Eigenvalue-free risk bounds for PCA projectors

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joint work with many people (G. Biau, E. Brunel, C. Crambes, N. Hilgert, A. Roche, F. Ruymgaart, N. Verzelen)

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Random Projections vs PCA

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- Principal components/PCA and variants : projection space depends on the data. Real projections i.e. $P^2 = P$.
- "Random projections" (RP) : projection space independent from the data. Not real projections but rectangle matrices with nrows<ncols filled with i.i.d. (Gaussian/Rademacher) entries.

RP are used in sparse recovery, compressed sensing, etc. Allow effective dimension reduction for sparse signals through Johnson-Lindenstrauss Lemma and Restricted Isometry Property.

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- Main feature : optimal linear reconstruction. Consider X random with cov. matrix Σ and $\mathcal{P}_k$ the set of orth. projections with rank k. Then, under general conditions :

$$\min_{P_k \in \mathcal{P}_k} \mathbb{E} \left\| X - P_k X \right\|^2 = \min_{P_k \in \mathcal{P}_k} \mathrm{tr} \left[P_k^{\perp} \Sigma P_k^{\perp} \right]$$

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  is obtained for principal components of X (= s.v.d. of Σ here).
- Numerous variants in ML : sparse PCA, kernel/non linear PCA...

Notations and Set-up

$\mathbf{H} = \mathbf{L}^2([0,1])$ or $\mathbf{W}^{2,m}([0,1])$ with inner product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$
$X_1, X_2, ...X_n$ sample of i.i.d random elements with values in $\mathbf{H}$ and $\mathbb{E}X_1 = 0$:

$$\Sigma = \mathbb{E}(X_1 \otimes X_1) = \mathbb{E}\langle X_1, \cdot \rangle X_1 = \sum_{i=1}^{+\infty} \lambda_k (\varphi_k \otimes \varphi_k),$$

$$\Sigma_n = \frac{1}{n} \sum_{k=1}^{n} X_k \otimes X_k \quad \Sigma_n \widehat{\varphi}_i = \widehat{\lambda}_i \widehat{\varphi}_i$$

- $(\lambda_k)_{k \in \mathbb{N}^*} \in l_1^+$,with $\lambda_1 > ... > \lambda_k > ... > 0$
- Rank one projector : $\pi_i = \varphi_i \otimes \varphi_i$.
- Projection onto $\mathrm{span}\{\varphi_1, ..., \varphi_k\}$: $\mathbf{P}_k = \sum_{i=1}^k \pi_i$.
- Empirical counterparts : $\widehat{\pi}_i = \widehat{\varphi}_i \otimes \widehat{\varphi}_i$ and $\widehat{\mathbf{P}}_k = \sum_{i=1}^k \widehat{\pi}_i$.

Smoothness of processes and eigenvalues decay

Karhunen-Loeve development : $X = \sum_{j=1}^{+\infty} \sqrt{\lambda_j}\xi_j\varphi_j$
[Kind of random generalized Fourier series]

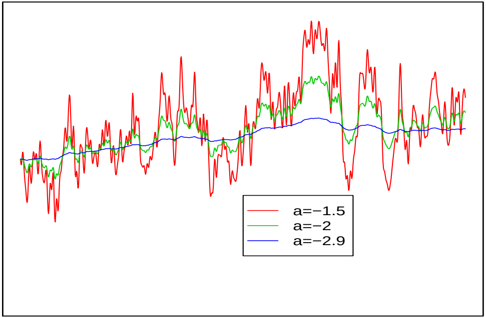

Figure: Three examples of random curves with $\lambda_j = j^a$ and the same ξ_j's.

Motivation-Goals

- $\Sigma \approx$ infinite size matrix, Σ trace-class, Σ^{-1} unbounded (not coercive)
- No specific model on X (e.g: signal$+$ noise) or Σ (spiked covariance structure not suited to functional setting)

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- Usually upper bounds are (roughly) $\|\widehat{\pi}_i - \pi_i\|_\infty^2 \prec 1/\left(n\lambda_i\right)$ or $1/\left(n\delta_i\right)$ with $\delta_i = \min\left(|\lambda_i - \lambda_{i+1}|, |\lambda_{i-1} - \lambda_i|\right)$
- Previous bound degenerates if $\lambda_i = e^{-mi}$ or $\lambda_i = i^{-\alpha}$ for large α
- Not that shocking if eig.vec. estimation seen as fixed point pb $\Sigma_n \hat{\varphi}_i / \hat{\lambda}_i = \hat{\varphi}_i$. If $i \uparrow \infty$ pb no more well posed $\mapsto$ price to pay...

