

# MATH 590: Meshfree Methods

## Accuracy and Optimality of RKHS Methods

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# Outline

- 1 Introduction
- 2 The Connection to Optimal Recovery
- 3 Orthogonality in Reproducing Kernel Hilbert Spaces
- 4 Optimality Theorems
- 5 The Basic Power Function Error Estimate
- 6 Sampling Inequalities



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In this chapter we will see that **within the native Hilbert spaces associated with strictly positive definite kernels (or, more specifically, radial functions) the kernel (RBF) interpolant provides the best approximation to a given data function.**



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In this chapter we will see that **within the native Hilbert spaces associated with strictly positive definite kernels (or, more specifically, radial functions) the kernel (RBF) interpolant provides the best approximation to a given data function.**

This **optimality of interpolants in Hilbert space** is the subject of the **theory of optimal recovery** described in the late 1950s by Michael Golomb and Hans Weinberger in [GW59].



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In [GW59] the authors studied the following general problem:

### Problem

Given the values  $f_1 = \lambda_1(f), \dots, f_N = \lambda_N(f) \in \mathbb{R}$ , where  $\{\lambda_1, \dots, \lambda_N\}$  is a linearly independent set of linear functionals (called *information functionals* yielding the *information* about  $f$ ), how does one “best” approximate the value  $\lambda(f)$  (called a *feature* of  $f$ ) where  $\lambda$  is a given linear functional and  $f$  is unknown?





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This is a *very general problem formulation* that includes

- interpolation of data such as
  - function values,
  - values of derivatives of  $f$ ,
  - integrals of  $f$  (such as averages or moments),
- as well as methods of approximation other than interpolation.

## Remark

*This kind of problem is known in the literature as an **optimal recovery problem**.*

*Besides the seminal work by Golomb and Weinberger, optimal recovery was also studied in detail in [MRW76, MR77, MR80, MR85].*



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More precisely, given a Hilbert space  $\mathcal{H}$  and data  $f_1 = \lambda_1(f), \dots, f_N = \lambda_N(f) \in \mathbb{R}$  with  $\{\lambda_1, \dots, \lambda_N\} \subseteq \mathcal{H}^*$  (the dual of  $\mathcal{H}$ ), the **minimum-norm interpolant** is that function  $\dot{g} \in \mathcal{H}$  which satisfies

$$\lambda_j(\dot{g}) = f_j, \quad j = 1, \dots, N,$$

and

$$\dot{g} = \underset{\substack{g \in \mathcal{H} \\ \lambda_j(g) = f_j, j=1, \dots, N}}{\operatorname{argmin}} \|g\|_{\mathcal{H}}.$$





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### Remark

The **kernel interpolant** with kernel  $K$  satisfies these criteria if  $\mathcal{H}$  is taken as the associated RKHS  $\mathcal{H}_K(\Omega)$ .

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### Remark

*The proofs of the first two “optimality theorems” require the following two lemmas.*



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## Lemma

Assume  $K$  is a symmetric strictly positive definite kernel on  $\mathbb{R}^d$  and let  $s$  be the usual kernel interpolant to  $f \in \mathcal{H}_K(\Omega)$  at the data sites  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subseteq \Omega$ , i.e.,

$$s(\mathbf{x}) = \sum_{j=1}^N c_j K(\mathbf{x}, \mathbf{x}_j),$$

where the  $c_j$  are determined by  $s(\mathbf{x}_i) = f(\mathbf{x}_i)$ ,  $i = 1, \dots, N$ .





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Then

$$\langle s, s - g \rangle_{\mathcal{H}_K(\Omega)} = 0$$

for any other interpolant  $g \in \mathcal{H}_K(\Omega)$ , i.e., with  $g(\mathbf{x}_i) = f(\mathbf{x}_i)$ ,  $i = 1, \dots, N$ .

Note that  $g \in \mathcal{H}_K(\Omega)$ , a **space that is larger** than  $\text{span}\{K(\cdot, \mathbf{x}_j) : \mathbf{x}_j \in \mathcal{X}\}$ .



**Proof.**

The interpolant  $s$  is of the form  $s = \sum_{j=1}^N c_j K(\cdot, \mathbf{x}_j)$ , where the  $c_j$  are determined by  $s(\mathbf{x}_i) = f(\mathbf{x}_i)$ ,  $i = 1, \dots, N$ .

