Learning sub-Gaussian classes: Upper and minimax bounds

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joint work with Shahar Mendelson

 $\mathsf{data}:\, (X_i,Y_i)_{i=1}^N \; \mathsf{i.i.d.} \sim (X,Y) \in \mathcal{X} \times \mathbb{R} \mathsf{,}$

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results : Fix 0 < δ < 1. With probability greater than 1 - δ ,

$$R(\hat{f}) \leq \inf_{f \in \mathcal{F}} R(f) + r_N(\mathcal{F}, \delta)$$

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- questions: a) How large is $r_N(\mathcal{F}, \delta)$? (complexity of \mathcal{F} , value of $\delta,...$)
 - b) Can we do better than ERM? (minimax results depending on δ , the complexity structure of $\mathcal{F},...$)

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1 the Gelfand k-width : $c_k(\mathcal{F}) = \inf_{L:L_2(\mu) \to \mathbb{R}^k} \operatorname{diam}(\mathcal{F} \cap \ker L, L_2(\mu))$.

How are they related?

$$\begin{array}{ccc} \sup_{\epsilon>0} \epsilon \log^{1/2} \textit{N}(\mathcal{F}, \epsilon D) & \lesssim & \mathbb{E} \|\textit{G}\|_{\mathcal{F}} & \lesssim & \int \log^{1/2} \textit{N}(\mathcal{F}, \epsilon D) d\epsilon \\ & \uparrow & \uparrow \\ & \textit{Sudakov} & \textit{Dudley} \end{array}$$

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ex. : $\mathcal{F} = \{\langle \cdot, t \rangle : t \in B_1^d \}$, $X \sim \mu$ is isotropic (i.e. $\mathbb{E}\langle X, t \rangle^2 = \|t\|_{\ell_2^d}^2$) then Sudakov, Carl and [P./T.-J.] are sharp $= \sqrt{\log d}$ but Dudley is not sharp $= (\log d)^{3/2}$.

Assumptions : sub-gaussian framework

 $\mathcal{F} \text{ is L-sub-Gaussian}: \forall f,g \in \mathcal{F} \cup \{0\},$ $\|f-g\|_{\psi_2(\mu)} \leq L \|f-g\|_{L_2(\mu)}$ $(\|f\|_{\psi_2(\mu)} = \inf \left(c>0: \mathbb{E} \exp(f^2(X)/c^2) \leq 2\right)).$

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- **3** \mathcal{F} is B-Bernstein : $\forall f \in \mathcal{F}$,

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 $\bullet \ \mathcal{F} - \mathcal{F} \text{ is star-shaped around 0 } ([f-g,0] \subset \mathcal{F} - \mathcal{F}, \forall f,g \in \mathcal{F}).$

Theorem [L.& Mendelson] : sharp oracle inequality for ERM in Sub-Gaussian framework

• If $\sigma \geq c_3 r_N^*$ then with probability at least $1 - 4 \exp(-c_4 N \sigma^{-2} (s_N^*)^2)$,

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where, for D the unit ball in $L_2(\mu)$,

$$\begin{split} s_N^* &= \inf \left\{ 0 < s \le d_{\mathcal{F}}(L_2) : \mathbb{E} \|G\|_{sD \cap (\mathcal{F} - \mathcal{F})} \le (c_0/\sigma) s^2 \sqrt{N} \right\}, \\ r_N^* &= \inf \left\{ 0 < r \le d_{\mathcal{F}}(L_2) : \mathbb{E} \|G\|_{rD \cap (\mathcal{F} - \mathcal{F})} \le c_1 r \sqrt{N} \right\}. \end{split}$$

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Classical fixed points - two main streams

<1996 Fixed points were associated to Dudley entropy integrals : [van de Geer, AOS90, AOS93, EP in M-estimation] or [Birgé, Massart PTRF93] : $\operatorname{residue} = (\sigma^*)^2$

