

Motivation: quantum mechanics

- Hamilton operator of the electronic Schrödinger equation

$$H = -\frac{1}{2} \sum_{i=1}^N \Delta_i - \sum_{i=1}^N \sum_{\nu=1}^K \frac{Z_\nu}{|x^i - a_\nu|} + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N \frac{1}{|x^i - x^j|}$$

- Operates on functions $f(x^1, \dots, x^N)$, $x^i \in \mathbb{R}^3$
- $\Delta_i \dots$ Laplace operator wrt. $x^i = (x_1^i, x_2^i, x_3^i) \in \mathbb{R}^3$
- $\{x^i\}_{i=1}^N$ Positions of N electrons
- $\{a_\nu\}_{\nu=1}^K$ Positions of the (fixed) nuclei
- $\{Z_\nu\}_{\nu=1}^K$ Charges of the nuclei
- Invariant states: **Eigenfunctions** of H

$$Hf = \lambda f$$

Mixed Sobolev regularity

- $f(x^1, \dots, x^N)$
- Number of electrons N large \implies increasing complexity!

$$d = 3N$$

- **Yserentant '04:** Some eigenfunctions of H possess **mixed weak derivatives** in L_2 with increasing order (in the number of electrons N)
- **product weights** on the “frequency space”

$$\|f\|_{mix}^2 = \int_{\mathbb{R}^{3N}} \left(1 + \sum_{i=1}^N |\omega^i|^2\right) \prod_{i \in I} \left(1 + |\omega^i|^2\right) |\hat{f}(\omega^1, \dots, \omega^N)|^2 d\omega < \infty$$

Approximation of the eigenfunctions

- **Motivation:** Galerkin methods
- Discretization of the problem \implies finite elements (hat functions)

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- Look for an “optimal” m -dimensional subspace in the sense of the **approximation/Kolmogorov numbers**
- **F**...function space, **X**...error norm

$$a_m(\mathbf{F}, X) := \inf_{\text{rank } A \leq m} \sup_{f \in \mathbf{F}} \|f - Af\|_X$$

- Fourier partial sum

$$Af = S_m f := \sum_{|k| \leq m} \hat{f}(k) e^{ik \cdot x}$$

- $1 = a_0 \geq a_1 \geq \dots \geq a_m$
- See talks by Sickel, Kühn, Mayer,...

Adaptive approximation

- Kolmogorov numbers: **worst-case error** with respect to a class \mathbf{F}

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- In practice: **One single instance** of the problem...
- \implies **Adaptive approximation**
- Requires **nonlinear methods**

A univariate example

- $f(x) = |\sin(x)|$

$$\|f - S_m(f)\|_\infty \asymp m^{-1}$$

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- Trigonometric system: $\{e^{ikx} : k \in \mathbb{Z}\}$

- **Majorov** (1970s): $|\Lambda_m| = m$

$$\left\| f - \sum_{k \in \Lambda_m} \lambda_k e^{ikx} \right\|_\infty \asymp m^{-3/2}$$

(Improves on a result by **Ismagilov**: $m^{-6/5+\varepsilon}$)

- Constructive approach!

Sparse approximation

- Best m -term approximation wrt. a dictionary $\mathcal{D} = \{\varphi_j\}_j$
- X quasi-Banach space, $f \in X$

$$\sigma_m(f, \mathcal{D})_X = \inf \left\{ \left\| f - \sum_{j \in \Lambda} \lambda_j \varphi_j \right\|_X : |\Lambda| \leq m, \lambda_j \in \mathbb{C}, \varphi_j \in \mathcal{D} \right\}$$

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- $f \in \mathbf{F}$
- Best m -term widths

$$\sigma_m(\mathbf{F}, \mathcal{D})_X := \sup_{f \in \mathbf{F}} \sigma_m(f, \mathcal{D})_X$$

- $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_m$

Largest coefficients?

