Cross-validation for estimator selection

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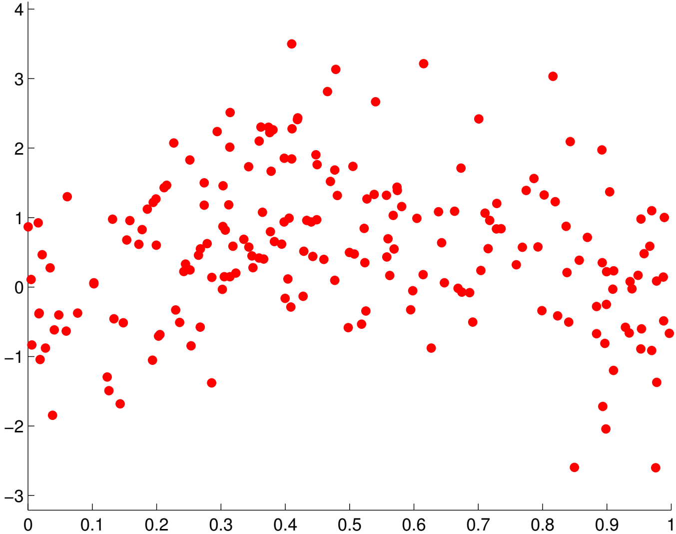
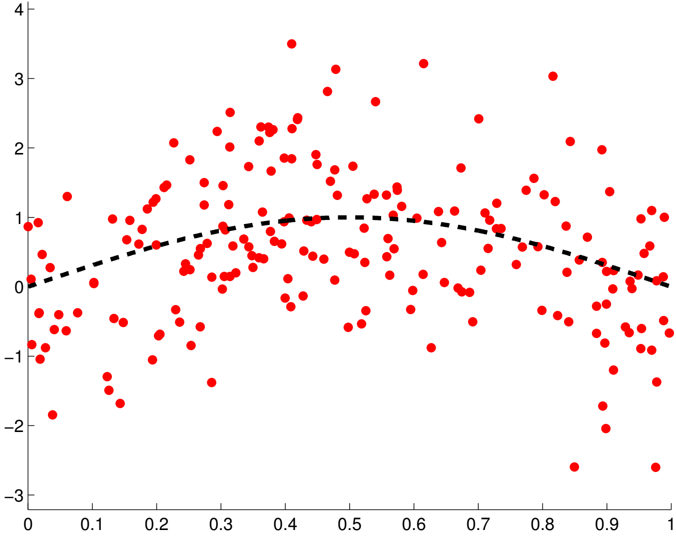
Main reference (survey paper): arXiv:0907.4728
Precise results in L^2 density estimation: arXiv:1210.5830