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>1996 Fixed points were associated to the expected supremum of the empirical process (indexed by localized classes) or weighted, symmetrized version, ...: [Massart, Saint Flour 2003] [Koltchinksii, Saint Flour 2008], [Bartlett, Mendelson, PTRF06], [Blanchard, Bousquet, Massart]:

$$\operatorname{residue} = \inf \left\{ s > 0 : \mathbb{E} \sup_{\{f \in \mathcal{F}: P\mathcal{L}_f \leq s\}} |(P - P_N)\mathcal{L}_f| \leq c_0 s \right\}.$$

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We want to be as good as $f_{\mathcal{F}}^*$ using observations $(X_i, Y_i)_{i=1}^N$. There are two different sources of statistical complexity :

• the projection $P_{\tau}: f \in L_2(\mu) \mapsto \big(f(X_i)\big)_1^N$ is a source of complexity because we want procedures having good "generalization" capabilities (being good even outside of the data sample).

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Decomposition of the excess loss function :

$$\mathcal{L}_{f}(x,y) = (\ell_{f} - \ell_{f_{\mathcal{F}}^{*}})(x,y) = (y - f(x))^{2} - (y - f_{\mathcal{F}}^{*}(x))^{2}$$
$$= (f - f_{\mathcal{F}}^{*})^{2}(x) + 2(y - f_{\mathcal{F}}^{*}(x))(f_{\mathcal{F}}^{*} - f)(x)$$

• The quadratic process $((P - P_N)(f - f_F^*)^2)_{f \in \mathcal{F} \cap rD}$. [Mendelson-Pajor-Tomczak] : w.h.p.

$$\sup_{h\in\mathcal{H}}\left|\frac{1}{N}\sum_{i=1}^Nh^2(X_i)-\mathbb{E}h^2\right|\lesssim \left(d_{\psi_2}(\mathcal{H})\frac{\mathbb{E}\|G\|_{\mathcal{H}}}{\sqrt{N}}+\frac{(\mathbb{E}\|G\|_{\mathcal{H}})^2}{N}\right).$$

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This measures the statistical complexity coming from the noise $(=\|\xi\|_{\psi_2}=\|Y-f_{\mathcal{F}}^*(X)\|_{\psi_2}=\sigma)$ via s_N^* .

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If \tilde{f}_N is a procedure such that, for every $f^* \in \mathcal{F}$, with probability at least $1-4\exp(-c_4N\sigma^{-2}(s_N^*)^2)$, $R(\tilde{f}_N) \leq \inf_{f \in \mathcal{F}} R(f) + \mathrm{residue}$, then necessarily $\mathrm{residue} \gtrsim (s_N^*)^2$.

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ERM is minimax in the Gaussian regression model over sub-Gaussian models (for this confidence bound and noise level $\sigma \gtrsim r_N^*$).

Corollary

In the Gaussian regression model with respect to a sub-Gaussian model for the confidence $1-4\exp(-c_4N\sigma^{-2}(s_N^*)^2)$ and for a noise level $\sigma\gtrsim r_N^*$, ERM is minimax.

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Theorem (L. & Mendelson)

If \tilde{f}_N is a procedure in the Gaussian model $Y=f^*(X)+W$ $(W\sim \mathcal{N}(0,\sigma^2I_N)$ ind. of X) such that for every $f^*\in \mathcal{F}$, with probability greater than 3/4, $R(\tilde{f}_N)\leq \inf_{f\in\mathcal{F}}R(f)+\operatorname{residue}$ then necessarily

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$$s_N^* = \inf_{0 < s < d_{\mathcal{F}}(L_2)} \left\{ \mathbb{E} \|G\|_{sD \cap (\mathcal{F} - \mathcal{F})} \le (c_0/\sigma) s^2 \sqrt{N} \right\}$$

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For the small noise regime, we obtain the following minimax bound.