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Using this, the symmetry of  $K$  and its reproducing property we have

$$\langle s, s - g \rangle_{\mathcal{H}_K(\Omega)} = \left\langle \sum_{j=1}^N c_j K(\cdot, \mathbf{x}_j), s - g \right\rangle_{\mathcal{H}_K(\Omega)}$$

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since both  $s$  and  $g$  interpolate  $f$  on  $\mathcal{X}$ . □

For the next result, we define

$$H_K(\mathcal{X}) = \text{span}\{K(\cdot, \mathbf{x}_j) : \mathbf{x}_j \in \mathcal{X}\}$$

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### Lemma

*Assume  $K$  is a strictly positive definite kernel on  $\mathbb{R}^d$  and let  $s \in H_K(\mathcal{X})$  be the interpolant to  $f \in \mathcal{H}_K(\Omega)$  on  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subseteq \Omega$ .*



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### Remark

In other words, the residual  $f - s$  is orthogonal to the subspace  $H_K(\mathcal{X})$  of  $\mathcal{H}_K(\Omega)$ . In particular,  $\langle f - s, s \rangle_{\mathcal{H}_K(\Omega)} = 0$ .

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since  $s$  interpolates  $f$  on  $\mathcal{X}$ .



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## Corollary

*The orthogonality property of the preceding lemma implies the **energy split***

$$\|f\|_{\mathcal{H}_K(\Omega)}^2 = \|f - s\|_{\mathcal{H}_K(\Omega)}^2 + \|s\|_{\mathcal{H}_K(\Omega)}^2.$$



Proof.

The statement follows from

$$\|f\|_{\mathcal{H}_K(\Omega)}^2 = \|f - s + s\|_{\mathcal{H}_K(\Omega)}^2$$



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and the fact that  $\langle f - s, s \rangle_{\mathcal{H}_K(\Omega)} = 0$  by the lemma since the interpolant  $s$  itself is a special linear combination from  $H_K(\mathcal{X})$ . □



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**Remark**

We will use the energy split in our *sampling inequality error estimates below*.



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### Theorem (Optimality I)

Suppose  $K \in C(\Omega \times \Omega)$  is a strictly positive definite kernel. If the values  $f_1, \dots, f_N$  are given, then the **interpolant  $s$  is the minimum-norm interpolant** to  $\{f_j\}_{j=1}^N$ , i.e.,

$$s = \underset{\substack{g \in \mathcal{H}_K(\Omega) \\ g(\mathbf{x}_j) = f_j, j=1, \dots, N}}{\operatorname{argmin}} \|g\|_{\mathcal{H}_K(\Omega)}.$$



Proof.

Let  $g \in \mathcal{H}_K(\Omega)$  be an arbitrary interpolant to  $f_1, \dots, f_N$ .

**Proof.**

Let  $g \in \mathcal{H}_K(\Omega)$  be an arbitrary interpolant to  $f_1, \dots, f_N$ .  
Then the first orthogonality lemma tells us

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Now

$$\|\mathbf{s}\|_{\mathcal{H}_K(\Omega)}^2 = \langle \mathbf{s}, \mathbf{s} - \mathbf{g} + \mathbf{g} \rangle_{\mathcal{H}_K(\Omega)}$$



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where the last step follows from the above orthogonality relation.  
The Cauchy-Schwarz inequality yields

$$\|\mathbf{s}\|_{\mathcal{H}_K(\Omega)}^2 \leq \|\mathbf{s}\|_{\mathcal{H}_K(\Omega)} \|\mathbf{g}\|_{\mathcal{H}_K(\Omega)},$$

so that the statement follows. □

## Example

The native space of (conditionally positive definite) **thin plate splines**

$$\kappa(r) = r^2 \log r,$$

$r = \|\mathbf{x}\|_2$  with  $\mathbf{x} = (x, y) \in \mathbb{R}^2$  is given by the **Beppo-Levi space**  $\text{BL}_2(\mathbb{R}^2)$ .

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The **corresponding semi-norm** in the Beppo-Levi space  $\text{BL}_2(\mathbb{R}^2)$  is (see [Fas07, Chapter 13])

$$|f|_{\text{BL}_2(\mathbb{R}^2)}^2 = \int_{\mathbb{R}^2} \left( \left| \frac{\partial^2 f}{\partial x^2}(\mathbf{x}) \right|^2 + 2 \left| \frac{\partial^2 f}{\partial x \partial y}(\mathbf{x}) \right|^2 + \left| \frac{\partial^2 f}{\partial y^2}(\mathbf{x}) \right|^2 \right) d\mathbf{x},$$

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which represents the **bending energy of a thin plate**.

