# Recent progress on boundary effects in kernel approximation

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# Boundary effects and error estimates

Radial basis function approximation over $\Omega$. Let $\Omega \subset \mathbb{R}^d$ and $\Xi \subset \Omega$ with $\#\Xi < \infty$. For a radial $k : \mathbb{R}^d \to \mathbb{R}$, approximate by using the finite dimensional spaces

$$S(\Xi) := \mathrm{span}_{\xi \in \Xi} k(\cdot - \xi)$$

Given $f : \Omega \to \mathbb{R}$, as $h := \max_{x \in \Omega} \mathrm{dist}(x, \Xi) \to 0$ estimate

$$\mathrm{dist}(f, S(\Xi))_{L_p(\Omega)}.$$

- Use the Matérn function of order $m > d/2$:

  $$k_m(x) : \mathbb{R}^d \to \mathbb{R} : x \mapsto K_{m-d/2}(|x|)\, |x|^{m-d/2}.$$

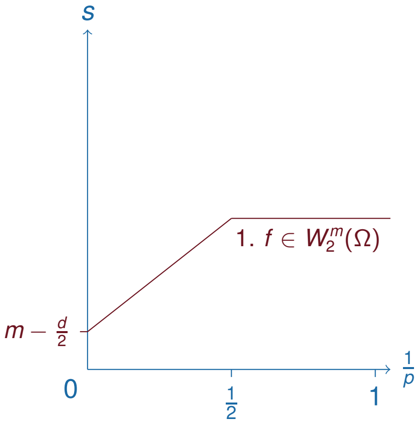
  Here $K_\nu$ is a modified Bessel function of the second kind.
- Fundamental solution of $(1 - \Delta)^m$ on $\mathbb{R}^d$.

# Boundary effects and error estimates

$\Omega$: compact, smooth boundary. $h := \max_{x\in\Omega} \operatorname{dist}(x, \Xi)$.

1. For $f \in W_2^m(\Omega)$:

$$\operatorname{dist}(f, S(\Xi))_{L_p(\Omega)} = O(h^{m-(d/2-d/p)_+})$$



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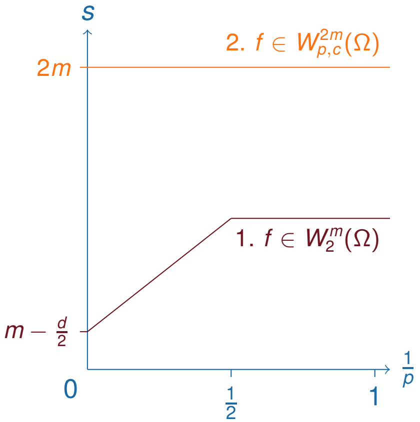
$$\operatorname{dist}(f, S(\Xi))_{L_p(\Omega)} = O(h^{2m})$$



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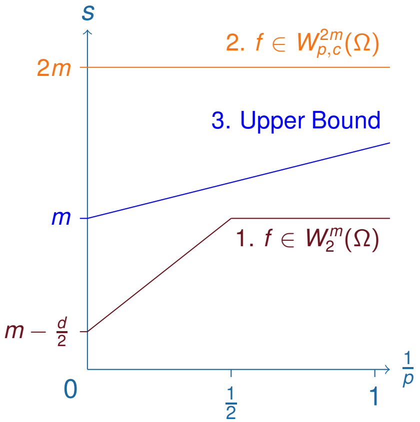
3. For certain $\Xi \subset \Omega$ there are $f \in C^\infty(\overline{\Omega})$ so that

$$\mathrm{dist}(f, S(\Xi))_p \neq o(h^{m+1/p}).$$



# Boundary effects

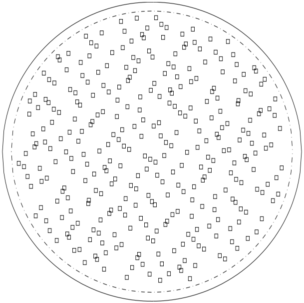
Let $0 < \alpha < 1$. Consider $\Xi \subset \Omega$ satisfying

$$\operatorname{dist}(\Xi, \partial\Omega) > \alpha h \tag{1}$$

## Theorem (Johnson (98))

*For $\Xi$ satisfying (1) there is $f \in C^\infty(\overline{\Omega})$ so that*

$$\operatorname{dist}(f, S(\phi_m, \Xi))_p \neq o(h^{m+1/p}).$$



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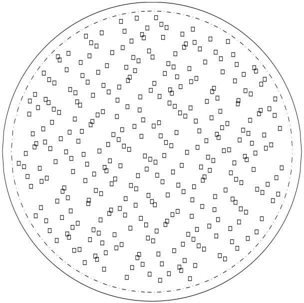
Q: Is $\mathcal{O}(h^{m+1/p})$ attainable for $f \in C^\infty(\overline{\Omega})$?

