Simultaneous adaptation for several criteria using an extended Lepskii principle

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Setting: linear regression in Hilbert space

We consider the observation model

$$Y_i = \langle f_\circ, X_i \rangle + \xi_i,$$

where

- X_i takes its values in a Hilbert space $\mathcal{H}$, with $\|X_i\| \leq 1$ a.s.;
- ξ_i is a random variable with $\mathbb{E}[\xi_i|X_i] = 0$, $\mathbb{E}\left[\xi^2|X_i\right] \leq \sigma^2$, $|\xi| \leq M$ a.s.;
- $(X_i, \xi_i)_{1 \leq i \leq n}$ are i.i.d.

The goal is to estimate $f_\circ$ (in a sense to be specified) from the data.
Note that if $\dim(\mathcal{H}) = \infty$, this is essentially a non-parametric model.

Why this model?

- Hilbert-space valued variables appear in standard models of **Functional Data Analysis**, where the observed data are modeled (idealized) as function-valued.
- Such models also appear in **reproducing kernel Hilbert space (RKHS) methods** in machine learning:
  - assume observations X_i take valued in some space $\mathcal{X}$
  - let $\Phi : \mathcal{X} \to \mathcal{H}$ be a "feature mapping" in a Hilbert space $\mathcal{H}$, and $\widetilde{X} = \Phi(X)$, then one considers the model

$$Y_i = \langle f_\circ, \widetilde{X}_i \rangle + \xi_i = \widetilde{f}_\circ(X_i) + \xi_i,$$

    where $\widetilde{f} \in \widetilde{H} := \{x \mapsto \langle f, \Phi(x) \rangle; f \in \mathcal{H}\}$ is a nonparametric model of functions (nonlinear in x!).
  - Usually all computations don't require explicit knowledge of Φ but only access to the **kernel** $k(x, x') = \langle \Phi(x), \Phi(x') \rangle$.

Why this model (II) - inverse learning

Of interest is also the **inverse learning** problem:

- X_i takes value in $\mathcal{X}$;
- if A is a linear operator from a Hilbert space $\mathcal{H}$ to a real function space on $\mathcal{X}$;
- inverse regression learning model:

$$Y_i = (Af_\circ)(X_i) + \xi_i.$$

- If A is a Carleman operator (i.e. evaluation functionals $f \mapsto (Af)(x)$ are continuous for all x), then this can be isometrically reduced to a reproducing kernel learning setting (De Vito, Rosasco, Caponnetto 2006; Blanchard and Mücke, 2017).

Two notions of risk

We will consider two notions of error (risk) for a candidate estimate $\widehat{f}$ of $f_\circ$:

- Squared prediction error:

$$\mathcal{E}(\widehat{f}) := \mathbb{E}\left[\left(\langle \widehat{f}, X \rangle - Y\right)^2\right].$$

- The associated (excess error) risk is

$$\mathcal{E}(\widehat{f}) - \mathcal{E}(f_\circ) = \mathbb{E}\left[\left(\left\langle \widehat{f} - f_\circ, X \right\rangle\right)^2\right] = \left\| \widehat{f}^* - f_\circ^* \right\|_{2,X}^2,$$

- Reconstruction error risk:

$$\left\| \widehat{f} - f_\circ \right\|_{\mathcal{H}}^2.$$

The goal is to find a suitable estimator $\widehat{f}$ of $f_\circ$ from the data having "optimal" convergence properties with respect to these two risks.

Finite-dimensional case

- The final dimensional case: $\mathcal{X} = \mathbb{R}^p$, $f_\circ$ now denoted $\beta_\circ$
- In usual matrix form:

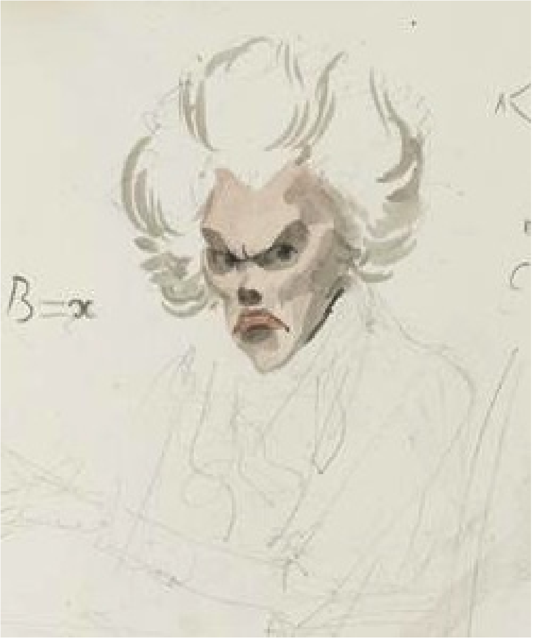
$$\boldsymbol{Y} = \boldsymbol{X}\beta_\circ + \boldsymbol{\xi}.$$

  - X_i^T form the lines of the (n, p) design matrix $\boldsymbol{X}$
  - $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^T$
  - $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n)^T$
- "Reconstruction" risk corresponds to $\left\|\beta_\circ - \widehat{\beta}\right\|^2$.
- Prediction risk corresponds to

$$\mathbb{E}\left[\langle \beta_\circ - \widehat{\beta}, X \rangle^2\right] = \left\|\Sigma^{1/2}(\beta_\circ - \widehat{\beta})\right\|^2,$$

  where $\Sigma := \mathbb{E}\left[XX^T\right]$.
- In Hilbert space, same relation with $\Sigma := \mathbb{E}[X \otimes X^*]$.

The founding fathers of machine learning?



A.M. Legendre

C.F. Gauß

The "ordinary" least squares (OLS) solution:

$$\widehat{\beta}_{OLS} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}.$$

Convergence of OLS in finite dimension

- We want to understand the behavior of $\widehat{\beta}_{OLS}$, when the data size n grows large. Will we be close to the truth $\beta_\circ$?
- Recall

$$\widehat{\beta}_{OLS} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{Y} = \Big(\underbrace{\frac{1}{n}\boldsymbol{X}^T\boldsymbol{X}}_{:=\widehat{\Sigma}}\Big)^{-1}\Big(\underbrace{\frac{1}{n}\boldsymbol{X}^T\boldsymbol{Y}}_{:=\widehat{\gamma}}\Big) = \widehat{\Sigma}^{-1}\widehat{\gamma},$$

- Observe by a vectorial LLN, as $n \to \infty$:

$$\widehat{\Sigma} := \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X} = \frac{1}{n}\sum_{i=1}^{n}\underbrace{X_iX_i^T}_{=:Z_i'} \longrightarrow \mathbb{E}\left[X_1X_1^T\right] =: \Sigma;$$

$$\widehat{\gamma} := \frac{1}{n}\boldsymbol{X}^T\boldsymbol{Y} = \frac{1}{n}\sum_{i=1}^{n}\underbrace{X_iY_i}_{=:Z_i} \longrightarrow \mathbb{E}[X_1Y_1] = \Sigma\beta_\circ =: \gamma;$$

- Hence $\widehat{\beta} = \widehat{\Sigma}^{-1}\widehat{\gamma} \to \Sigma^{-1}\gamma = \beta_\circ$. (Assuming Σ invertible.)

From OLS to Hilbert-space regression

- For ordinary linear regression with $\mathcal{X} = \mathbb{R}^p$ (fixed p, $n \to \infty$):
  - LLN implies $\widehat{\beta}_{OLS}(= \widehat{\Sigma}^{-1}\widehat{\gamma}) \to \beta_\circ(= \Sigma^{-1}\gamma)$;
  - CLT+Delta Method imply asymptotic normality and convergence in $\mathcal{O}(n^{-\frac{1}{2}})$.
- **How to generalize to $\mathcal{X} = \mathcal{H}$?**
- **Main issue:** $\Sigma = \mathbb{E}[X \otimes X^*]$ does not have a continuous inverse. ($\to$ ill-posed problem)
- Need to consider a suitable approximation $\zeta(\widehat{\Sigma})$ of Σ^{-1} **(regularization)**, where

$$\widehat{\Sigma} := \frac{1}{n}\sum_{i=1}^{m} X_i \otimes X_i^*$$

  is the empirical second moment operator.

