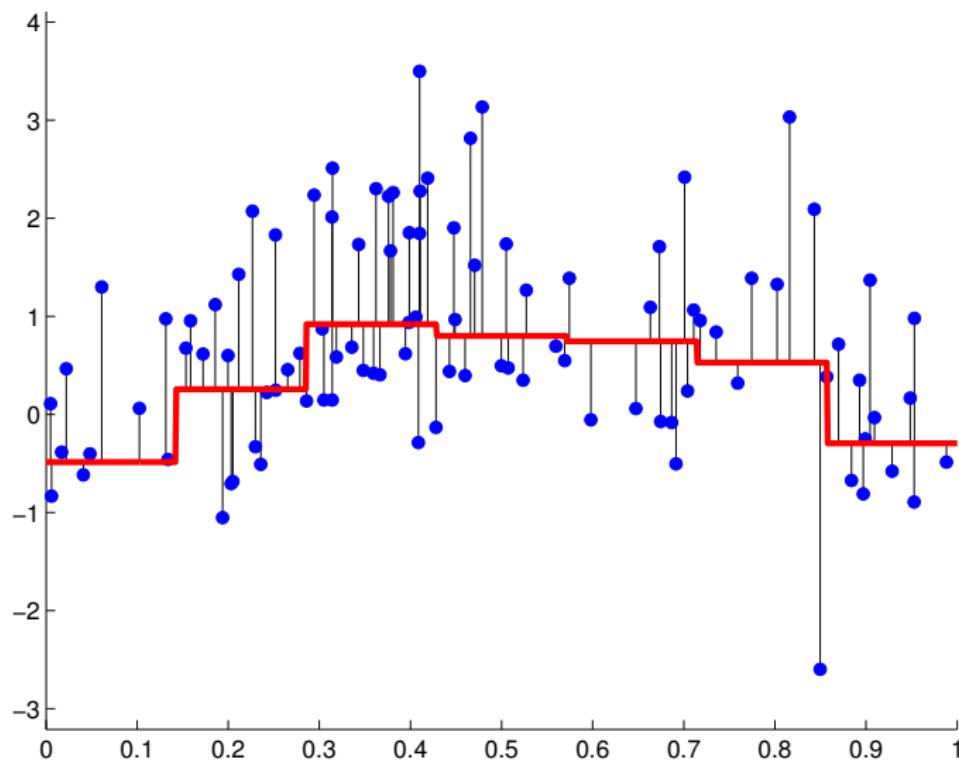
## Validation principle: learning sample



## Validation principle: validation sample



## Validation principle: validation sample



Estimator selection

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Cross-validation

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CV for risk estimation

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Large  $\mathcal{M}$ 

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Conclusion

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# Cross-validation

$$\underbrace{(X_1, Y_1), \dots, (X_{n_t}, Y_{n_t})}_{\text{Training set } D_n^{(t)} \Rightarrow \hat{s}_m^{(t)} = \hat{s}_m(D_n^{(t)})}$$

$$\underbrace{(X_{n_t+1}, Y_{n_t+1}), \dots, (X_n, Y_n)}_{\text{Validation set } D_n^{(v)} \Rightarrow \text{evaluate risk}}$$

Estimator selection

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# Cross-validation

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Training set  $D_n^{(t)} \Rightarrow \hat{s}_m^{(t)} = \hat{s}_m(D_n^{(t)})$

Validation set  $D_n^{(v)} \Rightarrow \text{evaluate risk}$

- hold-out estimator of the risk:

$$P_n^{(v)} \gamma \left( \hat{s}_m^{(t)} \right) = \frac{1}{n_v} \sum_{\xi \in D_n^{(v)}} \gamma \left( \hat{s}_m^{(t)}; \xi \right)$$

$n_v = |D_n^{(v)}| = n - n_t$

Estimator selection

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Cross-validation

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Conclusion

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# Cross-validation

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- hold-out estimator of the risk:

$$P_n^{(v)} \gamma \left( \hat{s}_m^{(t)} \right) = \frac{1}{n_v} \sum_{\xi \in D_n^{(v)}} \gamma \left( \hat{s}_m^{(t)}; \xi \right) \quad n_v = |D_n^{(v)}| = n - n_t$$

- cross-validation: average several hold-out estimators

$$\widehat{\mathcal{R}}^{\text{cv}} \left( \hat{s}_m; D_n; (I_j^{(t)})_{1 \leq j \leq B} \right) = \frac{1}{B} \sum_{j=1}^B P_n^{(v,j)} \gamma \left( \hat{s}_m^{(t,j)} \right) \quad D_n^{(t,j)} = (\xi_i)_{i \in I_j^{(t)}}$$

# Cross-validation

$$\underbrace{(X_1, Y_1), \dots, (X_{n_t}, Y_{n_t})}_{\text{Training set } D_n^{(t)} \Rightarrow \hat{s}_m^{(t)} = \hat{s}_m(D_n^{(t)})}$$

$$\underbrace{(X_{n_t+1}, Y_{n_t+1}), \dots, (X_n, Y_n)}_{\text{Validation set } D_n^{(v)} \Rightarrow \text{evaluate risk}}$$

Training set  $D_n^{(t)} \Rightarrow \hat{s}_m^{(t)} = \hat{s}_m(D_n^{(t)})$

Validation set  $D_n^{(v)} \Rightarrow \text{evaluate risk}$

- hold-out estimator of the risk:

$$P_n^{(v)} \gamma \left( \hat{s}_m^{(t)} \right) = \frac{1}{n_v} \sum_{\xi \in D_n^{(v)}} \gamma \left( \hat{s}_m^{(t)}; \xi \right) \quad n_v = |D_n^{(v)}| = n - n_t$$

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- estimator selection:

$$\hat{m} \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}^{\text{cv}} \left( \hat{s}_m; D_n \right) \right\}$$

## Cross-validation: examples

- Exhaustive data splitting: all possible subsets of size  $n_t$   
 $\Rightarrow$  leave-one-out ( $n_t = n - 1$ )

$$\widehat{\mathcal{R}}^{\text{loo}}(\widehat{s}_m; D_n) = \frac{1}{n} \sum_{j=1}^n \gamma\left(\widehat{s}_m^{(-j)}; \xi_j\right)$$

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- Monte-Carlo CV / Repeated learning testing:

$$I_1^{(t)}, \dots, I_B^{(t)} \text{ i.i.d. uniform}$$

# Outline

- 1 Estimator selection
- 2 Cross-validation
- 3 Cross-validation for risk estimation
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- 5 Large  $\mathcal{M}$
- 6 Conclusion

# Bias of cross-validation

- In this talk, we always assume:  $\forall j$ ,  $\text{Card}(D_n^{(t,j)}) = n_t$   
For  $V$ -fold CV:  $\text{Card}(B_j) = n/V$ .
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$$\mathbb{E}\left[\widehat{\mathcal{R}}^{\text{cv}}\left(\widehat{s}_m; D_n; \left(I_j^{(t)}\right)_{1 \leqslant j \leqslant B}\right)\right] = \mathbb{E}\left[P\gamma(\widehat{s}_m(D_{\textcolor{red}{n}}))\right]$$

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- Note: **bias can be corrected** in some settings (Burman, 1989).
- Note:  $D_n \rightarrow \widehat{s}_m(D_n)$  must be fixed **before seeing any data**; otherwise, stronger bias.