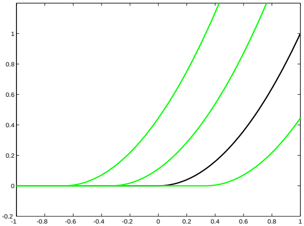
Q: By violating (1) can we get $\mathcal{O}(h^{2m})$?



# A useful kernel approximation scheme

In the integral representation $f(x) = \int_{\mathbb{R}^d} (1-\Delta)^m f(\alpha) k_m(x-\alpha)\mathrm{d}x$
Replace $k_m(x-\alpha) \leftrightsquigarrow K(x,\alpha) := \sum_{\xi\in\Xi} a(\alpha,\xi) k_m(x-\xi) \in S(\Xi)$ so that $|k_m(x-\alpha) - K(x,\alpha)|$ is suitably small.

$$
\begin{aligned}
T_\Xi f(x) &:= \int_{\mathbb{R}^d} (1-\Delta)^m f(\alpha) K(x,\alpha)\mathrm{d}x \\
&= \sum_{\xi\in\Xi} \left( \int_{\mathbb{R}^d} (1-\Delta)^m f(\alpha) a(\alpha,\xi)\mathrm{d}x \right) k_m(x-\xi) \in S(\Xi)
\end{aligned}
$$

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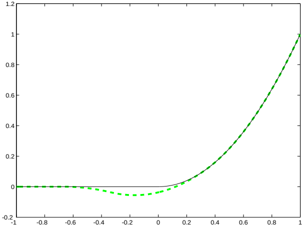

# Representation on bounded domains

Green's representation:

$$f(x) = \int_\Omega (1-\Delta)^m f(\alpha) k_m(x-\alpha)\,\mathrm{d}\alpha + \sum_{j=0}^{m-1} \int_{\partial\Omega} \left[S_j f(\alpha) \lambda_{j,\alpha} k_m(x-\alpha) - \lambda_j f(\alpha) S_{j,\alpha} k_m(x-\alpha)\right] \mathrm{d}\sigma(\alpha)$$

$\lambda_j$ - diff. operator of order $j$; $S_j$ - diff. operator of order $2m-j-1$

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Native space representation:

$$f(x) = \int_\Omega (1-\Delta)^m f(\alpha) k_m(x-\alpha)\,\mathrm{d}\alpha + \sum_{j=0}^{m-1} \int_{\partial\Omega} N_j f(\alpha)\ \lambda_{j,\alpha} k_m(x-\alpha)\,\mathrm{d}\sigma(\alpha)$$

Approximation scheme:

Replace each $\lambda_{j,\alpha} k_m(x-\alpha)$ by $K_j(x,\alpha) = \sum_{\xi\in\Xi} a_j(\alpha,\xi) k_m(x-\xi)$

$$s_f := \sum_{\xi\in\Xi} \left( \int_\Omega a(\alpha,\xi)\Delta^m f(\alpha)\,\mathrm{d}\alpha + \sum_{j=0}^{m-1} \int_{\partial\Omega} a_j(\alpha,\xi) N_j f(\alpha)\mathrm{d}\sigma(\alpha) \right) k_m(\cdot - \xi)$$

# Results

Let $\Omega$ be a bounded domain in $\mathbb{R}^d$ with smooth boundary.

- For $1 < p < \infty$, and $f \in B^s_{p,1}(\Omega)$, $0 < s \leq m + 1/p$

$$\operatorname{dist}(f, S(\Xi))_p \lesssim h^s \|f\|_{B^s_{p,1}(\Omega)}.$$

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- Use two fill distances:
    - $h_1 = h(\Omega, \Xi)$ – the global fill distance.
    - $h_2$ local fill distance around $\partial\Omega$. (In a $Kh_2$ neighborhood of $\partial\Omega$.)