Regularization methods

- Main idea: replace $\widehat{\Sigma}^{-1}$ by an approximate inverse, such as
- **Ridge regression/Tikhonov**:

$$\widehat{f}_{Ridge(\lambda)} = (\widehat{\Sigma} + \lambda I_p)^{-1}\widehat{\gamma}$$

- **PCA projection/spectral cut-off**: restrict $\widehat{\Sigma}$ on its k first eigenvectors

$$\widehat{f}_{PCA(k)} = (\widehat{\Sigma})^{-1}_{|k}\widehat{\gamma}$$

- **Gradient descent/Landweber Iteration/L^2 boosting**:

$$\widehat{f}_{LW(k)} = \widehat{f}_{LW(k-1)} + (\widehat{\gamma} - \widehat{\Sigma}\widehat{f}_{LW(k-1)})$$
$$= \sum_{i=0}^{k}(I - \widehat{\Sigma})^k\widehat{\gamma},$$

  (assuming $\|\widehat{\Sigma}\|_{op} \leq 1$).

General form spectral linearization

Bauer, Rosasco, Pereverzev 2007

- **General form** regularization method:

$$\widehat{f}_\lambda = \zeta_\lambda(\widehat{\Sigma})\widehat{\gamma}$$

  for some well-chosen function $\zeta_\lambda : \mathbb{R}_+ \to \mathbb{R}_+$ acting on the spectrum and "approximating" the function $x \mapsto x^{-1}$.

- $\lambda > 0$: regularization parameter; $\lambda \to 0 \Leftrightarrow$ less regularization
- Notation of (autoadjoint) functional calculus, i.e.

$$\widehat{\Sigma} = Q^T \mathrm{diag}(\mu_1, \mu_2, \ldots) Q \Rightarrow \zeta(\widehat{\Sigma}) := Q^T \mathrm{diag}(\zeta(\mu_1), \zeta(\mu_2), \ldots) Q$$

- Examples (revisited):
  - **Tikhonov**: $\zeta_\lambda(t) = (t+\lambda)^{-1}$
  - **Spectral cut-off**: $\zeta_\lambda(t) = t^{-1}\mathbf{1}\{t \geq \lambda\}$
  - **Landweber iteration**: $\zeta_k(t) = \sum_{i=0}^{k}(1-t)^i$.

Assumptions on regularization function

Standard assumptions on the regularization family $\zeta_\lambda : [0,1] \to \mathbb{R}$ are:

(i) There exists a constant $D < \infty$ such that

$$\sup_{0<\lambda\leq 1} \sup_{0<t\leq 1} |t\zeta_\lambda(t)| \leq D\,,$$

(ii) There exists a constant $E < \infty$ such that

$$\sup_{0<\lambda\leq 1} \sup_{0<t\leq 1} \lambda|\zeta_\lambda(t)| \leq E\,,$$

(iii) **Qualification:** for **residual** $r_\lambda(t) := 1 - t\zeta_\lambda(t)$,

$$\forall \lambda \leq 1 : \qquad \sup_{0<t\leq 1} |r_\lambda(t)| t^\nu \leq \gamma_\nu \lambda^\nu,$$

holds for $\nu = 0$ and $\nu = q > 0$.

Structural Assumptions (I)

- Denote $(\mu_i)_{i\geq 1}$ the sequence of positive eigenvalues of Σ in nonincreasing order.

- **Assumptions on spectrum decay:** for $s \in (0,1); \alpha > 0$:

$$\mathbf{IP}^{<}(s,\alpha): \quad \mu_i \leq \alpha i^{-\frac{1}{s}}$$

- This implies quantitative estimates of the "effective dimension"

$$\mathcal{N}(\lambda) := \mathrm{Tr}(\ (\Sigma+\lambda)^{-1}\Sigma\ ) \lesssim \lambda^{-s}.$$

Structural Assumptions (II)

- Denote $(\mu_i)_{i\geq 1}$ the sequence of positive eigenvalues of Σ in nonincreasing order.

- **Source condition** for the signal: for $r > 0$, define

$$\mathbf{SC}(r,R): \quad f_\circ = \Sigma^r h_\circ \text{ for some } h_\circ \text{ with } \|h_\circ\| \leq R,$$

  or equivalently, as a **Sobolev-type regularity**

$$\mathbf{SC}(r,R): \quad f_\circ \in \left\{ f \in \mathcal{H} : \sum_{i\geq 1} \mu_i^{-2r} f_i^2 \leq R^2 \right\},$$

  where f_i are the coefficients of h in the eigenbasis of Σ.