Outline

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



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

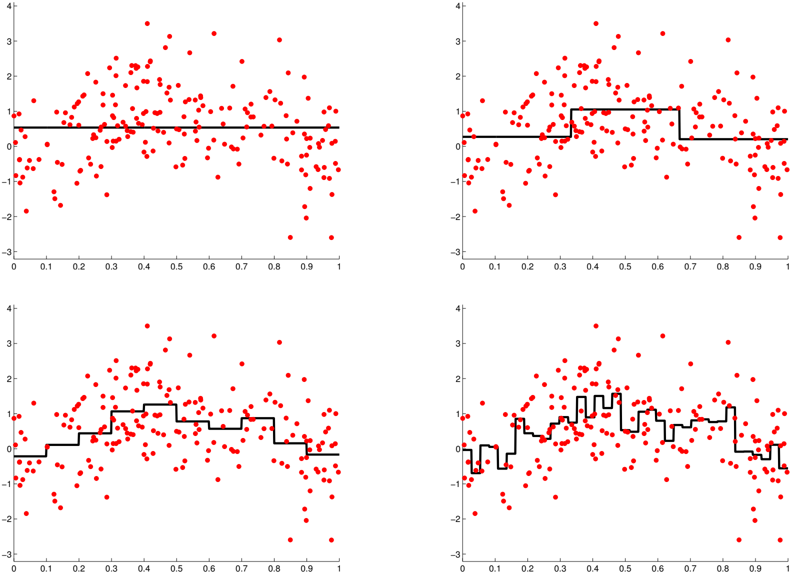


General setting: prediction

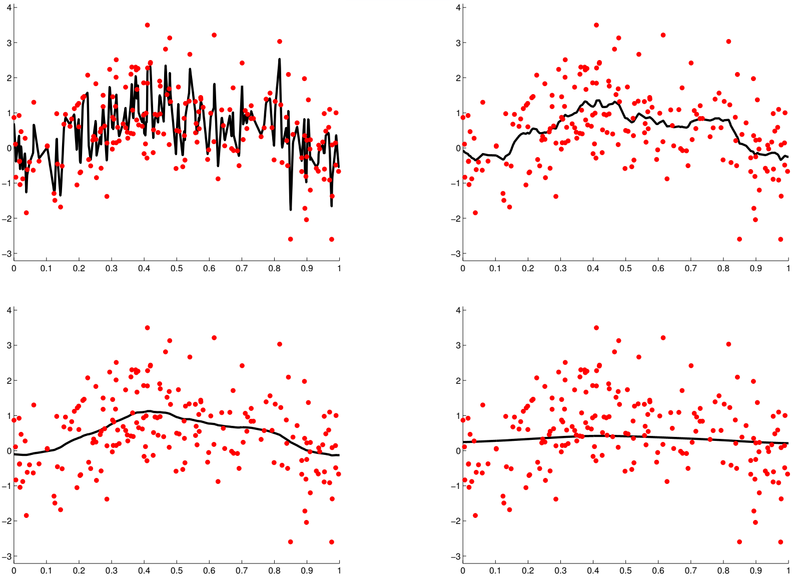
- Data: $D_n = (X_i, Y_i)_{1 \leqslant i \leqslant n} \in (\mathcal{X} \times \mathcal{Y})^n$ assumed i.i.d. $\sim P$
- Predictor: $f : \mathcal{X} \to \mathcal{Y}$ ($\mathcal{F}$: set of all predictors)
- Risk (prediction error): $\mathcal{R}(f) = \mathbb{E}\left[c(f(X), Y)\right]$
  minimal for $f = f^{\star}$

  LS regression: $c(y, y') = (y - y')^2$, $f^{\star}(X) = \mathbb{E}[Y | X]$ and
  $\mathcal{R}(f) - \mathcal{R}(f^{\star}) = \mathbb{E}\left[(f(X) - f^{\star}(X))^2\right]$
- Goal: from D_n only, find $f \in \mathcal{F}$ with $\mathcal{R}(f)$ minimal.
- Examples: regression, classification
- More general setting possible, including density estimation with LS or KL risk.

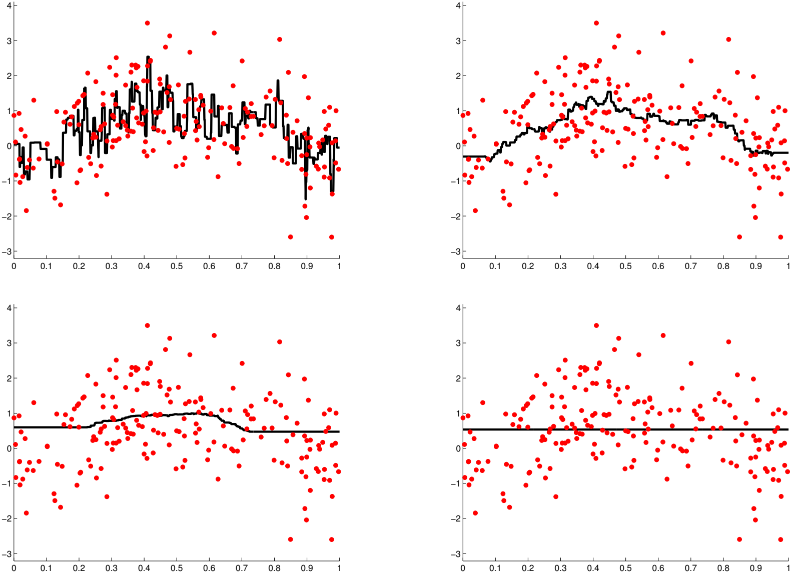
Estimator selection (regression): regular regressograms



Estimator selection (regression): kernel ridge



Estimator selection (regression): k nearest neighbours



Estimator selection

- Estimator/Learning algorithm: $\widehat{f} : D_n \mapsto \widehat{f}(D_n) \in \mathcal{F}$
- Example: least-squares estimator on some model $S_m \subset \mathcal{F}$

$$\widehat{f}_m \in \operatorname*{argmin}_{f \in S_m} \left\{ \widehat{\mathcal{R}}_n(f) \right\} \quad \text{where} \quad \widehat{\mathcal{R}}_n(f) := \frac{1}{n} \sum_{(X_i, Y_i) \in D_n} c\left(f(X_i), Y_i\right)$$