  Then, for $f \in W^{2m}_p(\Omega)$ (or $C^{2m}(\overline{\Omega})$ when $p = \infty$)

$$\operatorname{dist}(f, S(\Xi))_p \lesssim (h_1^{2m} + h_2^{m+\frac{1}{p}})\|f\|_{W^{2m}_p(\Omega)}.$$

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$$\operatorname{dist}(f, S(\Xi))_p \lesssim (h_1^{2m} + h_2^{m+\frac{1}{p}})\|f\|_{W^{2m}_p(\Omega)}.$$

- For $p = \infty$, if $h_2 \le h_1^2$,

$$\operatorname{dist}(f, S(\Xi))_\infty \lesssim h_1^{2m}\|f\|_{C^{2m}(\overline{\Omega})}$$

# Localized bases

Joint work with: Ed Fuselier, Fran Narcowich, Christian Rieger, Xingping Sun, Joe Ward, Grady Wright

# Matérn kernels

- $k_m$ is reproducing kernel for $W_2^m(\mathbb{R}^d)$: $f(x) = \langle f, k_m(x - \cdot)\rangle_{W_2^m(\mathbb{R}^d)}$
- $k_m$ is positive definite:
  for any finite set of centers $\Xi$, the collocation matrix
  $\mathsf{C}_\Xi := \big(k_m(\xi - \zeta)\big)_{(\xi,\zeta)\in\Xi\times\Xi}$ is symmetric, positive definite.
- $k_m$ provides best interpolation: the unique interpolant to $(y_\xi)_\Xi$ from $S(\Xi)$ has least $W_2^m(\mathbb{R}^d)$ norm.
- $\big(k_m(\cdot - \xi)\big)_{\xi\in\Xi}$ forms a basis for $S(\Xi) = \operatorname{span}_{\xi\in\Xi} k_m(\cdot - \xi)$
- So does the Lagrange basis $\big(\chi_\xi\big)_{\xi\in\Xi}$, where
  $\chi_\xi = \sum_{\eta\in\Xi} A_{\xi,\eta} k_m(\cdot - \eta)$ and for all $\zeta \in \Xi$, $\chi_\xi(\zeta) = \delta(\xi, \zeta)$.
- The matrix of Lagrange coefficients $\big(A_{\xi,\zeta}\big)_{(\xi,\zeta)\in\Xi\times\Xi}$ is the inverse of the collocation matrix $\mathsf{C}_\Xi$.
- The Lagrange function coefficients satisfy $A_{\xi,\eta} = \langle \chi_\xi, \chi_\zeta\rangle_{W_2^m}$.

$$\langle \chi_\xi, \chi_\zeta\rangle_{W_2^m} = \sum_{\eta\in\Xi} A_{\zeta,\eta}\langle \chi_\xi, k(\cdot,\eta)\rangle_{W_2^m} = \sum_{\eta\in\Xi} A_{\zeta,\eta}\delta(\xi,\eta) = A_{\xi,\eta}.$$

# Kernels on manifolds

$\mathbb{M}$ a compact $d$ dimensional Riemannian manifold. If $k : \mathbb{M} \times \mathbb{M} \to \mathbb{R}$ is the reproducing kernel for $W_2^m(\mathbb{M})$, $m > d/2$

- Lagrange function is bounded in native space norm

$$\|\chi_\xi\|_{W_2^m(\mathbb{M})} \le Cq^{d/2-m}.$$

  This is a bump estimate – compare $\chi_\xi$ to an interpolant with support in $B(\xi, q)$. Here $q := \min_{\xi\in\Xi} \mathrm{dist}(\xi, \Xi \setminus \{\xi\})$.