## Bias of cross-validation: generic example

Assume

$$\mathbb{E} \left[ P\gamma(\hat{s}_m(D_n)) \right] = \alpha(m) + \frac{\beta(m)}{n}$$

(e.g., LS/ridge/ $k$ -NN regression, LS/kernel density estimation).

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$\Rightarrow$   $V$ -fold: bias decreases when  $V$  increases, vanishes as  $V \rightarrow +\infty$ .

# Variance of cross-validation

- **Hold-out** (Nadeau & Bengio, 2003):

$$\begin{aligned} \text{var}\left(P_n^{(v)} \gamma\left(\hat{s}_m^{(t)}\right)\right) &= \frac{1}{n_v} \mathbb{E}\left[\text{var}\left(\gamma(u; \xi) \mid u = \hat{s}_m^{(t)}\right)\right] \\ &\quad + \text{var}\left(P \gamma\left(\hat{s}_m(D_{n_t})\right)\right) \end{aligned}$$

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- Monte-Carlo CV and number of splits: ( $p = n - n_t$ )

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- **V-fold CV**:  $B$ ,  $n_t$ ,  $n_v$  related  
leave-one-out: related to stability? (empirical results)

# Variance of the $V$ -fold CV criterion

- Least-squares density estimation (A. & Lerasle 2012), exact computation (non-asymptotic):

$$\begin{aligned} \text{var} \left( \widehat{\mathcal{R}}^{\text{vf}} (\widehat{s}_m; D_n; \mathcal{B}) \right) &= \frac{1 + \mathcal{O}(1)}{n} \text{var}_{\mathcal{P}}(s_m^*) \\ &+ \frac{2}{n^2} \left[ 1 + \frac{4}{V-1} + \mathcal{O}\left(\frac{1}{V} + \frac{1}{n}\right) \right] A(m) \end{aligned}$$

(simplified formula, histogram model with bin size  $d_m^{-1}$ ,  $A(m) \approx d_m$ )

- Linear regression, specific setting, asymptotic formula (Burman, 1989):

$$\text{var} \left( \widehat{\mathcal{R}}^{\text{vf}} (\widehat{s}_m; D_n; \mathcal{B}) \right) = \frac{2\sigma^2}{n} + \frac{4\sigma^4}{n^2} \left[ 4 + \frac{4}{V-1} + \frac{2}{(V-1)^2} + \frac{1}{(V-1)^3} \right] + o(n^{-2})$$

$\Rightarrow$  decreasing with  $V$ , dependence only in second order terms.

# Outline

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- 5 Large  $\mathcal{M}$
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Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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Large  $\mathcal{M}$ 

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Conclusion

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# Risk estimation and estimator selection are different goals

$$\hat{m} \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}^{\text{cv}} (\hat{s}_m) \right\} \quad \text{vs.} \quad m^* \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ P\gamma(\hat{s}_m(D_n)) \right\}$$

- For any  $Z$  (deterministic or random),

$$\hat{m} \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}^{\text{cv}} (\hat{s}_m) + Z \right\}$$

$\Rightarrow$  bias and variance meaningless.

Estimator selection

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Cross-validation

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Large  $\mathcal{M}$ 

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Conclusion

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$\Rightarrow \operatorname{var}(\widehat{\mathcal{R}}^{\text{vf}}(\hat{s}_m) - \widehat{\mathcal{R}}^{\text{vf}}(\hat{s}_{m'}))$  should be minimal (detailed heuristic: A. & Lerasle 2012)

Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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Large  $\mathcal{M}$ 

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Conclusion

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# Bias and estimator selection: generic example

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- Assume

$$\mathbb{E}[P\gamma(\hat{s}_m(D_n))] = \alpha(m) + \frac{\beta(m)}{n}$$

(e.g., LS/ridge/ $k$  NN regression, LS/kernel density estimation).

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- Key quantities:

$$\mathbb{E}[P\gamma(\hat{s}_m) - P\gamma(\hat{s}_{m'})] = \alpha(m) - \alpha(m') + \frac{\beta(m) - \beta(m')}{n}$$

$$\mathbb{E}[\widehat{\mathcal{R}}^{\text{cv}}(\hat{s}_m) - \widehat{\mathcal{R}}^{\text{cv}}(\hat{s}_{m'})] = \alpha(m) - \alpha(m') + \frac{\cancel{n} \beta(m) - \beta(m')}{n_t n}$$

$\Rightarrow$  CV favours  $m$  with smaller complexity  $\beta(m)$ , more and more as  $n_t$  decreases.

# CV with an estimation goal: the big picture ( $\mathcal{M}$ “small”)

- At first order, the **bias drives the performance** of:  
 leave- $p$ -out,  $V$ -fold CV,  
 Monte-Carlo CV if  $B \gg n^2$   
 or if  $n_v$  large enough (including hold-out)
- CV performs similarly to

$$\operatorname{argmin}_{m \in \mathcal{M}} \left\{ \mathbb{E} \left[ P\gamma(\hat{s}_m(D_{\textcolor{red}{n_t}})) \right] \right\}$$

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⇒ first-order optimality if  $n_t \sim n$

⇒ suboptimal otherwise

e.g.,  $V$ -fold CV with  $V$  fixed.

- Theoretical results for least-squares regression and density estimation at least.

Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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Large  $\mathcal{M}$ 

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Conclusion

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# Bias-corrected VFCV / $V$ -fold penalization

- Bias-corrected  $V$ -fold CV (Burman, 1989):

$$\widehat{\mathcal{R}}^{\text{vf,corr}}(\widehat{s}_m; D_n; \mathcal{B}) := \widehat{\mathcal{R}}^{\text{vf}}(\widehat{s}_m; D_n; \mathcal{B}) + P_n \gamma(\widehat{s}_m) - \frac{1}{V} \sum_{j=1}^V P_n \gamma\left(\widehat{s}_m^{(-j)}\right)$$

# Bias-corrected VFCV / $V$ -fold penalization

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(A. 2008)

- In least-squares density estimation (A. & Lerasle, 2012):

$$\widehat{\mathcal{R}}^{\text{vf}}(\widehat{s}_m; D_n; \mathcal{B}) = P_n \gamma(\widehat{s}_m(D_n)) + \underbrace{\left(1 + \frac{1}{2(V-1)}\right)}_{\text{overpenalization factor}} \text{pen}_{\text{VF}}(\widehat{s}_m; D_n; \mathcal{B})$$

$$\widehat{\mathcal{R}}^{\ell\text{po}}(\widehat{s}_m; D_n; \mathcal{B}) = P_n \gamma(\widehat{s}_m(D_n)) + \underbrace{\left(1 + \frac{1}{2\left(\frac{n}{p}-1\right)}\right)}_{\text{pen}_{\text{VF}}(\widehat{s}_m; D_n; \mathcal{B}_{\text{loo}})}$$

# Variance and estimator selection

$$\Delta(m, m', V) = \widehat{\mathcal{R}}^{\text{vf,corr}}(\widehat{s}_m) - \widehat{\mathcal{R}}^{\text{vf,corr}}(\widehat{s}_{m'})$$

Theorem (A. & Lerasle 2012, least-squares density estimation)

$$\begin{aligned} \text{var}(\Delta(m, m', V)) &= 4 \left( 1 + \frac{2}{n} + \frac{1}{n^2} \right) \frac{\text{var}_P(s_m^* - s_{m'}^*)}{n} \\ &\quad + 2 \left( 1 + \frac{4}{V-1} - \frac{1}{n} \right) \underbrace{\frac{B(m, m')}{n^2}}_{\geq 0} \end{aligned}$$

If  $S_m \subset S_{m'}$  are two histogram models with constant bin sizes  $d_m^{-1}, d_{m'}^{-1}$ , then,  $B(m, m') \propto \|s_m^* - s_{m'}^*\| d_m$ .