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

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

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

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):

$$\mathcal{R}(\widehat{f}_{\widehat{m}}) - \mathcal{R}(f^{\star}) \leqslant C \inf_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{f}_m) - \mathcal{R}(f^{\star})\} + R_n$$

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

$$\mathbb{P}(\widehat{m}(D_n) = m^{\star}) \xrightarrow[n \to \infty]{} 1 \, .$$

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

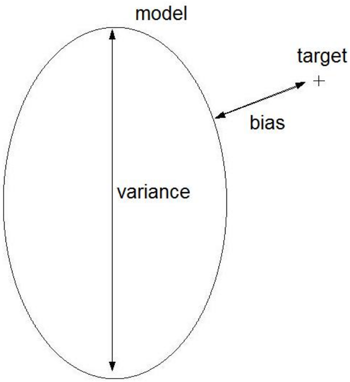
$$\mathbb{E}\left[\mathcal{R}(\widehat{f}_m)\right] - \mathcal{R}(f^\star) = \text{Bias} + \text{Variance}$$

Bias or Approximation error

$$\mathcal{R}(f_m^\star) - \mathcal{R}(f^\star) = \inf_{f \in S_m} \mathcal{R}(f) - \mathcal{R}(f^\star)$$

Variance or Estimation error

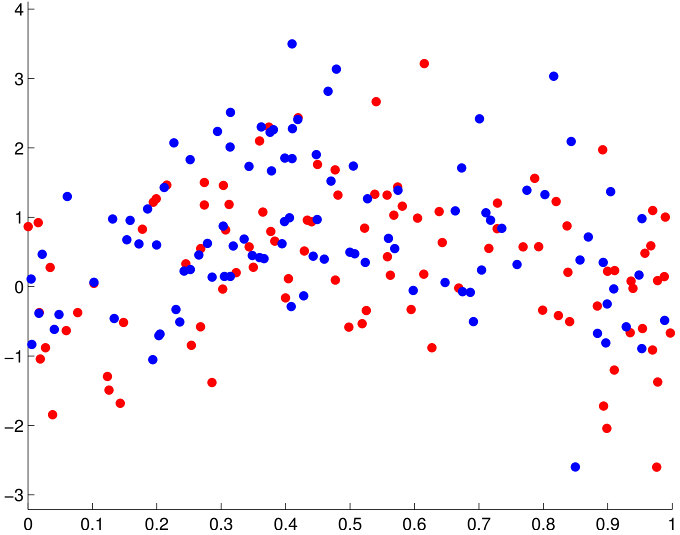
$$\text{OLS in regression:} \quad \frac{\sigma^2 \dim(S_m)}{n}$$



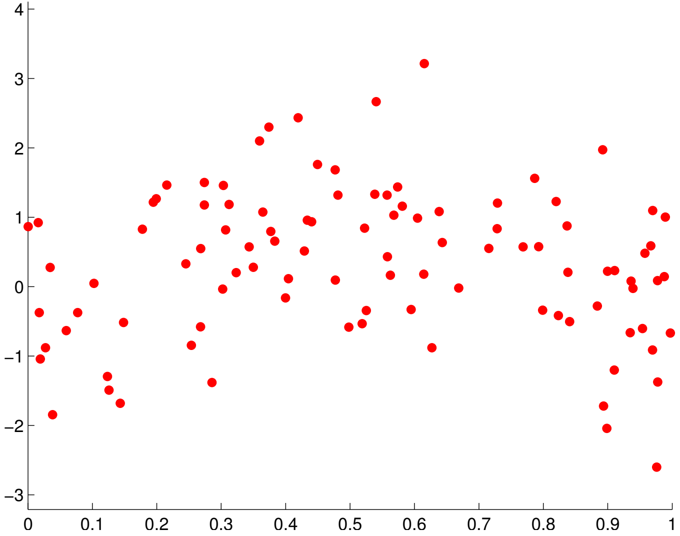
Bias-variance trade-off
$\Leftrightarrow$ avoid overfitting and underfitting