- Lagrange coefficients are uniformly bounded:

$$|A_{\xi,\zeta}| = |\langle \chi_\xi, \chi_\zeta \rangle_{W_2^m}| \le Cq^{d-2m}$$

$$\longrightarrow \|(\mathrm{C}_\Xi)^{-1}\|_\infty \le Cq^{d-2m}(\#\Xi)$$

- [De Marchi-Schaback, '10] If $\Xi$ is sufficiently dense in $\mathbb{M}$, then a zeros lemma ensures that the Lagrange function is bounded, independent of $\#\Xi$:

$$|\chi_\xi(x)| \le Cq^{d/2-m}h^{m-d/2} = C\rho^{m-d/2}$$

# Matérn kernels on manifolds (H-Narcowich-Ward, '10)

- For sufficiently dense $\Xi$, we have the **energy bound** for $R > 0$:

$$\text{For } R > 0, \quad \|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R))} \le C q^{d/2-m} e^{-\nu \frac{R}{h}}$$

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- Lagrange functions have pointwise bounds

$$|\chi_\xi(x)| \le C\rho^{m-d/2} e^{-\nu \frac{\mathrm{dist}(\xi,x)}{h}}$$

  - Boundedness of Lebesgue constant,
  - (H-N-Sun-W, '11) $L_p$ Stability: $\|\sum_{\xi\in\Xi} a_\xi \chi_\xi\|_p \sim q^{\frac{d}{p}} \|\vec{a}\|_{\ell_p(\Xi)}$,
  - (H-N-S-W, '11) $L_p$ boundedness of $L_2$ projector.

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- Centers more than $Kh|\log h|$ away from $\xi$:

$$\sum_{\mathrm{dist}(\zeta,\xi)>Kh|\log h|} |A_{\xi,\zeta}| \leq Cq^{d-2m}h^{\frac{\nu K}{2}} \leq C_\rho h^{\frac{\nu K}{2}+d-2m}$$

# Better bases: truncated and local Lagrange bases

From [Fuselier - H - Narcowich - Ward - Wright, '13]

- Let $\Upsilon_\xi := \Xi \cap B(\xi, Kh|\log h|)$.
- Consider the truncated Lagrange basis $\left(\widetilde{\chi_\xi}\right)_{\xi\in\Xi}$

$$\widetilde{\chi_\xi} := \sum_{\zeta\in\Upsilon_\xi} A_{\xi,\zeta} k_m(\cdot,\zeta) \qquad \longrightarrow \|\widetilde{\chi_\xi} - \chi_\xi\|_\infty \le C_\rho h^{(\frac{K\nu}{2}-2m)}$$

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- Still requires calculating all coefficients.
- Use $b_\xi \in S(\Upsilon_\xi)$, local Lagrange functions: $b_\xi(\zeta) = \delta_{\xi,\zeta}\ \forall \zeta \in \Upsilon_\xi$.
- Each element uses $K|\log N|^d$ centers
- For sufficiently large $K$, $(b_\xi)_{\xi\in\Xi}$ is an $L_p$-stable basis for $S(\Xi)$:

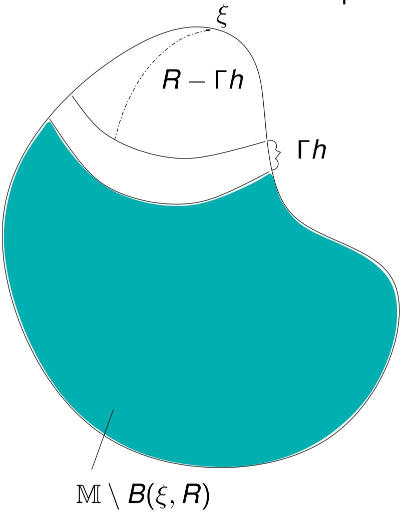
$$\|b_\xi - \chi_\xi\|_\infty \le C_\rho h^J \quad \text{when} \quad K = \frac{2}{\nu}(J + 4m + d)$$

- "Quasiinterpolation" $Q_\Xi f = \sum_{\xi\in\Xi} f(\xi) b_\xi$ gives near best approximation in $L_\infty$.

# Boundary Effects

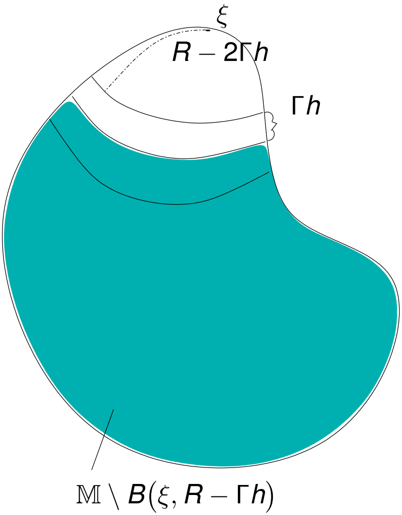
# How important is it to be "boundary-free"?