The two terms are of the same order if  $\|s_m^* - s_{m'}^*\| \approx d_m/n$ .

Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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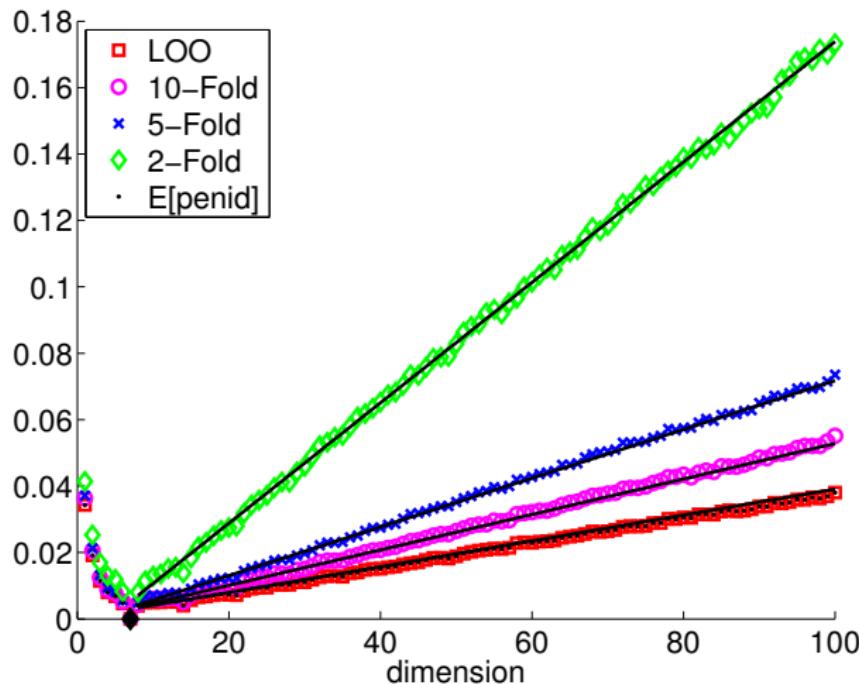
Large  $\mathcal{M}$ 

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Conclusion

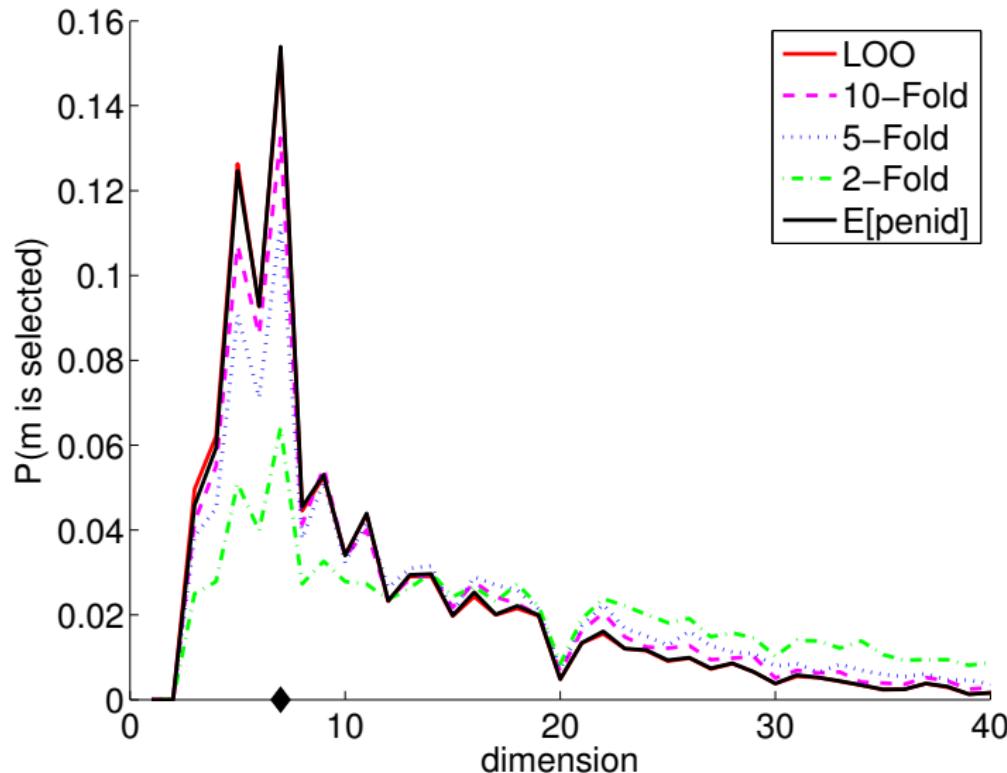
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# Variance of $\widehat{\mathcal{R}}^{\text{vf,corr}}(\widehat{s}_m) - \widehat{\mathcal{R}}^{\text{vf,corr}}(\widehat{s}_{m^*})$ vs. $(d_m, V)$

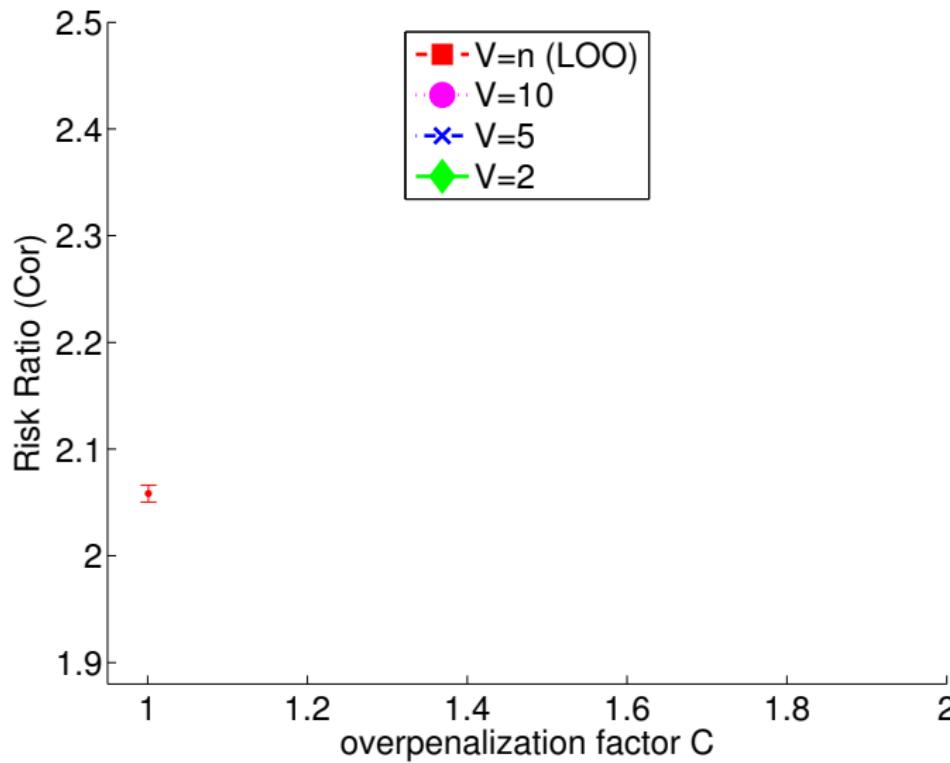


$$\text{var}(\Delta(m, m', V)) \approx n^{-2} [29(1 + \frac{0.8}{V-1}) + 3.7(1 + \frac{3.8}{V-1})(d_m - d_{m^*})]$$