Outline

Validation principle: data splitting



Validation principle: learning sample



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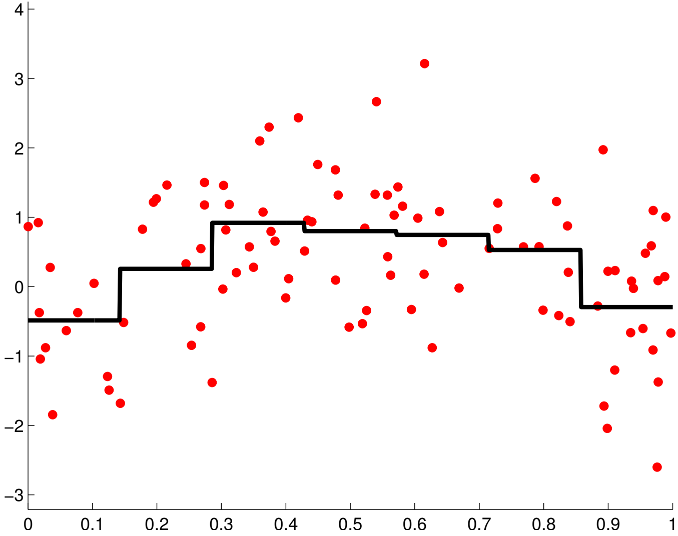

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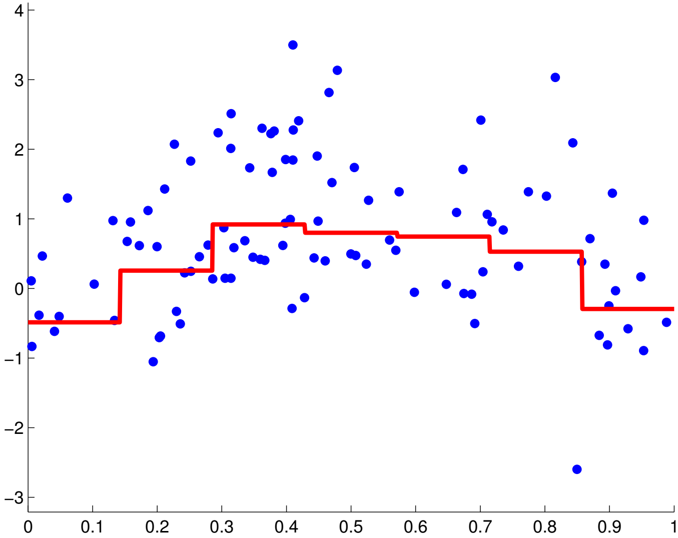

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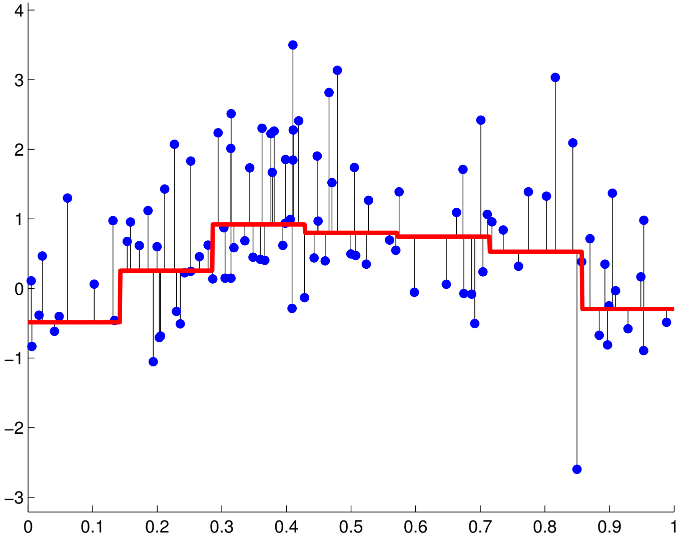

Cross-validation

$$\underbrace{(X_1, Y_1), \ldots, (X_{n_t}, Y_{n_t})}_{\text{Training set } D_n^{(t)} \Rightarrow \widehat{f}_m^{(t)} = \widehat{f}_m(D_n^{(t)})} \quad \underbrace{(X_{n_t+1}, Y_{n_t+1}), \ldots, (X_n, Y_n)}_{\text{Validation set } D_n^{(v)} \Rightarrow \text{ evaluate risk}}$$