By the optimality theorem the **thin plate spline interpolant minimizes this energy**. This explains the name of these functions.

Another nice property of the **kernel interpolant** is the fact that it **is at the same time the best Hilbert-space approximation to the given data.**



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### Theorem (Optimality II)

Let

$$H_K(\mathcal{X}) = \left\{ h = \sum_{j=1}^N c_j K(\cdot, \mathbf{x}_j) : \mathbf{x}_j \in \mathcal{X} \right\},$$

where  $K \in C(\Omega \times \Omega)$  is a strictly positive definite kernel.

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If only the values  $f_1 = f(\mathbf{x}_1), \dots, f_N = f(\mathbf{x}_N)$  are given, then **the interpolant  $s$  is the best approximation to  $f$  from  $H_K(\mathcal{X})$  in  $\mathcal{H}_K(\Omega)$ , i.e.,**

$$\|f - s\|_{\mathcal{H}_K(\Omega)} \leq \|f - h\|_{\mathcal{H}_K(\Omega)}$$

for all  $h \in H_K(\mathcal{X})$ .

Proof.

The native space  $\mathcal{H}_K(\Omega)$  is the completion of  $H_K(\Omega)$  with respect to the  $\|\cdot\|_{H_K}$ -norm (see Chapter 2) so that

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However, the second orthogonality lemma shows that  $\hat{g} = s$  satisfies this relation (and  $s$  qualifies since  $\mathcal{X} \subseteq \Omega$ ). □



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- *or the numerical solution of partial differential equations.*



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These contributions motivated our work on Green's kernels (see Chapter 6).



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### Theorem (Optimality III)

*Suppose  $K \in C(\Omega \times \Omega)$  is a strictly positive definite kernel and suppose that  $\mathbf{x} \in \Omega$  is fixed.*



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### Theorem (Optimality III)

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Then

$$\left| f(\mathbf{x}) - \sum_{j=1}^N f(\mathbf{x}_j) \dot{u}_j(\mathbf{x}) \right| \leq \left| f(\mathbf{x}) - \sum_{j=1}^N f(\mathbf{x}_j) u_j \right|$$

for all choices of  $u_1, \dots, u_N \in \mathbb{R}$ .



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- *It says that the minimum norm interpolant  $s$  is also more accurate (in the pointwise sense) than any linear combination of the given data values.*
- *This is very similar to the MSE-optimality of kriging.*



# Outline

- 1 Introduction
- 2 The Connection to Optimal Recovery
- 3 Orthogonality in Reproducing Kernel Hilbert Spaces
- 4 Optimality Theorems
- 5 The Basic Power Function Error Estimate**
- 6 Sampling Inequalities



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In their final form we will **want our estimates to depend on some kind of measure of the data distribution**.

The measure that is usually used in approximation theory is the so-called **fill distance**

$$h = h_{\mathcal{X}, \Omega} = \sup_{\mathbf{x} \in \Omega} \min_{\mathbf{x}_j \in \mathcal{X}} \|\mathbf{x} - \mathbf{x}_j\|_2$$

already introduced in Chapter 1.



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### Remark

*Most error bounds will focus on this **worst-case** setting. Some will be measured in the  $L_2$ -norm, i.e., for average case errors, or other  $L_p$ -norms.*

## Example

Let  $s^{(h)}$  denote the **interpolant** to data given

- at  $(2^n + 1)^d$ ,  $n = 1, 2, \dots$ , equally spaced points in the unit cube in  $\mathbb{R}^d$
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The definition of the fill distance also covers scattered data such as sets of Halton points.

In fact, since **Halton points are quasi-uniformly distributed** we can assume  $h \approx 2^{-n}$  for a set of  $(2^n + 1)^d$  Halton points in  $\mathbb{R}^d$ .



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## Remark

*These relations explain the specific sizes of the point sets we used in earlier examples.*



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We say that the interpolant  $s^{(h)}$  has  **$L_p$ -approximation order  $k$**  if

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### Remark

*We will concentrate mostly on the case  $p = \infty$  (i.e., pointwise estimates), but approximation order in other norms can also be studied.*



## Remark

Since we want to employ the machinery of *reproducing kernel Hilbert spaces* presented in the previous chapter we will *concentrate on error estimates for functions  $f \in \mathcal{H}_K$* .

In order to keep the following discussion as transparent as possible we will *restrict ourselves to strictly positive definite kernels*.

With (considerably) more technical details the following can also be formulated for strictly conditionally positive definite kernels (see [Wen05] for details).