- Under $(\mathbf{SC})(r,R)$ it is assumed that the **qualification** q of the regularization method satisfies $q \geq r + \frac{1}{2}$.

A general upper bound risk estimate

Theorem

Assume the source condition (**SC**)(r, R) *holds.*
If λ *is such that* $\lambda \gtrsim (\mathcal{N}(\lambda) \vee \log(\eta)^2)/n$, *then with probability at least* $1-\eta$, *it holds:*

$$\left\|(\Sigma+\lambda)^{1/2}\left(f_\circ - \widehat{f}_\lambda\right)\right\|_{\mathcal{H}} \lesssim \log(\eta)^2\left(R\lambda^{r+\frac{1}{2}} + \sigma\sqrt{\frac{\mathcal{N}(\lambda)}{n}} + \frac{1}{n\sqrt{\lambda}} + \mathcal{O}(n^{-\frac{1}{2}})\right).$$

This gives rise to estimates in both norms of interest since

$$\left\|f_\circ - \widehat{f}_\lambda\right\|_{\mathcal{H}} \leq \lambda^{-\frac{1}{2}}\left\|(\Sigma+\lambda)^{1/2}\left(f_\circ - \widehat{f}_\lambda\right)\right\|_{\mathcal{H}},$$

and

$$\left\|f_\circ^* - \widehat{f}_\lambda^*\right\|_{L^2(P_X)} = \left\|\Sigma^{\frac{1}{2}}(f_\circ - \widehat{f}_\lambda)\right\|_{\mathcal{H}} \leq \left\|(\Sigma+\lambda)^{1/2}\left(f_\circ - \widehat{f}_\lambda\right)\right\|_{\mathcal{H}}.$$

Upper bound on rates

Optimizing the obtained bound over λ (i.e. balancing the main terms) one obtains

Theorem

Assume r, R, s, α *are fixed positive constants and assume* $\mathbb{P}_{XY}$ *satisfies* **(IP**$^{<}$**)**(s,α), **(SC)**(r,R) *and* $\|X\| \leq 1$, $\|Y\| \leq M$, $\mathrm{Var}[Y|X]_\infty \leq \sigma^2$ *a.s. Define*

$$\widehat{\beta}_n = \zeta_{\lambda_n}(\widehat{\Sigma})\widehat{\gamma},$$

using a regularization family (ζ_λ) *satisfying the standard assumptions with qualification* $q \geq r + \frac{1}{2}$, *and the parameter choice rule*

$$\lambda_n = (R^2\sigma^2/n)^{-\frac{1}{2r+1+s}}.$$

Then it holds for any $p \geq 1$:

$$\limsup_{n\to\infty} \mathbb{E}^{\otimes n}\left(\left\|f_\circ - \widehat{f}_{\lambda_n}\right\|^p\right)^{1/p} \Big/ R\left(\frac{\sigma^2}{R^2 n}\right)^{\frac{r}{2r+1+s}} \leq C_\blacktriangle;$$

$$\limsup_{n\to\infty} \mathbb{E}^{\otimes n}\left(\left\|f_\circ^* - \widehat{f}_{\lambda_n}\right\|_{2,X}^p\right)^{1/p} \Big/ R\left(\frac{\sigma^2}{R^2 n}\right)^{\frac{r+1/2}{2r+1+s}} \leq C_\blacktriangle.$$

Towards adaptivity: existing approaches

- Cross-validation (or hold-out) will yield a tuning of the parameter which is **adaptive in the prediction risk**, it is based on a unbiased estimate of the risk **(URE)** principle.
- Standard Lepski's principle parameter selection can be applied for any fixed norm (provided a good estimate of the "variance" term $\sigma\sqrt{\mathcal{N}(\lambda)/n}$ is available)
- Despite the **existence** of a regularization parameter λ being optimal for both norms, there is no guarantee that **any** (close to) optimal parameter for prediction risk (eg. selected by cross-validation) will be close to optimal in reconstruction risk, or vice-versa.
- We want to construct a **simultaneously (for both norms) adaptive** data-driven parameter selection.

Generalized Lepskii's principle

We consider the following "deterministic" assumption to highlight the construction.