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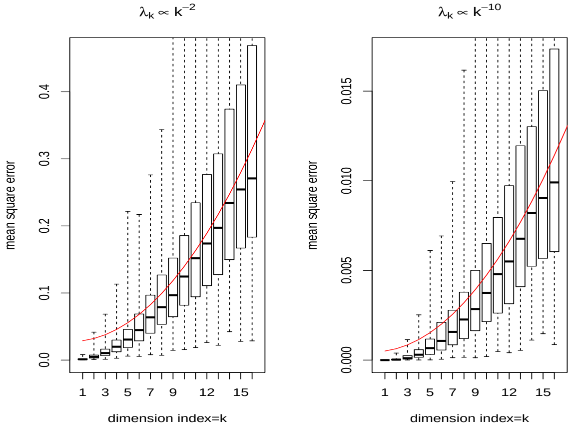
- But paradox ? X may be concentrated on low dimensional space $\rightarrow$ convergence of $\widehat{\pi}_i$ could be slow even for i in low dimensions.
- Why not some simulations now ?

Some simulations before theory...



MC simulation of $\mathbb{E}\,\|\widehat{\pi}_k - \pi_k\|_\infty^2$ with $M = 500$ replications, sample size $n = 500$ and $X = \sum_{j=1}^{kmax} \sqrt{\lambda_j}\xi_j e_j$ with $kmax = 20$, ξ_j Gaussian, e_j Fourier basis and $\mathrm{tr}\Sigma = 1$. Red curve : k^2 fit

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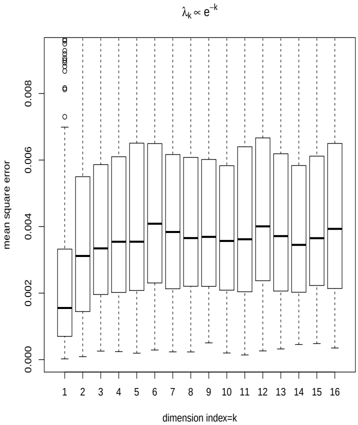

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From covariance to projectors : perturbation theory and functional calculus

Notice $\left|\widehat{\lambda}_k - \lambda_k\right| \leq \|\Sigma_n - \Sigma\|_\infty \leq \|\Sigma_n - \Sigma\|_2 .$

- Is it possible to get $\widehat{\pi}_k = f_k(\Sigma_n)$ and $\pi_k = f_k(\Sigma)$?
- So that $\widehat{\pi}_k - \pi_k = f_k(\Sigma_n) - f_k(\Sigma) \simeq g_k(\Sigma_n - \Sigma)$ with 'nice' g_k

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Functional calculus defines $f(M)$ where M and $f(M)$ matrices or operators for certain classes of functions f. Two kinds:

- **Spectral FC** $\diamond$ M selfadjoint $\diamond$ f Borel bounded on $\mathbb{R}$ $\diamond$ **Main tool :** Resolution of the identity (Spectral Theorem)
- **Perturbation FC** $\diamond$ any M $\diamond$ f holomorphic $\diamond$ **Main tool** : Resolvent (Kato's theory)

Projection via perturbation in a nutshell

- Take $\lambda_k \in \mathbb{C}$ and let Ω_k a closed oriented contour around λ_k (say a circle) separating λ_k from the other eigenvalues
- Use Cauchy integral properties to compute :

$$\frac{1}{2\pi\iota}\oint_{\Omega_k}\frac{dz}{z-\lambda_l}=\begin{cases}1 & k=l\\ 0 & k\neq l\end{cases}$$

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!!! $\widehat{\Omega}_k$ is a random contour of $\mathbb{C}$. Control of the location of eigenvalues (concentration inequalities) then $\widehat{\pi}_k = \frac{1}{2\pi\iota}\int_{\Omega_k}(zI-\Sigma_n)^{-1}\,dz + r_n$

