# 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.;
- $\xi_i$ 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 distribution of $X$ is **not known**.)

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 $\Phi$ 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 (**known**) linear operator from a Hilbert $\mathcal{G}$ to a real function space on $\mathcal{X}$;
- inverse regression learning model:

$$Y_i = (Ag_*)(X_i) + \xi_i,$$

- where $A$ is a Carleman operator
(i.e. evaluation functionals $f \mapsto (Af)(x)$ are continuous for all $x$),
- In this case the goal is to recover $g_* \in \mathcal{G}$.

# Why this model (III) - inverse learning, continued

- inverse regression learning model: $Y_i = \underbrace{(Ag_*)}_{f_\circ}(X_i) + \xi_i$.
  - If $A$ is a Carleman operator $\mathcal{G} \to \mathcal{F}_{\text{mes.}}(\mathcal{X}, \mathbb{R})$, then of evaluation functionals

    $$\text{For all } f \in \mathcal{G}, x \in \mathcal{X}: \qquad (Af)(x) = \langle F_x, f \rangle_{\mathcal{G}} \text{ for some } F_x \in \mathcal{G}$$

  - Then $\mathcal{H} := \mathrm{Im}(A)$ can be equipped with a RKHS structure with kernel

    $$k(x, x') := \langle F_x, F_{x'} \rangle_{\mathcal{G}}.$$

  - Furthermore, $A$ is then a **partial isometry** $\mathcal{H} \to \mathcal{G}$.
- Therefore, if $\widehat{f} \in \mathcal{H}$ is an estimate of $f_\circ = Ag_*$ and if we assume $g_* \in \mathrm{Ker}(A)^\perp$:

  $$\text{Put } \widehat{g} := A^{-1}\widehat{f}, \text{ then } \|\widehat{g} - g_*\|_{\mathcal{G}} = \left\| A^{-1}(\widehat{f} - f_\circ) \right\|_{\mathcal{G}} = \left\| \widehat{f} - f_\circ \right\|_{\mathcal{H}}$$

- Here the RKHS $\mathcal{H}$ is entirely determined by $A$. Mathematically speaking, we are back in the RKHS learning scenario, but **the convergence in $\mathcal{H}$-norm** is of major importance.

# Inverse regression vs inverse "learning"

- Bissantz, Hohage, Munk and Ruymgaart (2007) propose a very general analysis of general regularization methods for **statistical** inverse problems.

- Their model includes applications to the inverse regression model where the **design distribution** ($X$-marginal) is assumed to be known (the exact integral operator is used to construct the estimator).

- A proper characteristic of inverse **"learning"** is the absence of information a priori on the $X$-marginal – it has to be "learned" as well.

# 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 (especially relevant for **inverse learning**):

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

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

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

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

# Convergence of OLS in finite dimension

- The “ordinary” least squares (OLS) solution:

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

- 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 $\Sigma$ 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.
  ($\rightarrow$ ill-posed problem)

# From OLS to Hilbert-space regression

- For ordinary linear regression with $\mathcal{X} = \mathbb{R}^p$ (fixed $p$, $n \to \infty$):
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- **How to generalize to $\mathcal{X} = \mathcal{H}$?**

- **Main issue:** $\Sigma = \mathbb{E}[X \otimes X^*]$ does not have a continuous inverse.
  ($\longrightarrow$ ill-posed problem)

- Need to consider a suitable approximation $\zeta(\widehat{\Sigma})$ of $\Sigma^{-1}$ **(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**:

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

(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

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

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

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

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

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

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

# Structural Assumptions (I)

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

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

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

# Structural Assumptions (I)

- Denote $(\mu_i)_{i\geq 1}$ the sequence of positive eigenvalues of $\Sigma$ 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 $\Sigma$ 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 $\Sigma$.

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

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

# A general upper bound risk estimate

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*If* $\lambda$ *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 $\lambda$ (i.e. balancing the main terms) one obtains

## Theorem

*Assume* $r, R, s, \alpha$ *are fixed positive constants and assume* $\mathbb{P}_{XY}$ *satisfies* **(IP$^<$)**$(s, \alpha)$, **(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* $(\zeta_\lambda)$ *satisfying the standard assumptions with qualification* $q \geq r + \frac{1}{2}$, *and the parameter choice rule*

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

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

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

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

# Extensions to nonlinear operators

- Extensions possible to **nonlinear** inverse problems
- Need stronger assumptions (output space of $A$ has RKHS structure, $A$ is Lipschitz continuous)
- For Tikhonov regularization: see Abishake R, Blanchard, Mathé 2020.