Assumption

Let $\Lambda \subset \mathbb{R}_+$ be a finite set of candidate regularization parameters,

$$\Lambda := \{\lambda_j, \quad \lambda_0 > \lambda_1 > \ldots > \lambda_m = \lambda_{\min} > 0\},$$

The (known) family of elements of $\mathcal{H}$, $(f_\lambda)_{\lambda\in\Lambda}$, satisfies for any $\lambda \in \Lambda$:

$$\left\|(\Sigma+\lambda)^{1/2}(f_\circ - f_\lambda)\right\|_{\mathcal{H}} \leq C\sqrt{\lambda}(\mathcal{A}(\lambda)+\mathcal{S}(\lambda)),$$

where

- the function $\lambda \in \Lambda \mapsto \mathcal{A}(\lambda) \in \mathbb{R}_+$ is **non-decreasing** with $\mathcal{A}(0) = 0$ and possibly **unknown**;
- the function $\lambda \in \Lambda \mapsto \sqrt{\lambda}\mathcal{S}(\lambda) \in \mathbb{R}_+$ is **non-increasing** and **known**.

Generalized Lepskii's principle (II)

- Set

$$\mathcal{M}(\Lambda) := \Big\{ \lambda \in \Lambda \ : \ \left\| (\Sigma + \lambda')^{1/2} (f_\lambda - f_{\lambda'}) \right\|_{\mathcal{H}} \leq 4C\sqrt{\lambda'}\mathcal{S}(\lambda'), \\ \forall \lambda' \in \Lambda, \text{ s.t. } \lambda' \leq \lambda \Big\}.$$

- The balancing parameter is given as

$$\hat{\lambda} := \max \ \mathcal{M}(\Lambda) \ ;$$

(this quantity is always well-defined since $\lambda_{\min} \in \mathcal{M}(\Lambda)$.)

Generalized Lepskii's principle: bound

Theorem

Under the assumptions made previously, if

$$\lambda_* := \max\{\lambda \in \Lambda : \mathcal{A}(\lambda) \leq \mathcal{S}(\lambda)\},$$

and $\widehat{\lambda}$ is the parameter choice defined previously, then:

- *It holds*

$$\left\| (\Sigma + \lambda_*)^{\frac{1}{2}} (f_\circ - f_{\widehat{\lambda}}) \right\|_{\mathcal{H}} \lesssim \sqrt{\lambda_*}\mathcal{S}(\lambda_*);$$

- *Assuming it holds $\mathcal{S}(\lambda_k) \leq C_{\mathcal{S}}\mathcal{S}(\lambda_{k-1})$ for $k = 1, \ldots, m$, then:*

$$\left\| f_\circ - f_{\widehat{\lambda}} \right\|_{\mathcal{H}} \lesssim \min_{\lambda \in \Lambda} (\mathcal{A}(\lambda) + \mathcal{S}(\lambda));$$

$$\left\| \Sigma^{\frac{1}{2}} (f_\circ - f_{\widehat{\lambda}}) \right\|_{\mathcal{H}} \lesssim \min_{\lambda \in \Lambda} \sqrt{\lambda}(\mathcal{A}(\lambda) + \mathcal{S}(\lambda)).$$

Applying Lepski's principle

Looking at the main error bound obtained earlier, with high probability the assumption

$$\left\|(\Sigma+\lambda)^{1/2}(f_\circ - f_\lambda)\right\|_{\mathcal{H}} \le C\sqrt{\lambda}(\mathcal{A}(\lambda)+\mathcal{S}(\lambda))$$

is satisfied with

$$\mathcal{A}(\lambda) := \left(R\lambda^{r+\frac{1}{2}} + \mathcal{O}(n^{-\frac{1}{2}})\right),$$
$$\mathcal{S}(\lambda) := \sigma\sqrt{\frac{\mathcal{N}(\lambda)}{n}} + \frac{1}{n\sqrt{\lambda}}.$$

Remaining issues:

- Σ is not known;
- $\mathcal{N}(\lambda) = \mathrm{Tr}(\ (\Sigma+\lambda)^{-1}\Sigma)$ is not known;
- the noise variance σ^2 might not be known (issue ignored for now).