- hold-out estimator of the risk:

$$\widehat{\mathcal{R}}_n^{(v)}\left(\widehat{f}_m^{(t)}\right) = \frac{1}{n_v} \sum_{(X_i, Y_i) \in D_n^{(v)}} c\left(\widehat{f}_m^{(t)}(X_i); Y_i\right) \qquad n_v = |D_n^{(v)}| = n - n_t$$

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- cross-validation: average several hold-out estimators

$$\widehat{\mathcal{R}}^{\mathrm{cv}}\left(\widehat{f}_m; D_n; (I_j^{(t)})_{1\leqslant j\leqslant B}\right) = \frac{1}{B}\sum_{j=1}^{B} \widehat{\mathcal{R}}_n^{(v,j)}\left(\widehat{f}_m^{(t,j)}\right) \qquad D_n^{(t,j)} = (X_i, Y_i)_{i\in I_j^{(t)}}$$

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- estimator selection:

$$\widehat{m} \in \operatorname*{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}^{\mathrm{cv}}\left(\widehat{f}_m; D_n\right) \right\}$$

Cross-validation: examples

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

$$\widehat{\mathcal{R}}^{\mathrm{loo}}\left(\widehat{f}_m; D_n\right) = \frac{1}{n}\sum_{j=1}^{n} c\left(\widehat{f}_m^{(-j)}(X_j); Y_j\right)$$

  $\Rightarrow$ leave-p-out ($n_t = n - p$)

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$$\Rightarrow \widehat{\mathcal{R}}^{\mathrm{vf}}\left(\widehat{f}_m; D_n; \mathcal{B}\right) = \frac{1}{V}\sum_{j=1}^{V} \widehat{\mathcal{R}}_n^j\left(\widehat{f}_m^{(-j)}\right)$$

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- Monte-Carlo CV / Repeated learning testing:

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

Outline

Bias of cross-validation

- In this talk, we always assume: $\forall j$, $\mathrm{Card}\left(D_n^{(t,j)}\right) = n_t$
  For V-fold CV: $\mathrm{Card}(B_j) = n/V \Rightarrow n_t = n(V-1)/V$.
- Ideal criterion: $\mathcal{R}\left(\widehat{f}_m(D_n)\right)$

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- General analysis for the bias:

$$\mathbb{E}\left[\widehat{\mathcal{R}}^{\mathrm{cv}}\left(\widehat{f}_m; D_n; \left(I_j^{(t)}\right)_{1 \leqslant j \leqslant B}\right)\right] = \mathbb{E}\Bigl[\mathcal{R}\bigl(\widehat{f}_m(D_{n_t})\bigr)\Bigr]$$

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$\Rightarrow$ everything depends on $n \to \mathbb{E}\left[\mathcal{R}(\widehat{f}_m(D_n))\right]$

- Note: bias can be corrected in some settings (Burman, 1989).
- Note: $D_n \to \widehat{f}_m(D_n)$ must be fixed before seeing any data; otherwise (e.g., data-driven model m), stronger bias.

Bias of cross-validation: generic example

Assume:

$$\mathbb{E}\left[\mathcal{R}\left(\widehat{f}_m(D_n)\right)\right] = \alpha(m) + \frac{\beta(m)}{n}$$

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

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$$\Rightarrow \qquad \mathbb{E}\left[\widehat{\mathcal{R}}^{\mathrm{cv}}\left(\widehat{f}_m; D_n; \left(I_j^{(t)}\right)_{1\leqslant j\leqslant B}\right)\right] = \alpha(m) + \frac{n}{n_t}\frac{\beta(m)}{n}$$

$\Rightarrow$ Bias:

- decreases as a function of n_t,
- minimal for $n_t = n-1$,
- negligible if $n_t \sim n$.