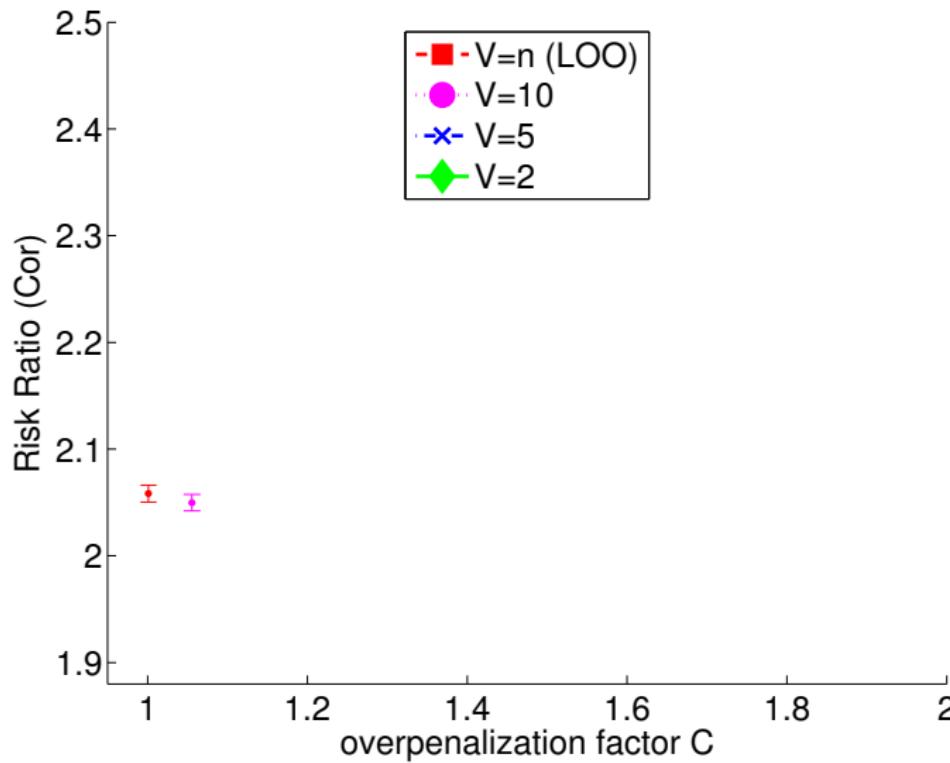
# Probability of selection of every $m$



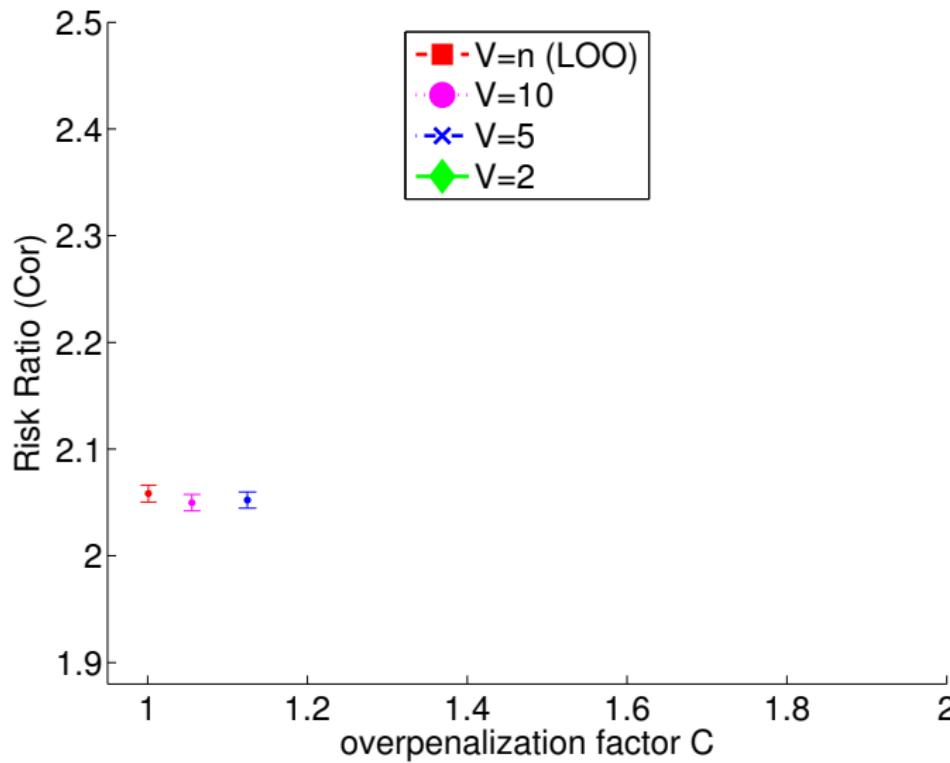
## Experiment (LS density estimation): $V$ -fold CV