# 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 $\lambda$ 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.

# Standard 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 $\lambda \in \Lambda$:

$$\|f_\circ - f_\lambda\|_{\mathcal{H}} \leq C(\mathcal{A}(\lambda) + \mathcal{S}(\lambda)),$$

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**.

# Standard Lepskii's principle (II)

Set

$$\hat{\lambda} := \max\left\{\lambda \in \Lambda \ : \ \|f_\lambda - f_{\lambda'}\|_{\mathcal{H}} \leq 4C\mathcal{S}(\lambda'), \forall \lambda' \in \Lambda, \text{ s.t. } \lambda' \leq \lambda \right\},$$

## Theorem

*Under the assumptions made previously, if*

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

- *then it holds:*

$$\|f_\circ - f_{\hat{\lambda}}\|_{\mathcal{H}} \lesssim \mathcal{S}(\lambda_*);$$

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

$$\|f_\circ - f_{\hat{\lambda}}\|_{\mathcal{H}} \lesssim \min_{\lambda \in \Lambda}(\mathcal{A}(\lambda) + \mathcal{S}(\lambda)).$$

# 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 $\lambda_{\text{min}} \in \mathcal{M}(\Lambda)$.)

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

# Applying Lepskii's principle

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

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

is satisfied with

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

$$\mathcal{S}(\lambda) := \frac{\sigma\sqrt{\mathcal{N}(\lambda)} + \mathcal{O}(1)}{\sqrt{\lambda n}}.$$

**Remaining issues:**

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

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

## Proposition

*If $\lambda$ is such that $\lambda \gtrsim \left(\mathcal{N}(\lambda) \vee \log(\eta)^2\right)/n$, 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 ($\sigma$, $M$ 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

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

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 $\lambda$ in the original bound, for **both norms of interest**.

# Estimating the unknown noise variance $\sigma^2$?

- 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 $\lambda$ small so that the "bias" $\mathcal{A}(\lambda)$ is expected to be much lower than the "variance" $\mathcal{S}(\lambda)$ (e.g., close to $\widehat{\lambda}_{\min}$.
  - 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.

# Estimation of the variance $\sigma^2$

- Assume we have two independent sample of the same size $n$, giving rise to estimators $\widehat{f}_\lambda^{(1)}, \widehat{f}_\lambda^{(2)}$ (using the same regularization parameter $\lambda > 0$).
- Consider the statistic

$$\begin{aligned}\Delta^2 &:= \left\| \frac{1}{2}(\widehat{\Sigma}^{(1)} + \widehat{\Sigma}^{(2)} + \lambda)^{\frac{1}{2}}(\widehat{f}_\lambda^{(1)} - \widehat{f}_\lambda^{(2)}) \right\|_{\mathcal{H}}^2 \\ &= \frac{1}{2n}\sum_{i=1}^{2n}(\widehat{f}_\lambda^{(1)} - \widehat{f}_\lambda^{(2)})^2(x_i) + \lambda \left\| \widehat{f}_\lambda^{(1)} - \widehat{f}_\lambda^{(2)} \right\|_{\mathcal{H}}^2,\end{aligned}$$

and

$$\widehat{\sigma}^2 := \frac{\Delta^2}{\sum_{i,j=1}^2 \|A_{ij}\|_{HS}^2},$$

where $A_{ij} = (\widehat{\Sigma}^{(i)} + \lambda)^{\frac{1}{2}} \zeta_\lambda(\widehat{\Sigma}^{(j)})(\widehat{\Sigma}^{(j)})^{\frac{1}{2}}$.

# Estimation of the variance $\sigma^2$

**Theorem**

*If $\lambda \geq \widehat{\lambda}_{min}$, where*

$$\widehat{\lambda}_{min} = \min\left\{\lambda > 0 : \lambda \geq 100(\widehat{\mathcal{N}}(\lambda) \vee \log(\eta^{-1})/2)\right\},$$

*then with probability at least $1 - \eta$, it holds*

$$\widehat{\sigma}^2 \in \left[\sigma^2 \pm \left(\lambda\sigma^2 + F(\lambda)\log(\eta^{-1})\right)\right],$$

*with $F(\lambda) \to 0$ as $\lambda \to 0$.*

**Conclusion:** the estimator $\widehat{\sigma}^2$ is consistent, and can be used as a proxy for $\sigma^2$ in the procedure, with the same conclusions (up to changes in numerical constants, and for $n$ big enough).

Thank you for your attention

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