- $0 < p < 1$

$$\|x\|_p := \left(\sum_{j=1}^{\infty} |x_j|^p \right)^{1/p} \leq 1$$

- $0 < p < q$, $\mathcal{D} = \{e_j\}_j$

$$\sigma_m(x, \mathcal{D})_{\ell_2} \lesssim m^{-(1/p-1/2)}$$

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- \mathcal{D} is an unconditional and democratic basis in ℓ_2
- Note, the trigonometric system is not an unconditional basis in L_p , $p \neq 2$
- **Temlyakov, Konyagin:** \mathcal{D} is **greedy**

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- **Pietsch/ DeVore, Popov** 1980s

$$\mathcal{A}_p^\alpha(\ell_2) = \ell_p \quad , \quad \alpha = 1/p - 1/2.$$

Functions with bounded mixed derivative

- r **smoothness**, $1 < p < \infty$ **integrability**
- r integer, $d = 2$

$$\|f\|_{S_p^r W} := \|f\|_p + \left\| \frac{\partial^r f}{\partial x_1^r} \right\|_p + \left\| \frac{\partial^r f}{\partial x_2^r} \right\|_p + \left\| \frac{\partial^{2r} f}{\partial x_1^r \partial x_2^r} \right\|_p$$

- $f : \mathbb{T}^d \rightarrow \mathbb{C}$, multivariate, periodic in every component
- $\hat{f}(k)$, Fourier coefficient of the “frequency” $k \in \mathbb{Z}^d$

$$\|f\|_{S_p^r W} := \left\| \sum_{k \in \mathbb{Z}^d} \hat{f}(k) \prod_{i=1}^d (1 + |k_i|^2)^{r/2} e^{i2\pi kx} \right\|_p$$

- $S_{2,2}^r B = H_{mix}^r = S_2^r W$

Tensor products

- $f_1, \dots, f_d \in W_p^r(\mathbb{R})$
- Consequence of the definition

$$f_1 \otimes \dots \otimes f_d \in S_p^r W(\mathbb{R}^d)$$

- p -nuclear tensor norm α_p (Grothendieck)

$$S_p^r W(\mathbb{R}^d) = W_p^r(\mathbb{R}) \otimes_{\alpha_p} \dots \otimes_{\alpha_p} W_p^r(\mathbb{R})$$

- Sobolev embedding: $1 < p < q < \infty$

$$S_p^r W(\mathbb{R}^d) \hookrightarrow S_q^{r-1/p+1/q} W(\mathbb{R}^d)$$

- **Compact embedding into $C(\mathbb{T}^d)$: $r > 1/p$**

$$S_p^r W(\mathbb{T}^d) \hookrightarrow C(\mathbb{T}^d)$$

Littlewood-Paley decomposition

- $f = \sum_j \delta_j f(x)$
- $1 < p < \infty$, Littlewood-Paley

$$\|f\|_p \asymp \left\| \left(\sum_{j \in \mathbb{Z}^d} |\delta_{(j_1, \dots, j_d)} f(x)|^2 \right)^{1/2} \right\|_p$$

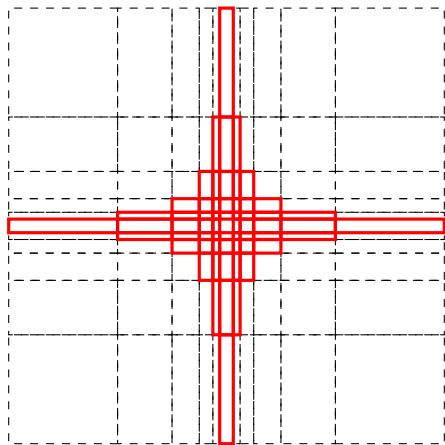
- Now for $S_p^r W$

$$\|f\|_{S_p^r W} \asymp \left\| \left(\sum_{j \in \mathbb{Z}^d} 2^{2(r_1 j_1 + \dots + r_d j_d)} |\delta_{(j_1, \dots, j_d)} f(x)|^2 \right)^{1/2} \right\|_p$$

- Recall: classical definition

$$\|f\|_{S_p^r W} := \left\| \sum_{k \in \mathbb{Z}^d} \hat{f}(k) \prod_{i=1}^d (1 + |k_i|^2)^{r/2} e^{i2\pi kx} \right\|_p$$