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Denote $f^*(X) = \mathbb{E}[Y|X]$. For every procedure \tilde{f}_N ,

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Similar lower bounds have been obtained in Compressed Sensing by [Donoho, IEEE06] or [Cohen, Dahmen, DeVore, JAMS09].

conclusion for large noise $\sigma \gtrsim r_N^* = \inf_r \left\{ \mathbb{E} \|G\|_{rD \cap (\mathcal{F} - \mathcal{F})} \le c_1 r \sqrt{N} \right\}$

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If "Sudakov is sharp at the level q_N^st ":

$$q_N^* \log^{1/2} N((\mathcal{F} - \mathcal{F}) \cap 2q_N^* D, q_N^* D) \sim \mathbb{E} \|G\|_{(\mathcal{F} - \mathcal{F}) \cap 2q_N^* D}$$

then upper and lower bounds match and therefore ERM is minimax in the Gaussian model for any subgaussian model for both exponentially large and constant confidences.

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In the Gaussian regression model, if a procedure satisfies (for any $f^* \in \mathcal{F}$) a sharp oracle inequality w.p.g. 1/2 then $\operatorname{residue} \gtrsim \sup_{f^* \in \mathcal{F}} \left(c_N(\mathcal{F} - f^*) \right)^2$. If "Pajor/Tomczak-Jaegermann is sharp at level N" (for some $f_0^* \in \mathcal{F}$):

$$\sqrt{N}c_N((\mathcal{F}-f_0^*)\cap r_N^*D)\sim \mathbb{E}\|G\|_{r_N^*D\cap(\mathcal{F}-\mathcal{F})}$$

then upper and lower bounds match and therefore ERM is minimax in the Gaussian model for any subgaussian model for both exponentially large and constant confidences.

 $\mathsf{data}:\, (X_i,Y_i)_{i=1}^N \;\mathsf{i.i.d.} \in \mathbb{R}^{p\times q} \times \mathbb{R},$

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 \begin{split} \text{data} : & (X_i, Y_i)_{i=1}^N \text{ i.i.d. } \in \mathbb{R}^{p \times q} \times \mathbb{R}, \\ \text{model} : & \mathcal{F} = \{ \left\langle \cdot, A \right\rangle : \|A\|_{\max} \leq R \}, \\ & \|A\|_{\max} = \min_{A = UV^\top} \|U\|_{2 \mapsto \infty} \|V\|_{2 \mapsto \infty}. \end{split}
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estimator: Emprical risk minimization (ERM):

$$\hat{A} \in \underset{\|A\|_{\max} \leq R}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} (Y_i - \langle X_i, A \rangle)^2.$$

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$$(X_i, Y_i)_{i=1}^N$$
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Assumptions :

- X is isotropic $(\mathbb{E}\langle A, X \rangle^2 = (pq)^{-1} ||A||_F^2)$ and subgaussian $(||\langle X, A \rangle||_{\psi_2} \leq L(pq)^{-1} ||A||_F)$,
- $A_{max}^* \in \operatorname{argmin}_{\|A\|_{max} \leq R} \mathbb{E}(Y \langle X, A \rangle)^2$ and $\|Y \langle X, A_{max}^* \rangle\|_{\psi_2} \leq \sigma$.

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Gaussian mean width : $\operatorname{conv} \mathcal{X}_+ \subset \mathcal{B}_{max} \subset K_G \operatorname{conv} \mathcal{X}_+$ where $\mathcal{X}_{+} = \{uv^{\top} : u \in \{\pm 1\}^{p}, v \in \{\pm 1\}^{q}\}.$

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$$\mathbb{E}\|G\|_{(\mathcal{F}-\mathcal{F})\cap sD} = \mathbb{E}\sup_{\|A\|_{max} < R; \|A\|_F < s\sqrt{pq}} \langle \mathfrak{G}, A \rangle$$

$$\lesssim R\mathbb{E}\sup_{A\in\mathcal{X}_{+}}\left\langle \mathfrak{G},A\right\rangle \leq K_{G}R\max_{A\in\mathcal{X}_{+}}\frac{\|A\|_{F}}{\sqrt{pq}}\sqrt{\log|\mathcal{X}_{\pm}|}\leq K_{G}R\sqrt{p+q}.$$

Therefore, $(s_N^*)^2 \sim \sigma R \sqrt{(p+q)/N}$ and $(r_N^*)^2 \sim R(p+q)/N$.