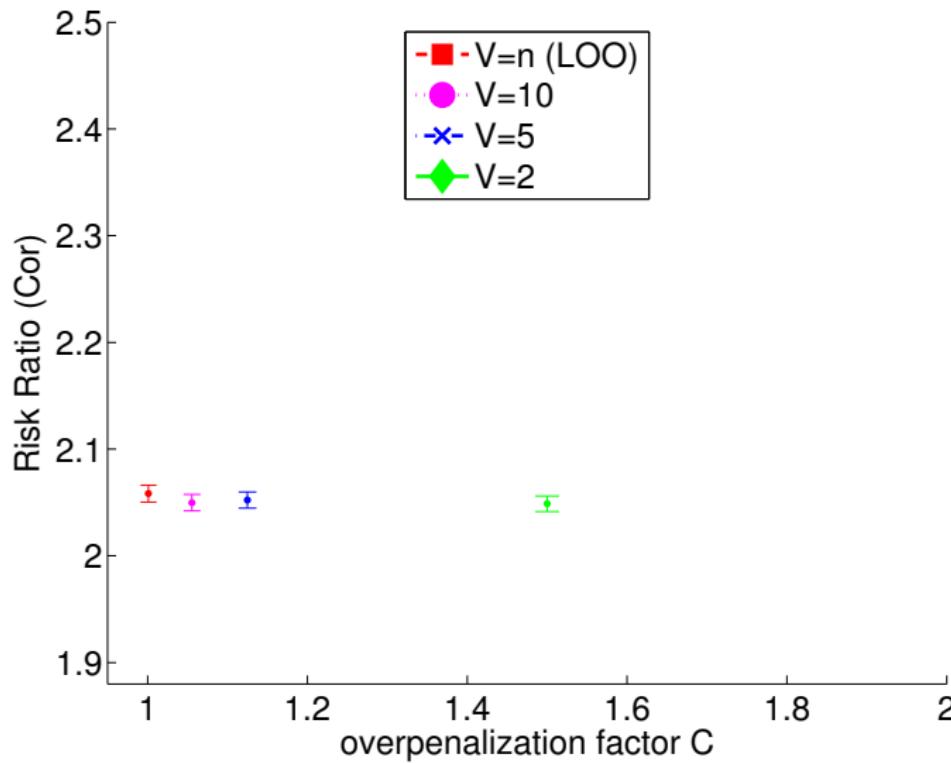
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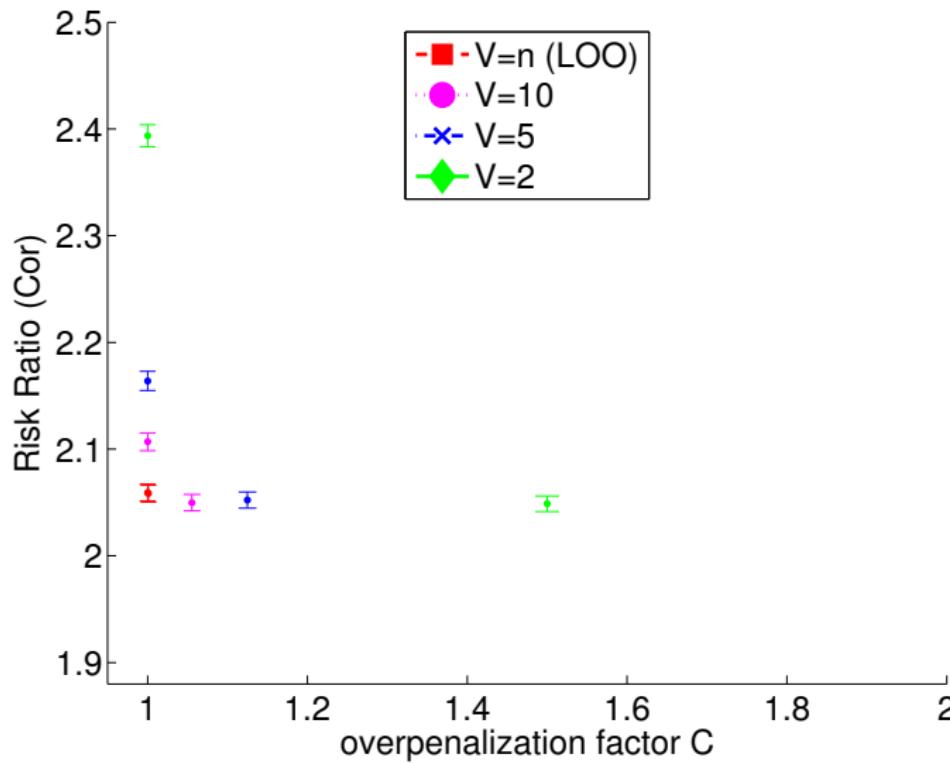
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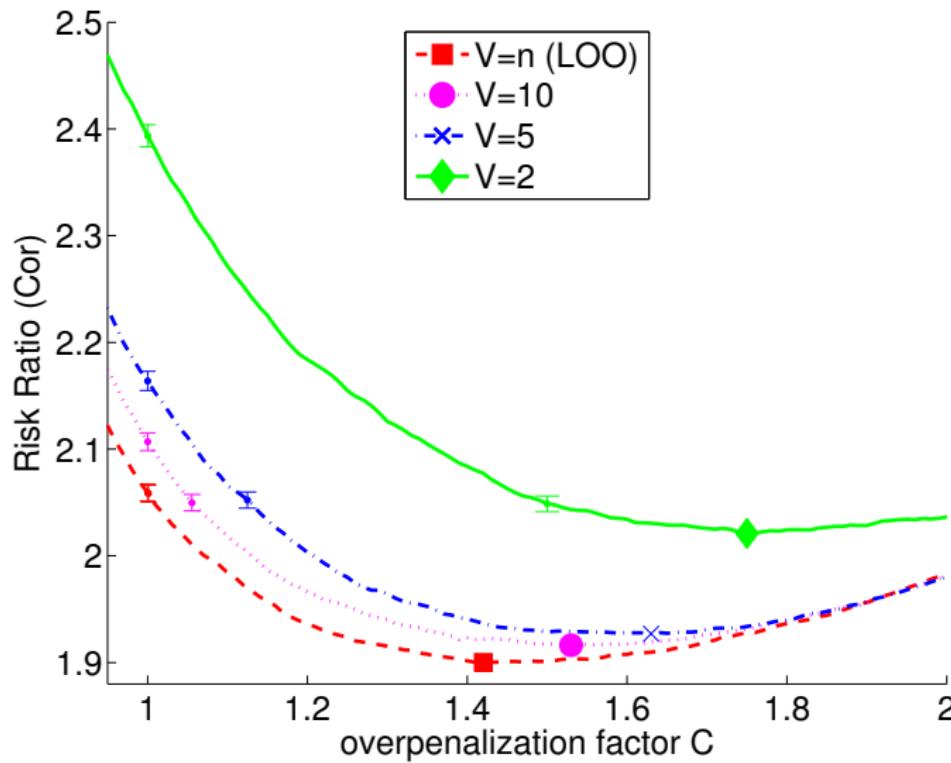
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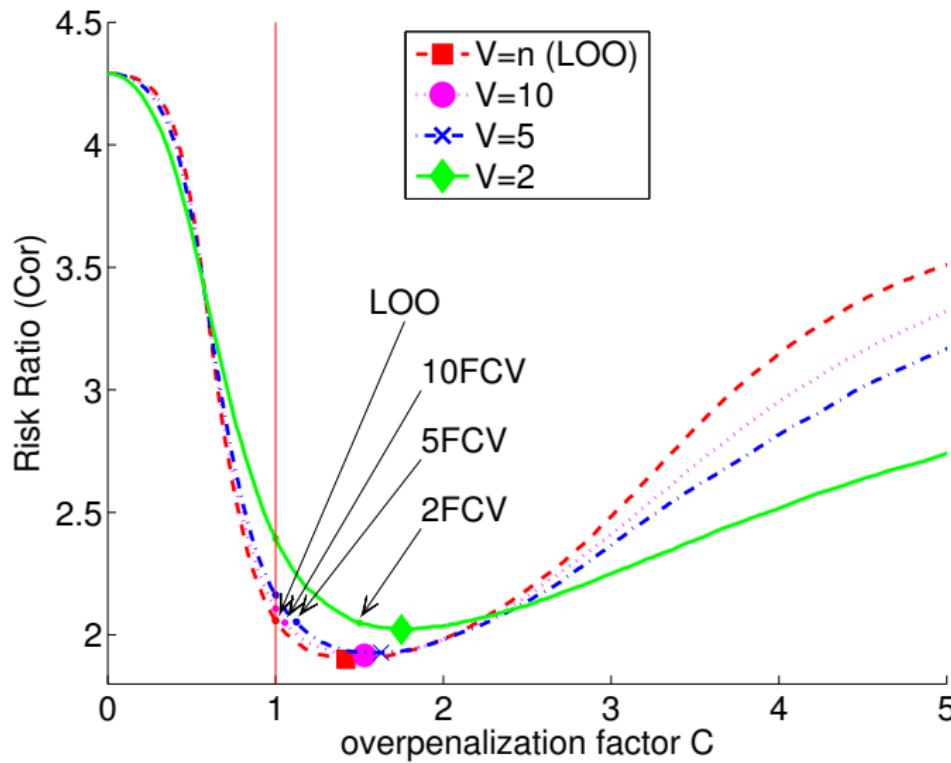
# Experiment (LS density estimation): $V$ -fold penalization