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

Variance of cross-validation: general case

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

$$\operatorname{var}\left(\widehat{\mathcal{R}}_n^{(v)}\left(\widehat{f}_m^{(t)}\right)\right) = \frac{1}{n_v}\mathbb{E}\left[\operatorname{var}\left(c(f(X),Y) \,\middle|\, f = \widehat{f}_m^{(t)}\right)\right] + \operatorname{var}\left(\mathcal{R}(\widehat{f}_m(D_{n_t}))\right)$$

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

$$\operatorname{var}\left(\widehat{\mathcal{R}}^{\mathrm{cv}}\left(\widehat{f}_m; D_n; \left(I_j^{(t)}\right)_{1\leqslant j\leqslant B}\right)\right) = \operatorname{var}\left(\widehat{\mathcal{R}}^{\ell\mathrm{po}}(\widehat{f}_m; D_n)\right) + \frac{1}{B}\underbrace{\mathbb{E}\left[\operatorname{var}_{I^{(t)}}\left(\widehat{\mathcal{R}}_n^{(v)}\left(\widehat{f}_m^{(t)}\right) \,\middle|\, D_n\right)\right]}_{\text{permutation variance}}$$

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

Variance of V-fold CV criterion

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

$$\operatorname{var}\left(\widehat{\mathcal{R}}^{\mathrm{vf}}\left(\widehat{f}_m; D_n; \mathcal{B}\right)\right) = \frac{1+\mathcal{O}(1)}{n} \operatorname{var}_P(f_m^\star) + \frac{2}{n^2}\left[1 + \frac{4}{V-1} + \mathcal{O}\left(\frac{1}{V}+\frac{1}{n}\right)\right] A(m)$$

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

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

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

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

Outline

Risk estimation and estimator selection are different goals

$$\widehat{m} \in \operatorname*{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}^{\mathrm{cv}} \left(\widehat{f}_m \right) \right\} \quad \text{vs.} \quad m^{\star} \in \operatorname*{argmin}_{m \in \mathcal{M}} \left\{ \mathcal{R}\left(\widehat{f}_m(D_n) \right) \right\}$$

- For any Z (deterministic or random),

$$\widehat{m} \in \operatorname*{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}^{\mathrm{cv}} \left(\widehat{f}_m \right) + Z \right\}$$

$\Rightarrow$ bias and variance meaningless.

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- Perfect ranking among $(\widehat{f}_m)_{m \in \mathcal{M}} \Leftrightarrow \forall m, m' \in \mathcal{M}$,

$$\operatorname{sign}\left(\widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_m) - \widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_{m'}) \right) = \operatorname{sign}\left(\mathcal{R}(\widehat{f}_m) - \mathcal{R}(\widehat{f}_{m'}) \right)$$

$\Rightarrow$ $\mathbb{E}\left[\widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_m) - \widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_{m'}) \right]$ should be of the good sign (unbiased risk estimation heuristic: AIC, C_p, leave-one-out...)

$\Rightarrow$ $\operatorname{var}\left(\widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_m) - \widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_{m'}) \right)$ should be minimal (detailed heuristic: A. & Lerasle 2012)

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

$$\operatorname*{argmin}_{m \in \mathcal{M}} \left\{ \mathbb{E}\left[\mathcal{R}\left(\widehat{f}_m(D_{n_t}) \right) \right] \right\}$$

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

$\Rightarrow$ suboptimal otherwise
e.g., V-fold CV with V fixed.

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

Bias-corrected VFCV / V-fold penalization

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

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

$$= \widehat{\mathcal{R}}_n\left(\widehat{f}_m(D_n)\right) + \underbrace{\mathrm{pen}_{\mathrm{VF}}(\widehat{f}_m; D_n; \mathcal{B})}_{V\text{-fold penalty (A. 2008)}}$$

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

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

$$\widehat{\mathcal{R}}^{\ell\mathrm{po}}(\widehat{f}_m; D_n; \mathcal{B}) = \widehat{\mathcal{R}}_n(\widehat{f}_m(D_n)) + \overbrace{\left(1 + \frac{1}{2\left(\frac{n}{p} - 1\right)}\right)} \mathrm{pen}_{\mathrm{VF}}(\widehat{f}_m; D_n; \mathcal{B}_{\mathrm{loo}})$$

Variance and estimator selection

$$\Delta(m, m', V) = \widehat{\mathcal{R}}^{\mathrm{vf,corr}}\left(\widehat{f}_m\right) - \widehat{\mathcal{R}}^{\mathrm{vf,corr}}\left(\widehat{f}_{m'}\right)$$