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In the Gaussian linear model ($Y = \langle A^*, X \rangle + W$), we obtain a minimax bound (for constant and exponentially large confidence)

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via the entropy estimate of [Cai&Wenxin, 2013].

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Therefore, ERM is minmax over the MAX-norm model in the Gaussian linear model. A similar result was obtained in [Cai&Wenxin, 2013] for the ERM over $R\mathcal{B}_{max} \cap (\alpha \mathcal{B}_{\infty}^{pq})$.

Complexity is important but geometry is even more important

Theorem

Let $X \sim \mu$. Let $\mathcal{F} \subset L_2(\mu)$ be locally compact. The following are equivalent :

i) for any real valued random variable $Y \in L_2$, $\exists f_{\mathcal{F}}^* \in \operatorname{argmin}_{f \in \mathcal{F}} \mathbb{E}(Y - f(X))^2$ and for every $f \in \mathcal{F}$,

$$\mathbb{E}\big(f(X) - f_{\mathcal{F}}^*(X)\big)^2 \le \mathbb{E}\big((Y - f(X))^2 - (Y - f_{\mathcal{F}}^*(X))^2\big). \tag{1}$$

ii) \mathcal{F} is non-empty and convex.

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For non-convex model, ERM cannot do better than $1/\sqrt{N}$.

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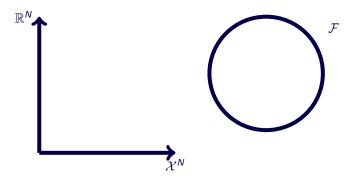
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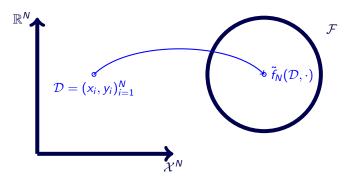
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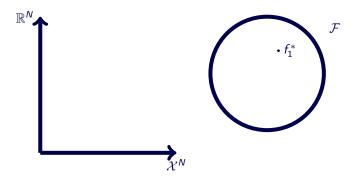
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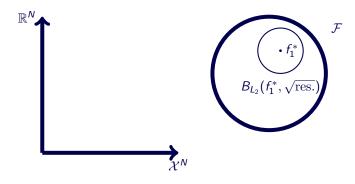
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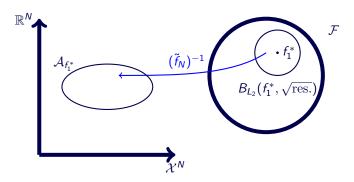
⇒ the shape of the model really matters in Learning theory.



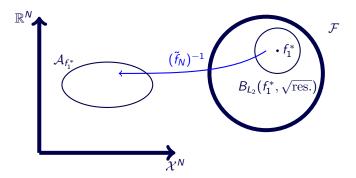




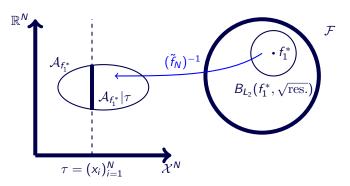




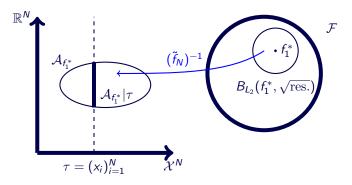
$$\mathcal{A}_{f_1^*} = (\tilde{f}_N)^{-1}(B_{L_2}(f_1^*, \sqrt{\mathrm{res.}}))$$



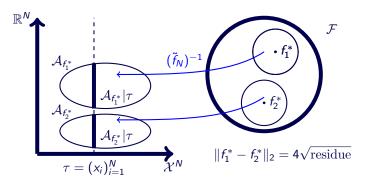
$$\begin{split} \mathcal{A}_{f_1^*} &= (\tilde{f}_N)^{-1}(B_{L_2}(f_1^*, \sqrt{\mathrm{res.}})) \\ (\nu_{f_1^*} \otimes \mu^N)(\mathcal{A}_{f_1^*}) &\geq 1 - \delta \\ \end{split} \qquad \nu_{f_1^*} \sim \mathcal{N}((f_1^*(x_i)_1^N, \sigma^2 I_N)), \ X \sim \mu \end{split}$$