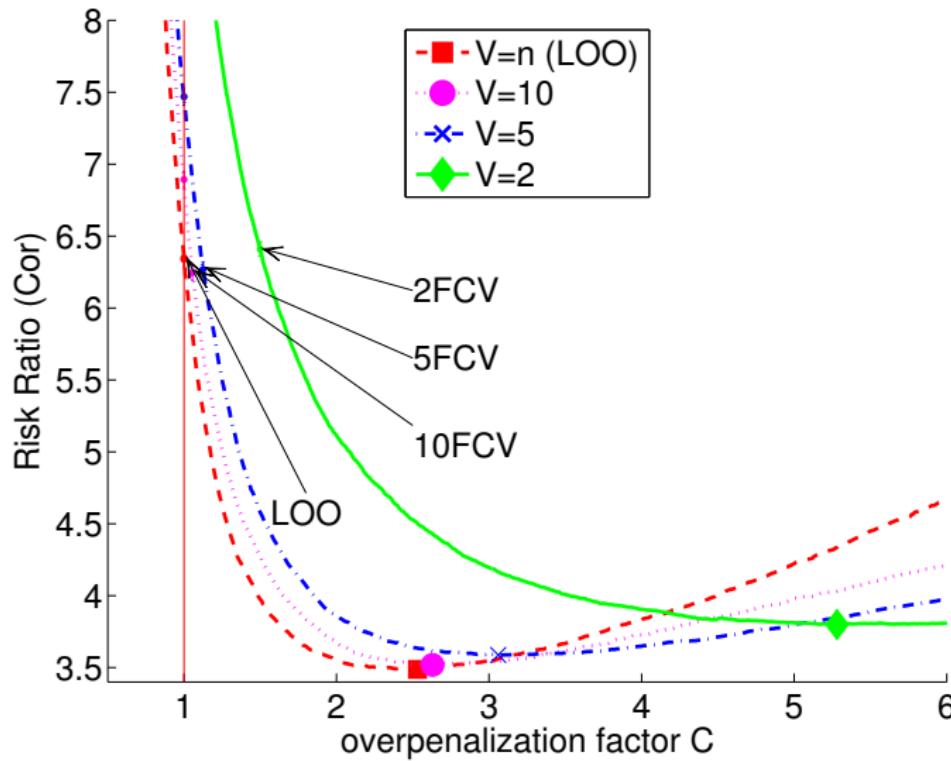
# Experiment (LS density estimation): overpenalization



# Experiment (LS density estimation): conclusion



# Experiment (LS density estimation): other setting



Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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Large  $\mathcal{M}$ 

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Conclusion

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## Estimator selection with $V$ -fold: conclusion

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    - ... if optimal overpenalization factor  $C^* \approx 1$  (various behaviours possible).
- $V$ -fold penalization:
  - Decoupling of bias and variance ⇒ easier to understand.
  - Bias: chosen directly through  $C$ , without any constraint.
  - Variance: decreases with  $V$  / almost minimal with  $V \in [5, 10]$ .

# Outline

- 1 Estimator selection
- 2 Cross-validation
- 3 Cross-validation for risk estimation
- 4 Cross-validation for estimator selection
- 5 Large  $\mathcal{M}$
- 6 Conclusion

# Large collection of estimators/models

- Estimator/model selection with an “exponential” collection (implicitly excluded in all results above).  
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# Large collection of estimators/models

- Estimator/model selection with an “exponential” collection (implicitly excluded in all results above).  
⇒ Expectations do not drive the first order!
- Examples: variable selection with  $p \geq n$  variables, change-point detection.
- Solution: group the models ⇒ one estimator per dimension (e.g., empirical risk minimizer)  
works for change-point detection (A. & Celisse, 2010).

# Change-point detection and model selection

$$Y_i = \eta(t_i) + \sigma(t_i)\varepsilon_i \quad \text{with} \quad \mathbb{E}[\varepsilon_i] = 0 \quad \mathbb{E}[\varepsilon_i^2] = 1$$

- Goal: detect the **change-points of the mean  $\eta$**  of the signal  $Y$
- ⇒ Model selection, collection of regressograms with  
 $\mathcal{M}_n = \mathfrak{P}_{\text{interv}}(\{t_1, \dots, t_n\})$  (partitions of  $\mathcal{X}$  into intervals)
- No assumption on the variance  $\sigma(t_i)^2$

# Classical approach (Lebarbier, 2005; ...)

- “Birgé-Massart” penalty (assumes  $\sigma(t_i) \equiv \sigma$ ):

$$\hat{m} \in \operatorname{argmin}_{m \in \mathcal{M}_n} \left\{ P_n \gamma(\hat{s}_m) + \frac{C\sigma^2 D_m}{n} \left( 5 + 2 \log \left( \frac{n}{D_m} \right) \right) \right\}$$

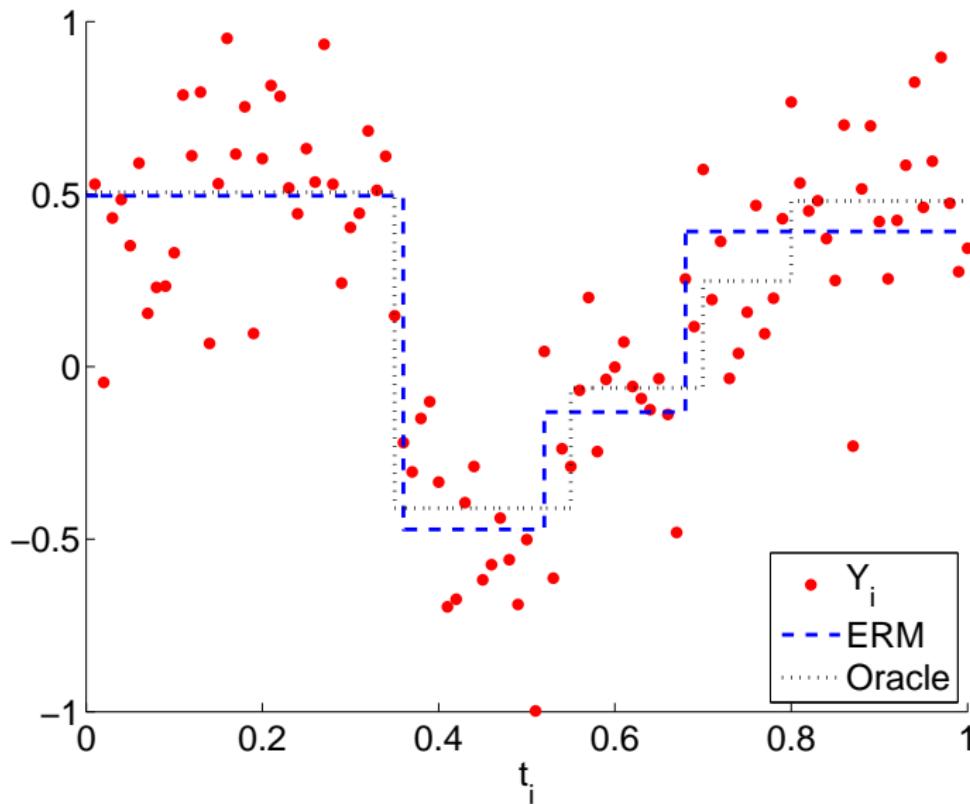
- Equivalent to aggregating models of the same dimension:

$$\tilde{S}_D := \bigcup_{m \in \mathcal{M}_n, D_m = D} S_m$$

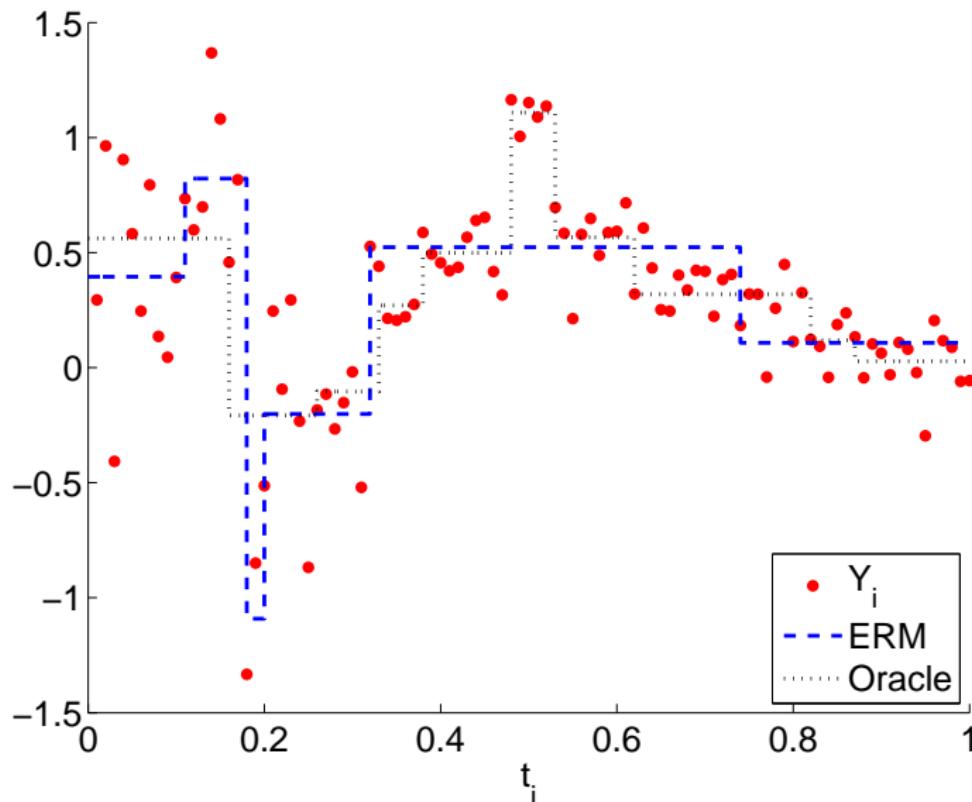
$$\hat{s}_D \in \operatorname{argmin}_{t \in \tilde{S}_D} \{ P_n \gamma(t) \} \quad \text{dynamic programming}$$

$$\hat{D} \in \operatorname{argmin}_{1 \leqslant D \leqslant n} \left\{ P_n \gamma(\hat{s}_D) + \frac{C\sigma^2 D}{n} \left( 5 + 2 \log \left( \frac{n}{D} \right) \right) \right\}$$

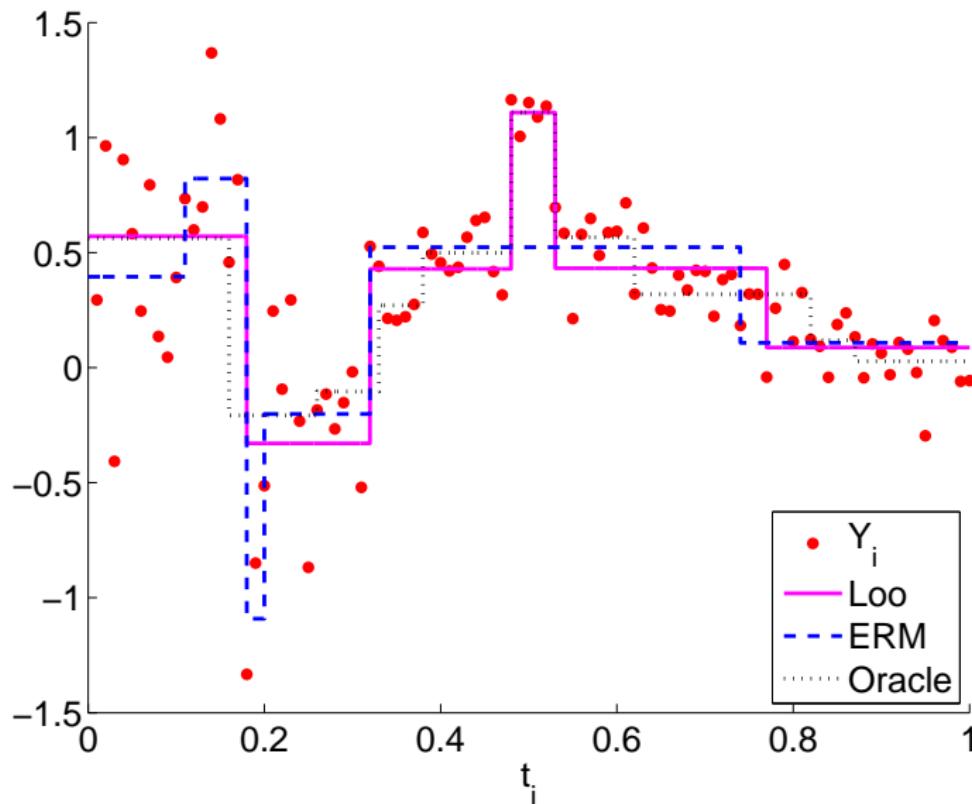
$D = 4$ , homoscedastic;  $n = 100$ ,  $\sigma = 0.25$



$D = 6$ , heteroscedastic;  $n = 100$ ,  $\|\sigma\| = 0.30$



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# Change-point detection algorithms (A. & Celisse, 2010)