We must be able to decompose $\mathbb{M}$ into annuli around $\xi$.



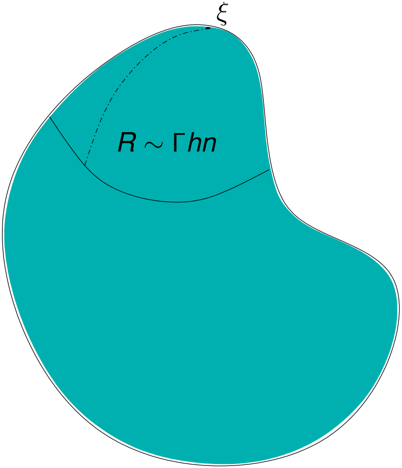

**1-step energy:**
$\exists \epsilon < 1$, $\Gamma > 0$, (depending only on $m$ and $\mathbb{M}$) so that

$$\|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R))} \le \epsilon \|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R-\Gamma h))}$$




## Bulk Chasing

$$
\begin{aligned}
&\|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R))} \\
&\le \epsilon \|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R-\Gamma h))} \\
&\le \epsilon^2 \|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R-2\Gamma h))} \\
&\vdots \\
&\le \epsilon^n \|\chi_\xi\|_{W_2^m(\mathbb{M})}
\end{aligned}
$$




**Energy estimate**

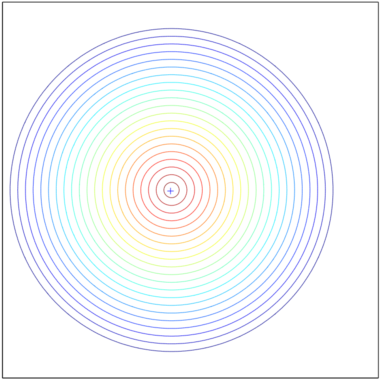
For $R < \mathrm{r}_{\mathbb{M}}/2$

$$\begin{aligned}&\|\chi_\xi\|_{W_2^m(\mathbb{M}\setminus B(\xi,R))}\\ &\lesssim e^{-\nu(\frac{R}{h})}\|\chi_\xi\|_{W_2^m(\mathbb{M})}\\ &\lesssim e^{-\nu(\frac{R}{h})}\, q^{d/2-m}\end{aligned}$$

# How important is it to be “boundary-free”?

Consider $\Omega = [0, 1]^2$:

There are 22 annuli around the center (.45, .5)



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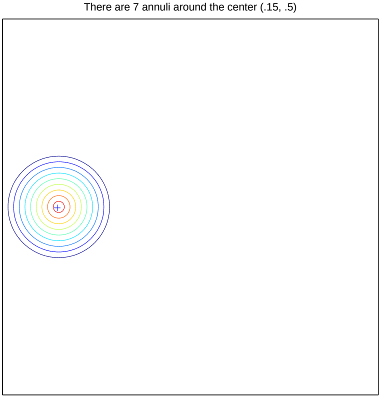
Consider $\Omega = [0,1]^2$: This argument breaks down for centers near the boundary where we can place fewer annuli.

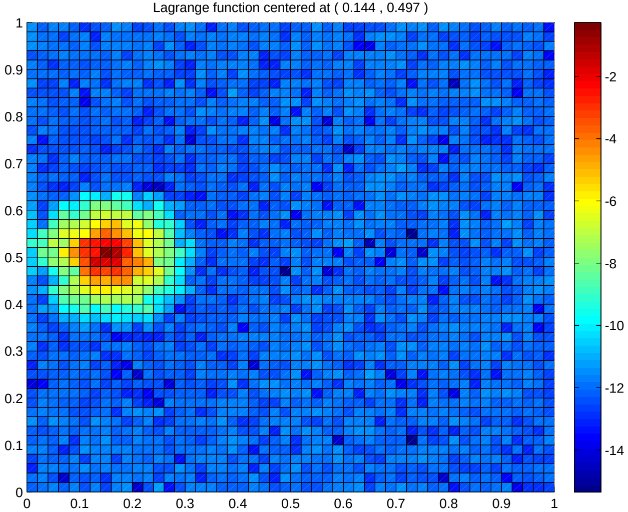



For $R < \mathrm{dist}(\xi, \partial\Omega)$

$$\|\chi_\xi\|_{W_2^m(\Omega\setminus B(x,R))} \le C q^{d/2-m} e^{-\nu\frac{R}{h}}.$$