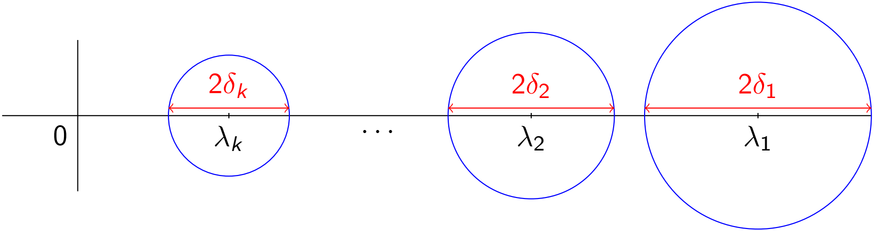

Figure: Contour made of disjoint circles (court. A. Roche)

Typical contour to define one or more π_k's

Two examples of classical contours

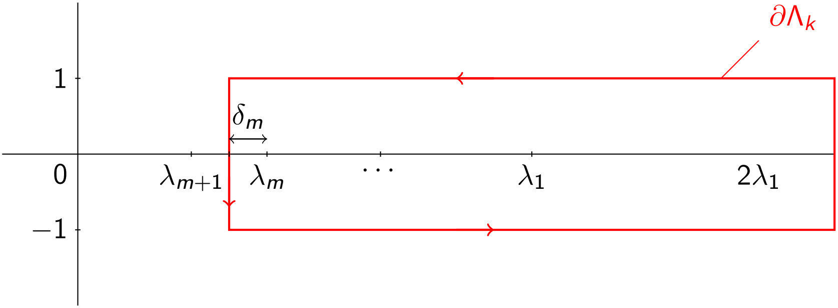

Figure: Rectangular contour (court. A. Roche)

Typical contour to define P_m, projector associated with the m first eigenvalues.

Main results 1/2:

Let $\mathbf{a}_k = \sum_{i \neq k} \frac{\lambda_i}{|\lambda_i - \lambda_k|} + \frac{\lambda_k}{\delta_k}$.
Theorem (lower bound) Take X Gaussian and $\mathbf{a}_k/\sqrt{n} < 0.5$ then :

$$\mathbb{E}\left\|\widehat{\pi}_k - \pi_k\right\|_\infty^2 \geq \underbrace{\frac{1}{2n}\sum_{j \neq k} \lambda_k \lambda_j / \left(\lambda_j - \lambda_k\right)^2}_{\mathrm{M}_k} - 4\frac{\mathbf{a}_k^4}{n^2}$$

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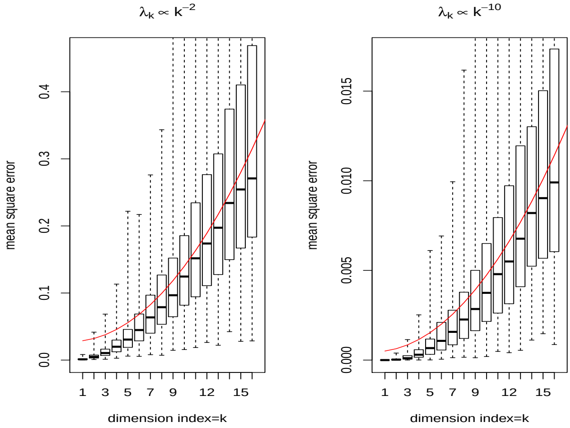
- N.B.1 : the constants depend on the eigenvalues, the rate *not really*.
- N.B.2 : If $\exists \gamma > 0, j\lambda_j \log^{1+\gamma}(j) \downarrow 0$, then $\mathbf{a}_k \leq c\left(\gamma\right) k \log k$.

Back to simulations



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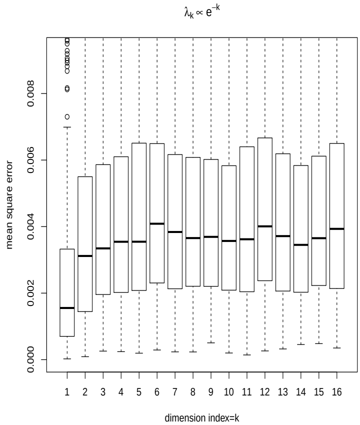

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Theorem (Upper bound for reconstruction) : Take $\mathbf{u} = X_i$ or $\mathbf{u} = X_{n+1}$ or $\mathbf{u}$ nonrandom with $\sup_i |\langle \mathbf{u}, \varphi_i \rangle|^2 / \lambda_i < 1$ then for all $n \geq 2$ and $k \geq 2$:

$$\mathbb{E} \left\| \left(\widehat{\mathbf{P}}_k - \mathbf{P}_k \right) \mathbf{u} \right\|^2 \leq \underbrace{\kappa c_0 \exp \left(-c_1 \frac{n}{\mathbf{a}_k^2} \right)}_{\mathcal{E}_{k,n}} + c_2 \cdot \frac{\mathbf{a}_k^2}{n} \log^2 n \cdot \left(\sum_{j=1}^{k} \sqrt{j \delta_j} \right)^2$$