Step hyperbolic cross

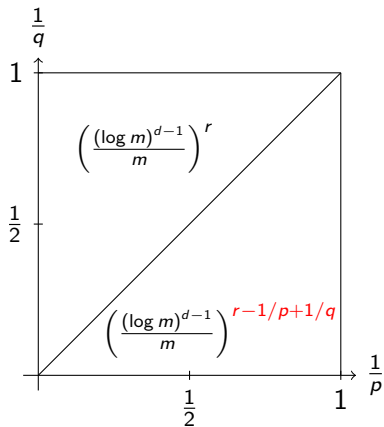


- Take the dyadic blocks from the (step-)hyperbolic cross \mathcal{H}_n

$$P_{\mathcal{H}_n} f := \sum_{j_1 + \dots + j_d \leq n} \delta_{j_1, \dots, j_d} f$$

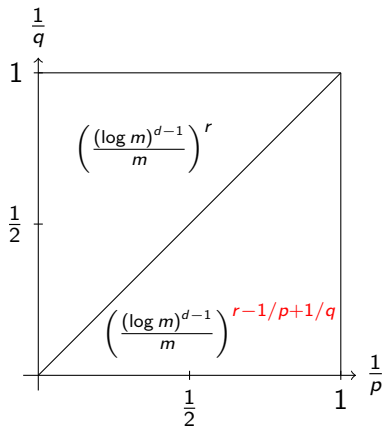
- $f - P_{\mathcal{H}_n} f = \sum_{j_1 + \dots + j_d > n} \delta_{j_1, \dots, j_d} f$
- **L_p -Error:** $\lesssim 2^{-r \cdot n}$
- **Cost:** $m \asymp 2^n n^{d-1}$
- **Rate:** $m^{-r} (\log m)^{(d-1)r}$

Hyperbolic cross and sparse trig. approximation



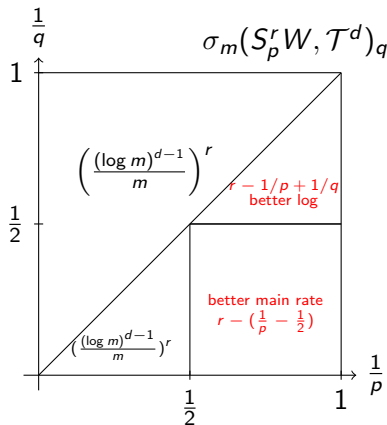
Best approximation from the
hyperbolic cross

Hyperbolic cross and sparse trig. approximation



Best approximation from the hyperbolic cross

Temlyakov (recently)



Sparse trigonometric approximation "large" smoothness

Wavelet dictionaries

- $(\psi_{j,k})_{j,k}$ univariate wavelet basis $j \in \mathbb{N}_0, k \in \mathbb{Z}$
- Hyperbolic wavelets, **tensorization over all scales**

$$\psi_{\vec{j}, \vec{k}}(x_1, \dots, x_d) := \psi_{j_1, k_1}(x_1) \cdot \dots \cdot \psi_{j_d, k_d}(x_d) \quad , \quad \vec{j} \in \mathbb{N}_0^d, \vec{k} \in \mathbb{Z}^d$$

- In contrast to $\mathcal{T}^d = \{e^{ik \cdot x}\}_{k \in \mathbb{Z}^d}$ the wavelet dictionary $\Psi^d = \{\psi_{\vec{j}, \vec{k}}\}_{\vec{j}, \vec{k}}$ is an unconditional basis in L_p for all $1 < p < \infty$

$$\|f\|_p \asymp \left\| \left(\sum_{\vec{j} \in \mathbb{N}_0^d} \left| \sum_{\vec{k} \in \mathbb{Z}^d} 2^{|\vec{j}|_1} \langle f, \psi_{\vec{j}, \vec{k}} \rangle \chi_{\vec{j}, \vec{k}} \right|^2 \right)^{1/2} \right\|_p$$

- **Disadvantage:** the basis is **not** “democratic” for $d \geq 2$

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- Instead of greedy: levelwise thresholding!