# Boundary effects for Lagrange functions

## A Lagrange function centered in the interior of $[0,1]^2$.



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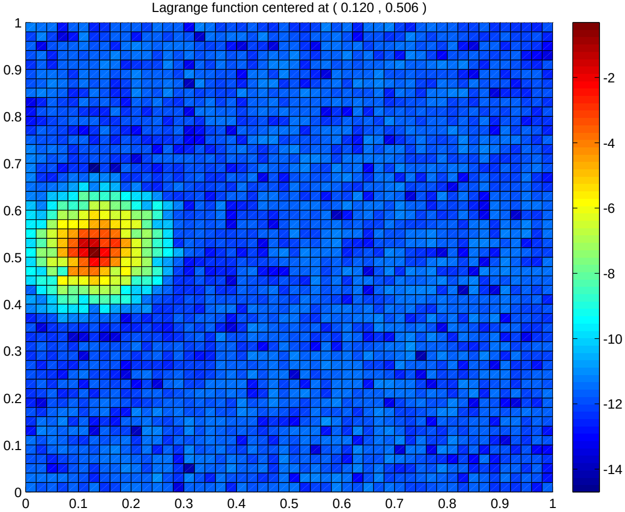

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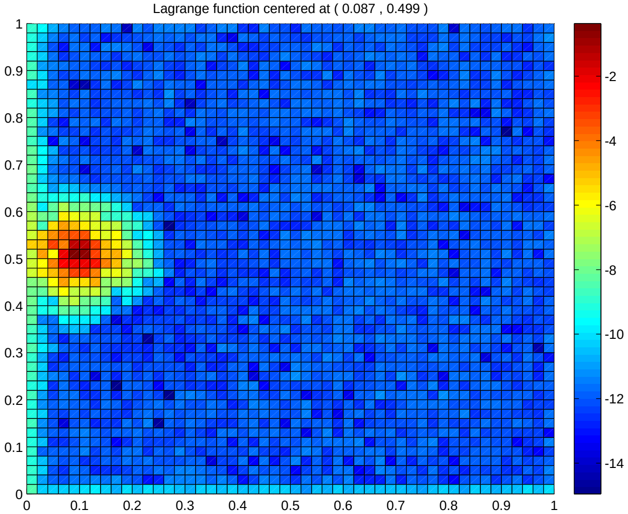

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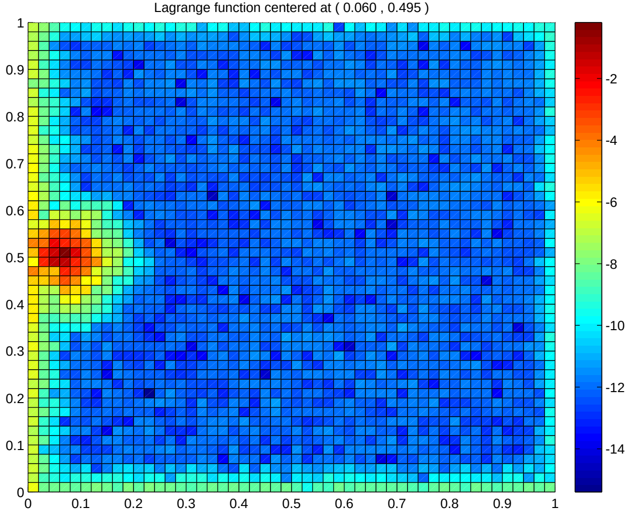

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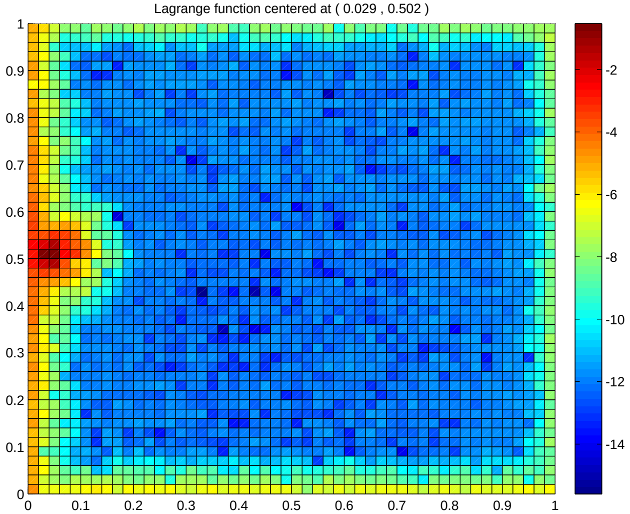