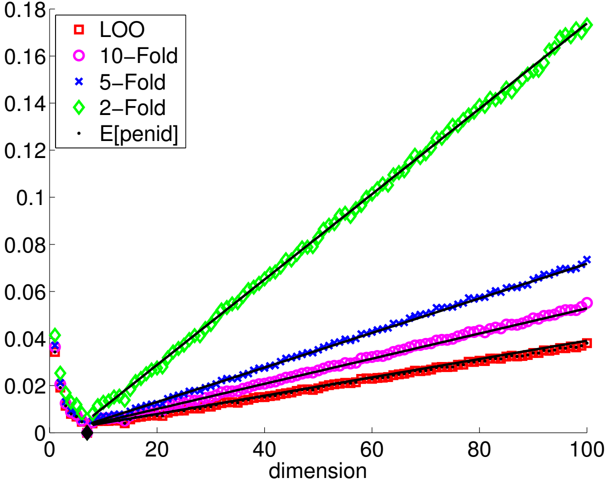
Theorem (A. & Lerasle 2012, least-squares density estimation)

$$\operatorname{var}\left(\Delta(m, m', V)\right) = 4\left(1 + \frac{2}{n} + \frac{1}{n^2}\right)\frac{\operatorname{var}_P\left(f_m^\star - f_{m'}^\star\right)}{n} + 2\left(1 + \frac{4}{V-1} - \frac{1}{n}\right)\underbrace{\frac{B(m, m')}{n^2}}_{\geqslant 0}$$

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

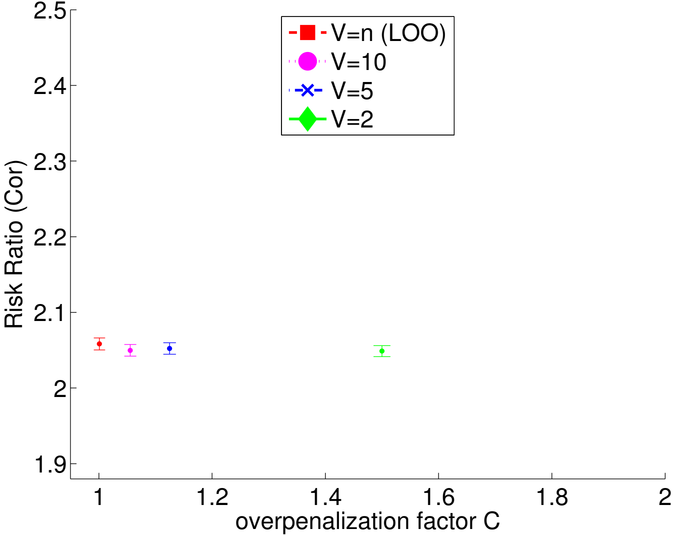
The two terms are of the same order if $\|f_m^\star - f_{m'}^\star\| \approx d_m/n$.

Variance of $\widehat{\mathcal{R}}^{\mathrm{vf,corr}}(\widehat{f}_m) - \widehat{\mathcal{R}}^{\mathrm{vf,corr}}(\widehat{f}_{m^\star})$ vs. (d_m, V)

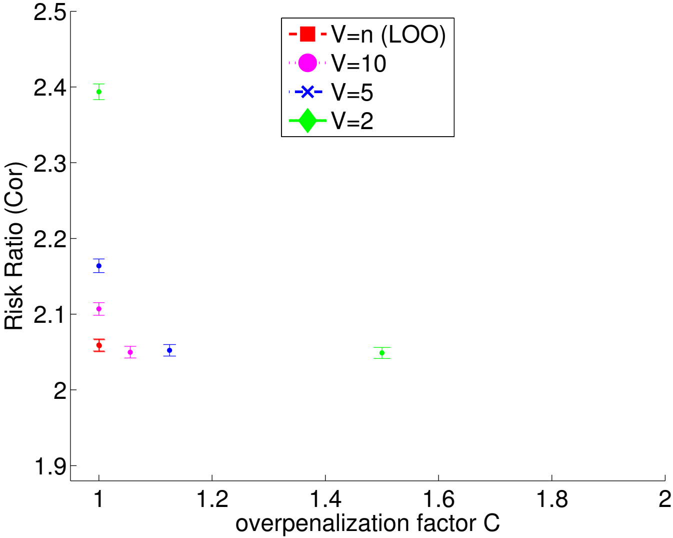


$$\mathrm{var}(\Delta(m, m', V)) \approx n^{-2}\left[29\left(1 + \frac{0.8}{V-1}\right) + 3.7\left(1 + \frac{3.8}{V-1}\right)(d_m - d_{m^\star})\right]$$