Best m -term widths

- $(\psi_{j,k})_{j,k}$ wavelet with sufficient smoothness and vanishing moments

Theorem (Hansen, Sickel '09)

Let $1 < p, q < \infty$ and $r > (1/p - 1/q)_+$. Then

$$\sigma_m(S_p^r W, \Psi^d)_q \asymp m^{-r} (\log m)^{(d-1)r}, \quad m \in \mathbb{N}$$

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- Non-compact embedding: $S_p^{1/p-1/q} W \hookrightarrow L_q$

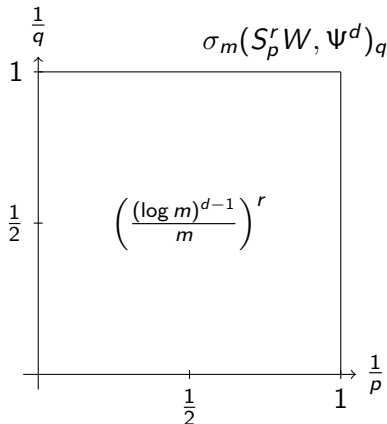
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Sparse hyperbolic wavelet approximation

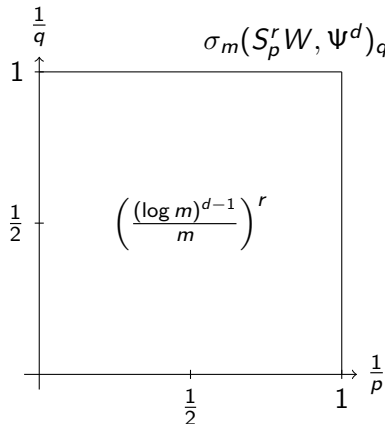
Temlyakov, Hansen, Sickel, Dũng, ...



Sparse wavelet approximation

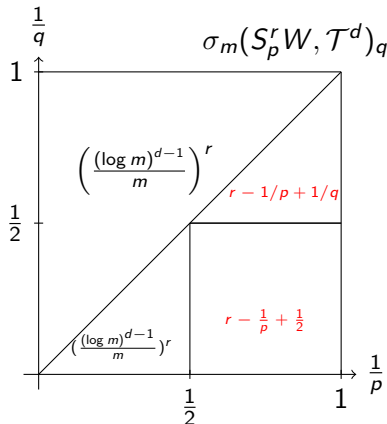
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Temlyakov

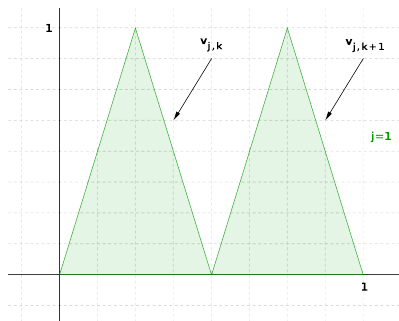
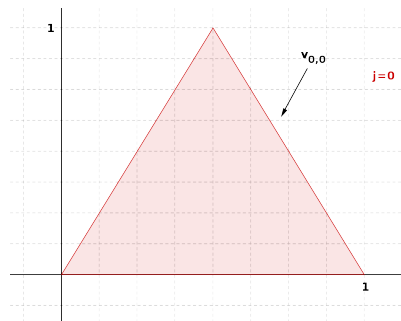


Sparse trigonometric approximation

The Faber-Schauder basis

- **Faber 1908:** Univariate hat functions: decomposition of $f \in C(\mathbb{T})$

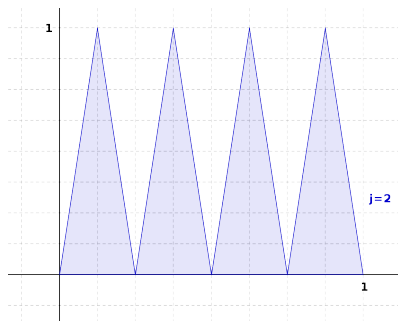
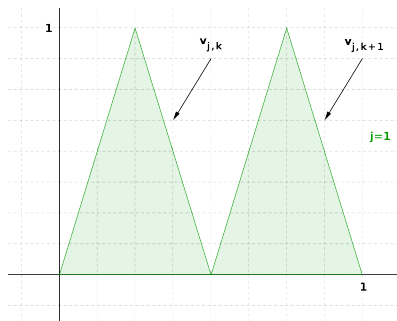
$$f(x) = f(0) - \frac{1}{2} \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} d_{j,k}(f) v_{j,k}$$