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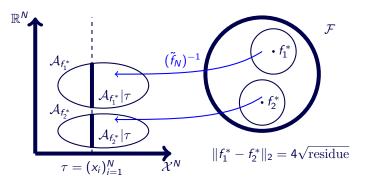


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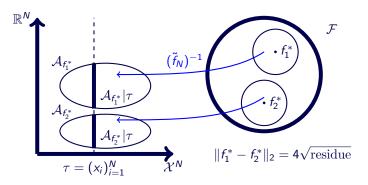


$$\begin{split} \mathcal{A}_{f_1^*} &= (\tilde{f}_{\textit{N}})^{-1} (\mathcal{B}_{\textit{L}_2}(f_1^*, \sqrt{\mathrm{res.}})) & \mathcal{A}_{f_1^*} | \tau \subset \mathbb{R}^{\textit{N}} : \mathsf{fiber} \; \mathsf{of} \; \mathcal{A}_{f_1^*} \\ (\nu_{f_1^*} \otimes \mu^{\textit{N}}) (\mathcal{A}_{f_1^*}) &\geq 1 - \delta \Longrightarrow \mu^{\textit{N}} \big(\tau : \nu_{f_1^*, \tau} (\mathcal{A}_{f_1^*} | \tau) \geq 1 - \sqrt{\delta} \big) \geq 1 - \sqrt{\delta}. \end{split}$$

 \tilde{f}_N a procedure such that, for every $f^* \in \mathcal{F}$, with probability greater than $1 - \delta$, $R(\tilde{f}_N) \leq \inf_{f \in \mathcal{F}} R(f) + \text{residue}$ i.e. $\|\tilde{f}_N - f^*\|_{L_2(\mu)}^2 \leq \text{res}$.



 $\mathcal{A}_{f_1^*}|\tau,\mathcal{A}_{f_2^*}|\tau\subset\mathbb{R}^{\textit{N}} \text{ disjoint. } \nu_{f_1^*,\tau}\big(\mathcal{A}_{f_1^*}|\tau\big),\nu_{f_2^*,\tau}\big(\mathcal{A}_{f_2^*}|\tau\big)\geq 1-\sqrt{\delta} \text{ for many } \tau\text{'s.}$



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- **1** $\mathcal{A}_{f_1^*}|\tau, \mathcal{A}_{f_2^*}|\tau \subset \mathbb{R}^N$ disjoint.
- $\nu_{f_1^*,\tau}(A_{f_1^*}|\tau), \nu_{f_2^*,\tau}(A_{f_2^*}|\tau) \ge 1 \sqrt{\delta}$ for many τ 's.
- $\bullet \ \nu_{f_1^*,\tau} \sim \mathcal{N}\big((f_1^*(x_i))_1^N, \sigma^2 I_N \big) \text{ and } \nu_{f_2^*,\tau} \sim \mathcal{N}\big((f_2^*(x_i))_1^N, \sigma^2 I_N \big).$

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- $\Rightarrow \ \nu_{f_1^*,\tau}\big(\mathcal{A}_{f_2^*}|\tau\big) < \sqrt{\delta} \ \text{and} \ \nu_{f_2^*,\tau}\big(\mathcal{A}_{f_2^*}|\tau\big) \geq 1 \sqrt{\delta} \ \text{for many } \tau\text{'s.}$

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Theorem ("Gaussian shift theorem". Li & Kuelbs, 98)