- ①  $\forall D \in \{1, \dots, D_{\max}\}$ , select

$$\hat{m}(D) \in \operatorname{argmin}_{m \in \mathcal{M}_n, D_m=D} \left\{ \text{crit}_1(m; (t_i, Y_i)_i) \right\}$$

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$$\hat{D} \in \operatorname{argmin}_{D \in \{1, \dots, D_{\max}\}} \left\{ \text{crit}_2(D; (t_i, Y_i)_i; \text{crit}_1(\cdot)) \right\}$$

Examples for  $\text{crit}_2$ : penalized empirical criterion,  $V$ -fold estimator of the risk

Estimator selection

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Cross-validation

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CV for risk estimation

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CV for estimator selection

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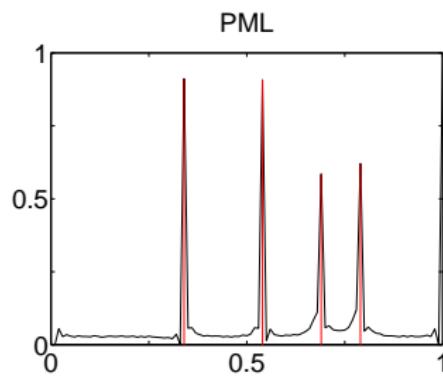
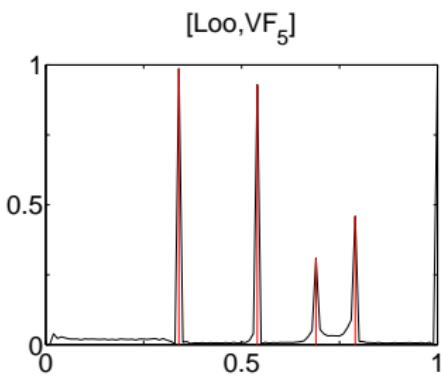
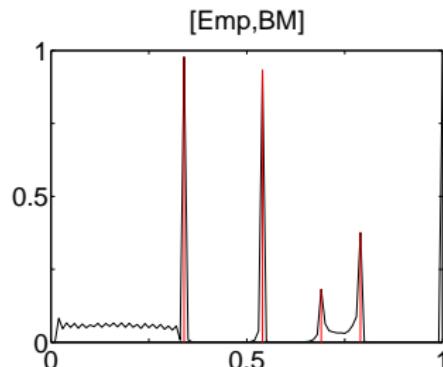
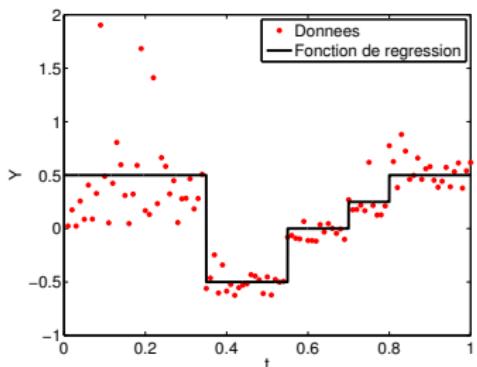
Large  $\mathcal{M}$ 

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Conclusion

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# Simulations: position of the change-points



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Otherwise: use repeated  $V$ -fold or Monte-Carlo CV with a well-chosen  $n_t$ .

- Variance: different behaviours can occur in other settings (experiments).
- Everything can be checked on synthetic data: plot

$$n \rightarrow \mathbb{E}\left[P\gamma(\hat{s}_m(D_n))\right] \quad \text{and} \quad m \rightarrow \text{var}\left(\widehat{\mathcal{R}}^{\text{cv}}(\hat{s}_m) - \widehat{\mathcal{R}}^{\text{cv}}(\hat{s}_{m^*})\right) .$$

# Cross-validation with an identification goal

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- Remark: **estimation goal, parametric setting**  $\Rightarrow$  similar behaviour.

# Dependent data

- $D_n^{(t)}, D_n^{(v)}$  dependent  $\Rightarrow$  CV heuristic fails!
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- $D_n^{(t)}, D_n^{(v)}$  dependent  $\Rightarrow$  CV heuristic fails!
- $\Rightarrow$  possible troubles for risk estimation (Hart & Wehrly, 1986; Opsomer et al., 2001).
- **Solution for short-term dependence:**  
remove some data at each split  $\Rightarrow$  gap between training and validation samples.

# Questions?

## Part I

### Appendix

# Outline

## 1 Change-point detection

# Competitors

- [Emp, BM]: assume  $\sigma(\cdot) \equiv \sigma$

$$\operatorname{argmin}_{m \in \mathcal{M}_n} \left\{ P_n \gamma(\hat{s}_m) + \frac{C\hat{\sigma}^2 D_m}{n} \left( 5 + 2 \log \left( \frac{n}{D_m} \right) \right) \right\}$$

- BGH (Baraud, Giraud & Huet 2009): multiplicative penalty,  $\sigma(\cdot) \equiv \sigma$

$$\operatorname{argmin}_{m \in \mathcal{M}_n} \left\{ P_n \gamma(\hat{s}_m) \left[ 1 + \frac{\text{pen}_{\text{BGH}}(m)}{n - D_m} \right] \right\}$$

- ZS (Zhang & Siegmund, 2007): modified BIC,  $\sigma(\cdot) \equiv \sigma$
- PML (Picard *et al.*, 2005): penalized maximum likelihood, looks for change-points of  $(\eta, \sigma)$ , assuming a Gaussian model

$$\operatorname{argmin}_{m \in \mathcal{M}_n} \left\{ \sum_{\lambda \in m} n \hat{p}_\lambda \log \left( \frac{1}{n \hat{p}_\lambda} \sum_{t_i \in \lambda} (Y_i - \hat{s}_m(t_i))^2 \right) + \hat{C}'' D_m \right\}$$

## Simulations: comparison to the oracle (quadratic risk)

$$\frac{\mathbb{E} [\ell(s^*, \hat{s}_{\hat{m}})]}{\mathbb{E} [\inf_{m \in \mathcal{M}_n} \{\ell(s^*, \hat{s}_m)\}]} \quad N = 10\,000 \text{ sample}$$

$\mathcal{L}(\varepsilon)$	Gaussian	Gaussian	Gaussian
$\sigma(\cdot)$	homosc.	heterosc.	heterosc.
$\eta$	$s_2$	$s_2$	$s_3$
[Loo, VF <sub>5</sub> ]	$4.02 \pm 0.02$	$4.95 \pm 0.05$	$5.59 \pm 0.02$
[Emp, VF <sub>5</sub> ]	$3.99 \pm 0.02$	$5.62 \pm 0.05$	$6.13 \pm 0.02$
[Emp, BM]	$3.58 \pm 0.02$	$9.25 \pm 0.06$	$6.24 \pm 0.02$
BGH	$3.52 \pm 0.02$	$10.13 \pm 0.07$	$6.31 \pm 0.02$
ZS	$3.62 \pm 0.02$	$6.50 \pm 0.05$	$6.61 \pm 0.02$
PML	$4.34 \pm 0.02$	$2.73 \pm 0.03$	$4.99 \pm 0.03$

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BGH	<b><math>3.52 \pm 0.02</math></b>	$11.67 \pm 0.09$	$6.42 \pm 0.04$
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