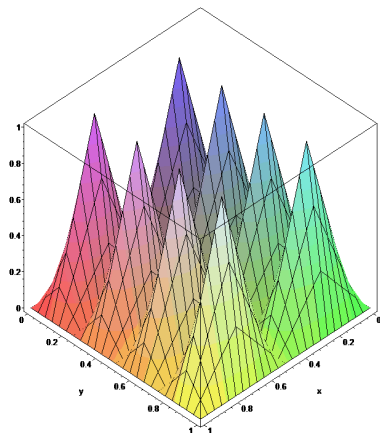
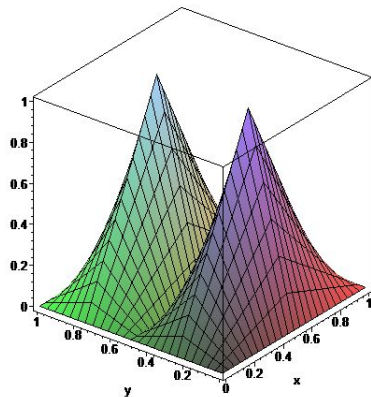
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Tensorized Faber-Schauder basis



Sparse Faber-Schauder approximation

- Let $\mathcal{F}^d := (v_{\bar{j}, \bar{k}})_{\bar{j}, \bar{k}}$ be the Faber-Schauder dictionary
- **Problem:** No unconditional basis in any $L_q(\mathbb{T}^d)$
- Solution: $f = \sum_j \sum_k d_{j, \bar{k}}^2(f) v_{j, \bar{k}}$

$$\|f\|_q \leq \sum_{\bar{j}} \left\| \sum_{\bar{k}} d_{j, \bar{k}}^2(f) v_{j, \bar{k}} \right\|_q$$

right-hand side is related to $s_{q,1}^0 b$ sequence space

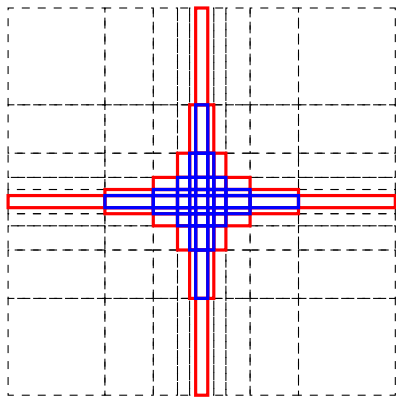
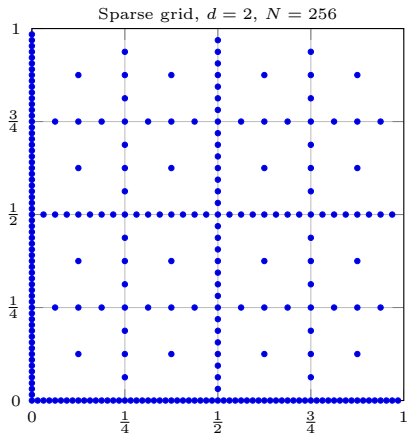
- Those target spaces have been considered by **Hansen, Sickel '09**

Theorem (Byrenheid, U.)

Let $1 < p < \infty$, $1 \leq q \leq \infty$ and $2 > r > \max\{1/p, 1/2\}$ then

$$\sigma_m(S_p^r W, \mathcal{F}^d)_q \lesssim m^{-r} (\log m)^{(d-1)(r+1/2)}$$

Which coefficients (points) are used?



Linear approximation, sampling recovery

- **Sampling nodes** $\xi = \{\xi^1, \dots, \xi^m\}$
- Linear recovery operators of type

$$R_{\xi, \psi} f := \sum_{i=1}^m f(\xi^i) \psi^i(\cdot)$$

- Sampling numbers

$$\varrho_m(\mathbf{F}, X) := \inf_{\substack{\xi^1, \dots, \xi^m \\ \psi^1, \dots, \psi^m}} \sup_{f \in \mathbf{F}} \|f - R_{\xi, \psi} f\|_X$$

- **Temlyakov '93, Ismagilov '74:** $r > 1/2$

$$a_m(H_{mix}^r, L_\infty) \asymp \varrho_m(H_{mix}^r, L_2) \asymp m^{-(r-1/2)} (\log m)^{(d-1)r}$$

Unconditional tensor Faber basis

Theorem (Byrenheid, U. '16, Triebel '10)

Let $1 < p < \infty$. The tensorized Faber-Schauder system $\{v_{\bar{j}, \bar{k}}\}_{\bar{j} \in \mathbb{N}_{-1}, \bar{k} \in \mathbb{Z}}$ is an uncond. basis in $S_p^r W(\mathbb{T}^d)$ if