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- Same kind of bounds for $\mathbb{E} \left\| \widehat{\pi}_k - \pi_k \right\|_\infty^2$ and for $\mathbb{E} \left\| \hat{\varphi}_k - \varphi_k \right\|^2$
- Previous rates may be improved with projection MS error:

$$\underbrace{\|P_k - P_k\|_\infty}_{uniform} \gg \underbrace{\|(P_k - P_k)\, u\|}_{strong} \gg \underbrace{\langle (P_k - P_k)\, u, v \rangle}_{weak}$$

Application to high-dimensional kernel estimation

Take X in high dim. space, $Y \in \mathbb{R}$ and consider modified non parametric regression : $r_k(x) = \mathbb{E}(Y|\mathbf{P}_k X = x)$ with $x \in \mathrm{Im}(\mathbf{P}_k)$

$$\widehat{r}(x) = \frac{\sum_{i=1}^n Y_i K\left(\left\|\widehat{\mathbf{P}}_k(X_i - x)\right\|/h\right)}{\sum_{i=1}^n K\left(\left\|\widehat{\mathbf{P}}_k(X_i - x)\right\|/h\right)}.$$

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Prop : Non asymptotic bound for all h and k subject to $k > 2$, $0 \leq h \leq h_{\max} < 1$

$$\mathbb{E}[\widehat{r}(x) - r^*(x)]^2 \leq c_6 \frac{k^4}{nh^2} \log^2 n \log\left(\frac{h\sqrt{n}}{k^2}\right).$$

Application to linear inference for functional data

Model generalizes linear regression to functional input/ouput

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- Main goal not β_n but predictor $\langle \beta_n, X_{n+1} \rangle$

Why PCA ?

- Consider bias=approx error for prediction after projection with $\mathcal{P}_k$ (which is any k-dimensional projector)

$$\mathbb{E}\left\langle \mathcal{P}_k\beta - \beta, X\right\rangle^2 = \mathbb{E}\left\langle \beta, \left(I - \mathcal{P}_k\right) X\right\rangle^2 \leq \left\|\beta\right\|^2 \mathbb{E}\left\|\left(I - \mathcal{P}_k\right) X\right\|^2$$

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- Avoids decoupling assumptions : smoothness of X / smoothness of β
- Provide minimax adaptive estimators
- Allows minimax adaptive testing as well
- Mean Square Pred. Risk : $\log n/n$ even if eigenvalues AND β Fourier coeff decay at exponential rate $\approx$ highly ill-posed.

Example of estimation results : Set $L = \left\| \Sigma^{1/2} \beta \right\|$, $\varphi(j) = \lambda_j \langle \beta, \varphi_j \rangle^2 / L^2$ and k_n^* as the integer part of the unique solution of the integral equation (in x) :

$$\frac{1}{x} \int_x^{+\infty} \varphi(x)\, dx = \frac{1}{n} \frac{\sigma_\varepsilon^2}{L^2}. \tag{1}$$

then with $\mathcal{R}_n(L, \varphi) = \sup_{\Sigma^{1/2}\beta \in \mathcal{L}_2(L,\varphi)} \mathbb{E} \langle \beta_n - \beta, X_{n+1} \rangle^2$

$$\lim \sup_{n \to +\infty} \frac{n}{k_n^*} \mathcal{R}_n(L, \varphi) = 2\sigma_\varepsilon^2$$

If $\varphi_a(j) \propto \left(j^{2+\alpha} (\log j)^\beta \right)^{-1}$,$\mathcal{R}_n(L, \varphi_a) \propto \frac{(\log n)^{\beta/(2+\alpha)}}{n^{(1+\alpha)/(2+\alpha)}}$,
If $\varphi_b(j) \propto \exp(-\alpha j)$,$\mathcal{R}_n(L, \varphi_b) \leq \frac{\log n}{\alpha n}$.
Besides $\inf_{\widehat{T}} \sup_{\Sigma^{1/2}\beta \in \mathcal{L}_2(\varphi, L)} \mathbb{E} \left\| \widehat{T}(X_{n+1}) - S(X_{n+1}) \right\|^2 \asymp \frac{k_n^*}{n}$

Thank you for your attention.