Let $\nu \sim \mathcal{N}(0, I_N)$. Let $H_+ = \{x \in \mathbb{R}^N : \langle x, w \rangle \geq b\}$ for some $w \in \mathbb{R}^N$, $b \in \mathbb{R}$. Let $B \subset \mathbb{R}^N$ such that $\nu(H_+) = \nu(B)$. Then,

$$\nu(w+B) \geq \nu(w+H_+).$$

- $\bullet \ \mathcal{A}_{f_1^*}|\tau,\mathcal{A}_{f_2^*}|\tau\subset\mathbb{R}^N \text{ disjoint.}$
- **2** $\nu_{f_1^*,\tau}(\mathcal{A}_{f_1^*}|\tau), \nu_{f_2^*,\tau}(\mathcal{A}_{f_2^*}|\tau) \ge 1 \sqrt{\delta}$ for many τ 's.
- **3** $\nu_{f_1^*,\tau} \sim \mathcal{N}((f_1^*(x_i))_1^N, \sigma^2 I_N)$ and $\nu_{f_2^*,\tau} \sim \mathcal{N}((f_2^*(x_i))_1^N, \sigma^2 I_N)$.
- $\Rightarrow \nu_{f_*,\tau}(\mathcal{A}_{f_*^*}|\tau) < \sqrt{\delta} \text{ and } \nu_{f_*,\tau}(\mathcal{A}_{f_*^*}|\tau) \geq 1 \sqrt{\delta} \text{ for many } \tau$'s.
- \Rightarrow This forces the residue to be large.

Theorem ("Gaussian shift theorem". Li & Kuelbs, 98)

Let $\nu \sim \mathcal{N}(0, I_N)$. Let $H_+ = \{x \in \mathbb{R}^N : \langle x, w \rangle \geq b\}$ for some $w \in \mathbb{R}^N$, $b \in \mathbb{R}$. Let $B \subset \mathbb{R}^N$ such that $\nu(H_+) = \nu(B)$. Then,

$$\nu(w+B) \geq \nu(w+H_+).$$

If $\nu_u \sim \mathcal{N}(u, \sigma^2 I_N)$ and $\nu_v \sim \mathcal{N}(v, \sigma^2 I_N)$ then

$$u_u(A) \ge 1 - \Phi(\Phi^{-1}(1 - \nu_v(A)) + \|u - v\|_{\ell^N_2}/\sigma)$$

for
$$\Phi(t) = \mathbb{P}[\mathcal{N}(0,1) \leq t]$$
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The result follows for $\delta = 4 \exp(-c_4 N \sigma^{-2}(s_N^*)^2)$.

Thanks for your attention

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- **⑤** $X \in \mathcal{M}_{p,q}$ uniformly distributed over $\{E_{ij}: 1 \leq i \leq p, 1 \leq j \leq q\}$ (matrix completion design) and $\mathcal{B} \subset \mathcal{M}_{p,q}$ such that $|A_{ij}| \leq R, \forall i,j,A \in \mathcal{B}$. Then $\{\langle \cdot,A \rangle : A \in \mathcal{B}\}$ is *L*-sub-gaussian for X.

We do have : $\forall t \geq c_0$, with probability greater than $1-4\exp(-c_0t^2N(s_N^*/\sigma)^2)$,

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Classical results in the bounded case are written like (cf. Koltchinksii or Massart) : $\forall t \geq c_0$, with probability greater than $1 - 4 \exp(-c_1 t)$,

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The trade-off is obtained for $t = N(s_N^*)^2$.

- below $t \leq N(s_N^*)^2$ the probability estimate is damaged (the residue is still $(s_N^*)^2$).
- 2 above $t \geq N(s_N^*)^2$, the residue is damaged.

Other examples of Gaussian mean widths

- **1** If $p \ge 2$ then $\ell_*(B_p^d \cap sB_2^d) = \ell_*(sB_2^d) = s\sqrt{d}$.
- ② If p<2 then set 1=1/p+1/q and put 1/r=1/2-1/q. For any $d^{-1/r}< s \le 1$,

$$\ell_*(\mathcal{B}_p^d \cap s \mathcal{B}_2^d) \sim \left\{ \begin{array}{cc} \sqrt{q} d^{1/q} & \text{if } 2 < q < \log(2d) \text{ and } s^{-1} \leq c_1^{q/r} d^{1/r} \\ \sqrt{\log\left(2ds^2\right)} & \text{if } q \geq \log(2d) \end{array} \right.$$

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Furthermore, if $s \leq d^{-1/r}$, then $\ell_*(B^d_p \cap sB^d_2) = \ell_*(sB^d_2) = s\sqrt{d}$.