$\max\{1/2, 1/p\} < r < \min\{3/2, 1 + 1/p\}$. Then

$$\|f\|_{S_p^r W} \asymp \left\| \left(\sum_{\bar{j} \in \mathbb{N}_0^d} 2^{|\bar{j}|_1 r} \left| \sum_{\bar{k} \in D_{\bar{j}}} d_{\bar{j}, \bar{k}}^2(f) \chi_{\bar{j}, \bar{k}}(\cdot) \right|^2 \right)^{1/2} \right\|_p$$

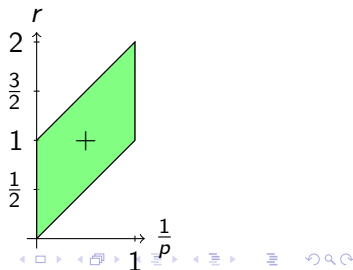
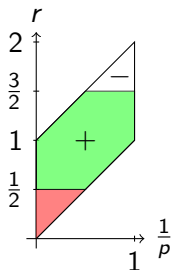
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Comments on the proof

- Conjecture by **Triebel '10**
- Extending the univariate proof technique to d dimensions requires a non-trivial **direction-adapted** use of complex interpolation by **Mendez, Mitrea**
- Vector-smoothness $r = (r_1, \dots, r_d)$

Small smoothness effect?

Theorem (Byrenheid, U. '16)

Let $2 < p < \infty$, $1 \leq q \leq \infty$ and $1/p < r \leq 1/2$. Then

$$\sigma_m(S_p^r W, \mathcal{F}^d)_q \lesssim m^{-r} (\log m)^{(d-1)(1+\epsilon)}$$

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Recall: large smoothness...

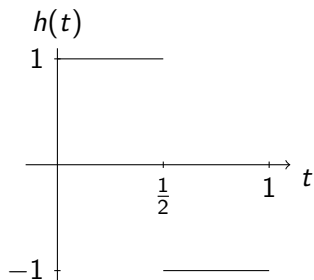
Theorem

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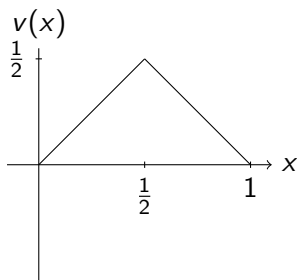
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- Is there a small smoothness effect?
- Faber basis for spaces in the red region?

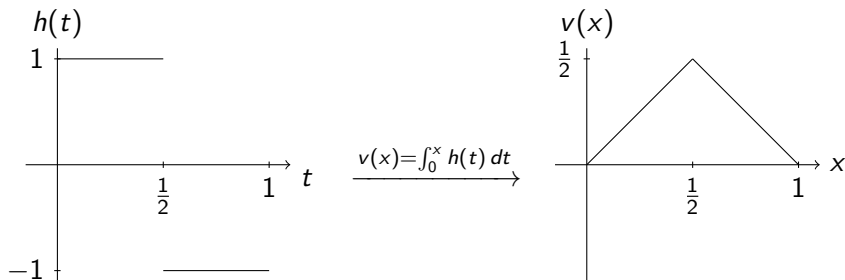
Faber = \int Haar



$$v(x) = \int_0^x h(t) dt$$



Faber = \int Haar



- The Haar wavelet-system

$$h_{j,k}(x) := 2^{j/2} h(2^j x - k) \quad , \quad j, k \in \mathbb{Z}.$$

is an orthonormal basis in $L_2(\mathbb{R})$

100 years Haar and Faber basis

- **1908 Faber**, Über stetige Funktionen, Math. Ann. 66
- **1910 Haar**, Zur Theorie der orthogonalen Funktionensysteme, Math. Ann. 69
- **1910 Faber**, Über die Orthogonalfunktionen des Herrn Haar, DMV Jahresber.
- **1928 Schauder**, Eine Eigenschaft der Haarschen Orthog.-systeme, Math. Z. 28
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- **2010 Triebel** Discrepancy, numerical integration, and hyperbolic cross approximation, EMS Zürich

100 years Haar and Faber basis

- **1908 Faber**, Über stetige Funktionen, Math. Ann. 66
- **1910 Haar**, Zur Theorie der orthogonalen Funktionensysteme, Math. Ann. 69
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- Haar basis in the Sobolev space $W_p^r(\mathbb{R})$?