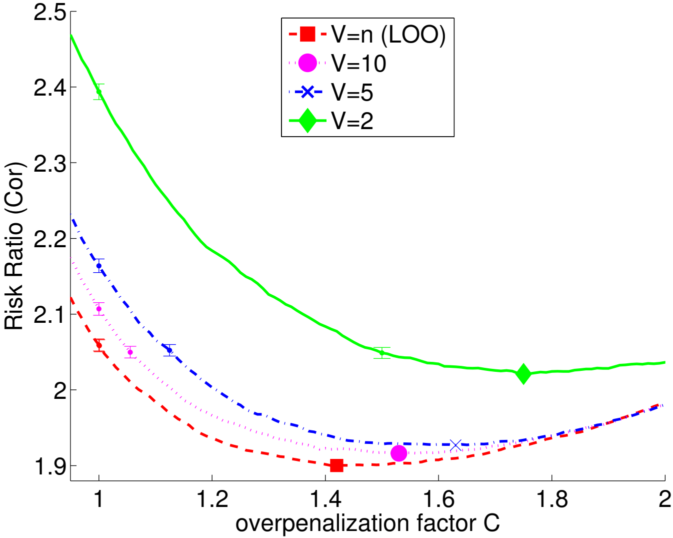
Experiment (LS density estimation): V-fold CV



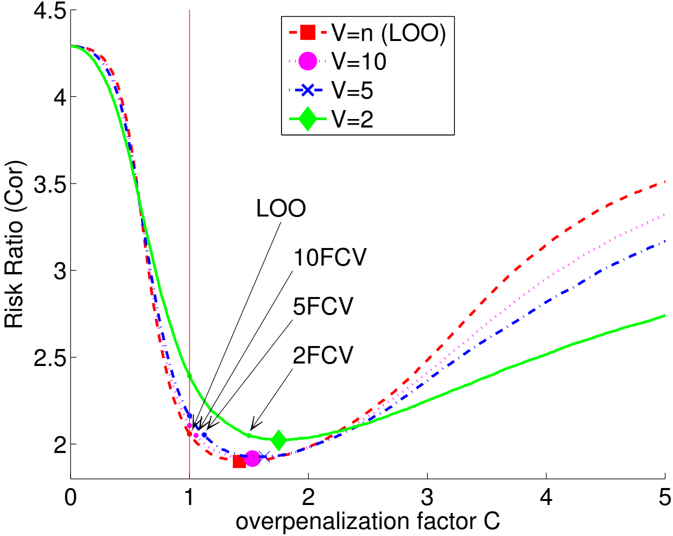
Experiment (LS density estimation): V-fold penalization



Experiment (LS density estimation): overpenalization



Experiment (LS density estimation): conclusion



Outline

Estimator selection with V-fold: conclusion

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

Generality of the results

- At least valid for least-square regression / density estimation, kernel density estimation.
- Bias-correction / V-fold penalization: valid if

$$\mathbb{E}\left[(\mathcal{R} - \widehat{\mathcal{R}}_n)(\widehat{f}_m)\right] \approx \frac{\gamma(m)}{n} \quad .$$

  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

$$n \to \mathbb{E}\left[\mathcal{R}\left(\widehat{f}_m(D_n)\right)\right] \qquad \text{and} \qquad m \to \operatorname{var}\left(\widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_m) - \widehat{\mathcal{R}}^{\mathrm{cv}}(\widehat{f}_{m^\star})\right) .$$

Large collection of estimators/models

- Estimator/model selection with an "exponential" collection (implicitly excluded in all results above).
  $\Rightarrow$ Expectations do not drive the first order!

- Examples: variable selection with $p \geqslant n$ variables, change-point detection.

- Solution: group the models $\Rightarrow$ one estimator per "dimension" (e.g., empirical risk minimizer)
  works for change-point detection (A. & Celisse, 2010).

Cross-validation with an identification goal

- Main change: value of the optimal overpenalization factor $C^\star$, often $C^\star \to +\infty$ when $n \to +\infty$.

$\Leftrightarrow$ Cross-validation paradox (Yang, 2006, 2007): $n_t \ll n$ can be necessary!

- Why? Smaller $n_t \Rightarrow$ easier to distinguish the two best procedures... if n_t large enough (asymptotic regime).

- 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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- Solution for short-term dependence:
  remove some data at each split $\Rightarrow$ gap between training and validation samples.

Questions?