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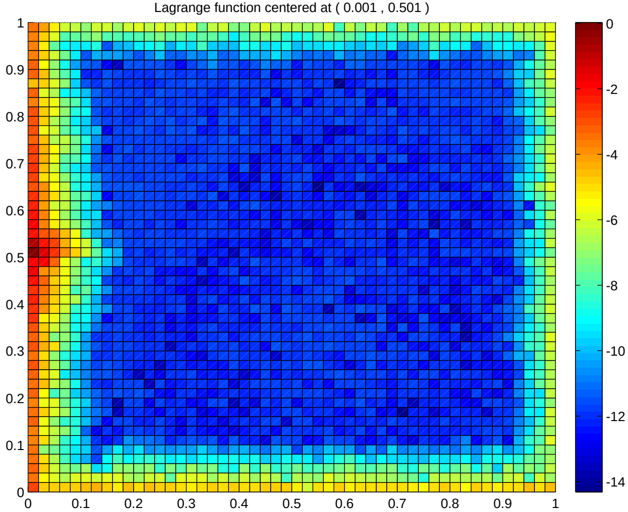
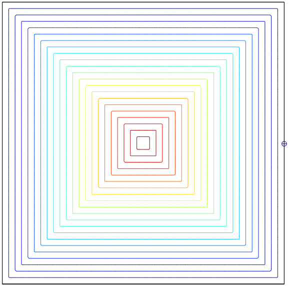


# How important is it to be "boundary-free"?

For compact $\Omega \subset \mathbb{R}^d$, and $0 \le R$, $\Omega_R := \{x \in \Omega \mid \operatorname{dist}(x, \partial\Omega) \ge R\}$.




There exist positive constants $C$, $h_0$ and $\nu$ depending only on $\partial\Omega$ and $m$ so that for $h < h_0$ and $\operatorname{dist}(\xi, \partial\Omega) \le R$, we have

$$\|\chi_\xi\|_{W_2^m(\Omega_R)} \le C q^{d/2-m} e^{-\nu \frac{R-\operatorname{dist}(\xi,\partial\Omega)}{h}}.$$

Question: For $\xi \in \partial\Omega$, does $|\chi_\xi(x)|$ decay along boundary?

# Recent work: Inverse Estimates

# Bernstein estimates

Consider $\Omega \subset \mathbb{R}^d$, bounded. Let $\tilde{\Omega} = \{x \in \mathbb{R}^d \mid \mathrm{dist}(x, \Omega) < Kh|\log h|\}$ be a small neighborhood of $\Omega$.

Avoiding boundary effects: For a discrete set $\Xi \subset \Omega$ with $h(\Xi, \Omega)$ sufficiently small, consider the spaces

$$V_\Xi = \operatorname*{span}_{\xi \in \Xi} b_\xi$$

Given $\Xi \subset \Omega$, one can easily extend this to $\tilde{\Xi} \subset \tilde{\Omega}$.

Bernstein estimates (H-Narcowich-Rieger-Ward, to appear):
For $0 \leq \tau \leq m - (d/2 - d/p)_+$

$$\|\sum_{\xi \in \Xi} a_\xi b_\xi\|_{W_p^\tau(\Omega)} \leq C_\rho h^{\frac{d}{p} - \tau} \|a\|_{\ell_p(\Xi)}$$

# Inverse estimates on $\Omega$

Lower Riesz bound (H-Narcowich-Rieger-Ward, to appear):

$$\|\mathbf{a}\|_{\ell_p(\Xi)} \leq C_\rho h^{-d/p} \|s\|_{L_p(\Omega)}.$$

for all $s = \sum_{\xi \in \Xi} a_\xi b_\xi \in V_\Xi$.

Inverse estimate (H-Narcowich-Rieger-Ward, to appear):
For $s \in V_\Xi$, $0 \leq \tau \leq m - (d/2 - d/p)_+$

$$\|s\|_{W_p^\tau(\Omega)} \leq C_\rho h^{-\tau} \|s\|_{L_p(\Omega)}.$$