Replacing $\Sigma, \mathcal{N}(\lambda)$ by empirical quantities

Proposition

If λ is such that $\lambda \gtrsim (\mathcal{N}(\lambda) \vee \log(\eta)^2)\,/\,n$, then with probability at least $1-\eta$, it holds:

$$\left\|(\Sigma+\lambda)^{\frac{1}{2}}(\widehat{\Sigma}+\lambda)^{-\frac{1}{2}}\right\| \lesssim 1+\log(\eta^{-1}).$$

Proposition

If $\lambda \gtrsim n^{-1}$, it holds with probability at least $1-\eta$, for $\widehat{\mathcal{N}}(\lambda) := \mathrm{Tr}(\widehat{\Sigma}(\widehat{\Sigma}+\lambda)^{-1})$:

$$\max\left(\frac{\mathcal{N}(\lambda)\vee 1}{\widehat{\mathcal{N}}(\lambda)\vee 1}, \frac{\widehat{\mathcal{N}}(\lambda)\vee 1}{\mathcal{N}(\lambda)\vee 1}\right) \lesssim (1+\log\eta^{-1})^2.$$

Fully empirical procedure (σ, M known)

- Put $L := 2\log(8\log n/(\eta \log q))$ and let

$$\widehat{\Lambda} := \left\{\lambda_i = q^{-i}, i \in \mathbb{N}, \text{ s.t. } \lambda_i \geq 100(\widehat{\mathcal{N}}(\lambda) \vee L^2/n)\right\}.$$

- Define the parameter choice

$$\widehat{\lambda} = \max\Big\{\lambda \in \widehat{\Lambda} : \forall \lambda' \in \widehat{\Lambda}, \text{ s.t. } \lambda' \leq \lambda :$$
$$\left\|(\widehat{\Sigma} + \lambda')^{\frac{1}{2}}(\widehat{f}_\lambda - \widehat{f}_{\lambda'})\right\| \leq cL\sqrt{\lambda'}\widehat{S}(\lambda')\Big\},$$

where

$$\widehat{\mathcal{S}}(\lambda) := \frac{\sigma\sqrt{2(\widehat{\mathcal{N}}(\lambda) \vee 1)} + M/5}{\sqrt{\lambda n}}.$$

Result for the empirical selection procedure

Theorem

Assume the source condition $(\mathbf{SC})(r, R)$ *holds.*
Then for the generalized-Lepski parameter choice $\widehat{\lambda}$*, with probability at least* $1 - \eta$*:*

$$\left\|(\Sigma + \lambda)^{\frac{1}{2}}(\widehat{f}_{\widehat{\lambda}} - f_\circ)\right\| \lesssim L^3 \min_{\lambda \in [\lambda_{\min}, 1]} \left(R\lambda^{r+\frac{1}{2}} + \sigma\sqrt{\frac{\mathcal{N}(\lambda)}{n}} + \frac{1}{n\sqrt{\lambda}} + \mathcal{O}(n^{-\frac{1}{2}})\right).$$

where

$$\lambda_{\min} = \min\left\{\lambda \in [0, 1] : \lambda \gtrsim (\mathcal{N}(\lambda) \vee L^2/n)\right\}.$$

Conclusion: as a direct byproduct we get the same rates (up to $\log\log n$ factor) as the optimal choice of λ in the original bound, for **both norms of interest**.

Perspective: estimation of unknown noise variance σ

- Observe that in general, there is no identifiability in the model

$$y_i = f(x_i) + \sigma \xi_i,$$

  if the function f can be "arbitrary".
- There is a hope when we assumed that f has some regularity (here: linearity)
- **Idea:**
  - Take λ small so that the "bias" $\mathcal{A}(\lambda)$ is expected to be much lower than the "variance" $\mathcal{S}(\lambda)$ (e.g., close to $\widehat{\lambda}_{\mathrm{min}}$.
  - Split the sample into two subsamples giving rise to $\widehat{f}_\lambda^{(1)}, \widehat{f}_\lambda^{(2)}$.
  - The hope is that by considering $\left\| \widehat{f}_\lambda^{(1)} - \widehat{f}_\lambda^{(2)} \right\|^2$ in a suitable norm, we cancel the bias and observe twice the "variance".
- Need somewhat precise concentration (upper and lower) for this quantity.