An unconditional basis in L_p

- In contrast to the trigonometric system $\{e^{ikx}\}_{k \in \mathbb{Z}}$ the Haar wavelet system is an unconditional basis in L_p for $p \neq 2$

Theorem (Marcinkiewicz '37, Paley '32)

Let $1 < p < \infty$.

- (i) The Haar system $\{h_{j,k}\}_{j,k \in \mathbb{Z}}$ is an unconditional basis in $L_p(\mathbb{R})$.
- (ii) There exist constants $0 < c < C$ such that

$$c \|f\|_p \leq \left\| \left(\sum_{j \in \mathbb{Z}} \left| \sum_{k \in \mathbb{Z}} 2^j \langle f, h_{j,k} \rangle \chi_{j,k} \right|^2 \right)^{1/2} \right\|_p \leq C \|f\|_p$$

- The statement does neither hold in case $p = 1$ nor $p = \infty$!

The Haar-basis in Sobolev spaces

Theorem (Seeger, U. '16)

Let $1 < p < \infty$. The Haar system $\{h_{j,k}\}_{j \in \mathbb{N}_{-1}, k \in \mathbb{Z}}$ is an unconditional basis in $W_p^r(\mathbb{R})$ *if and only if*

$$\max \left\{ \frac{1}{p} - 1, -\frac{1}{2} \right\} < r < \min \left\{ \frac{1}{p}, \frac{1}{2} \right\}.$$

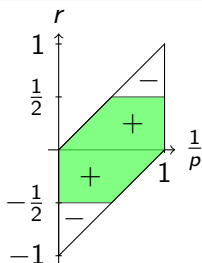


Figure: Unconditional basis in W_p^r

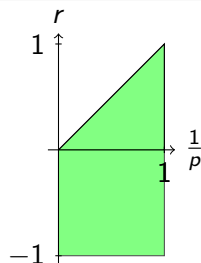


Figure: Haar functions in W_p^r

Unconditional bases

Definition

Let X be a Banach space. Any biorthogonal system (x_n, x_n^*) with a countable index set A is an unconditional basis in X if

- $\overline{\text{span}}\{x_n\}_n = X$
- There exists a constant $C > 0$ such that for every $x \in X$ and every finite index set $B \subset A$

$$\left\| \sum_{n \in B} x_n^*(x) x_n \right\|_X \leq C \|x\|_X$$

- **In other words:** the norm of **any projection**

$$P_B(x) := \sum_{n \in B} x_n^*(x) x_n$$

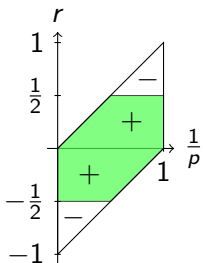
is uniformly bounded by C

Large projection norms

- Let $E \subset \{h_{j,k}\}_{j \in \mathbb{N}_{-1}, k \in \mathbb{Z}}$ a finite subset of the Haar system
- Associated projections

$$P_E(f) := \sum_{h_{j,k} \in E} 2^j \langle f, h_{j,k} \rangle h_{j,k}$$

“grow” with $\#E$ (in the “lower” and “upper” triangle)



- **Probabilistic** construction
- **Quantitative** version
(sharp growing rates)

Figure: Unconditional basis in $S_p^r W$

A probabilistic argument

- $\#A \sim 2^{N+1}$
- Random operator

$$T_{A,\varepsilon}g(x) = \sum_{2^j \in A} \varepsilon_j \sum_{\mu=0}^{2^j-1} 2^j \langle h_{j,\mu}, g \rangle h_{j,\mu}(x)$$

- Random test function

$$f_{A,\varepsilon'} = \sum_{2^k \in A} \varepsilon'_k 2^{-(k+N)r} \sum_{\mu=1}^{2^k} \eta_{k+N,2^N\mu}$$

- Via **Khinchine's inequality**

$$\left(\mathbb{E}_{\varepsilon'} \mathbb{E}_{\varepsilon} \| T_{A,\varepsilon} f_{A,\varepsilon'} \|_{H_p^r}^2 \right)^{1/2} \geq c 2^{N(-r-1/2)}$$

Thank you for your attention!