# Lagrange Form of the Interpolant and Cardinal Basis Functions

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In earlier chapters we established that, for any strictly positive definite kernel  $K$ , the linear system

$$K\mathbf{c} = \mathbf{y}$$

with  $K_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ ,  $i, j = 1, \dots, N$ ,  $\mathbf{c} = (c_1, \dots, c_N)^T$ , and  $\mathbf{y} = (f(\mathbf{x}_1), \dots, f(\mathbf{x}_N))^T$  **has a unique solution**.



In order to obtain the cardinal basis functions  $\hat{u}_j$ ,  $j = 1, \dots, N$ , with the property  $\hat{u}_j(\mathbf{x}_i) = \delta_{ij}$ , i.e.,

$$\hat{u}_j(\mathbf{x}_i) = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases}$$



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we consider the linear system

$$K\hat{\mathbf{u}}(\mathbf{x}) = \mathbf{k}(\mathbf{x}), \quad (1)$$

where the matrix  $K$  is as above (and therefore invertible),  $\hat{\mathbf{u}} = (\hat{u}_1, \dots, \hat{u}_N)^T$ , and  $\mathbf{k}(\mathbf{x}) = (K(\mathbf{x}, \mathbf{x}_1), \dots, K(\mathbf{x}, \mathbf{x}_N))^T$ .





# Existence of Cardinal Functions

## Theorem

Suppose  $K$  is a strictly positive definite kernel on  $\mathbb{R}^d \times \mathbb{R}^d$ . Then, for any distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$ , there exist functions  $\hat{u}_j \in \text{span}\{K(\cdot, \mathbf{x}_j), j = 1, \dots, N\}$  such that  $\hat{u}_j(\mathbf{x}_i) = \delta_{ij}$ . They are *determined pointwise* by solving the linear system (1), i.e.,

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$$K\hat{\mathbf{u}}(\mathbf{x}) = \mathbf{k}(\mathbf{x}).$$

Therefore — **if we know the cardinal functions** — we can write the interpolant  $s$  to  $f$  at  $\mathbf{x}_1, \dots, \mathbf{x}_N$  in the cardinal form

$$s(\mathbf{x}) = \sum_{j=1}^N f(\mathbf{x}_j) \hat{u}_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d.$$



## Remark

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- Once the data sites are fixed and the basic function is chosen with an appropriate shape parameter (whose optimal value will depend on the data sites and values), then the cardinal functions are determined by the linear system (1).



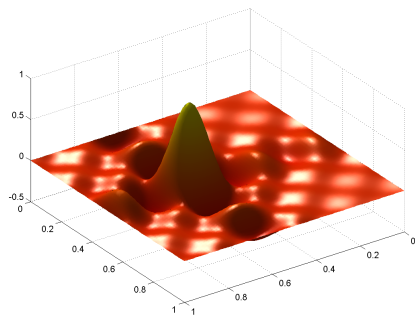
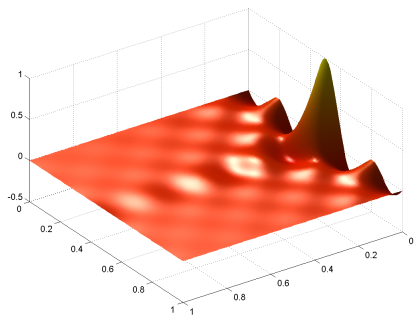
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- The cardinal functions are formally identical to the *optimal kriging weights* of Chapter 4.



## Example

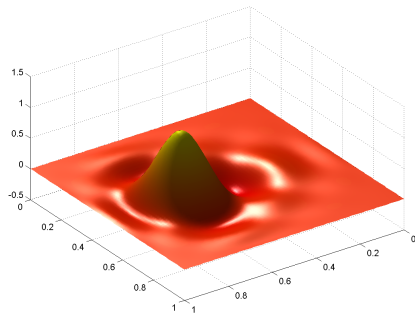
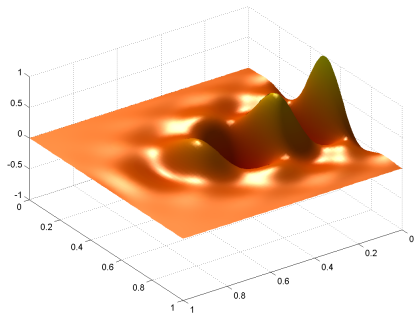
### Gaussian Cardinal Functions



**Figure:** Cardinal functions for Gaussian interpolation (with  $\varepsilon = 5$ ) on 81 uniformly gridded points in  $[0, 1]^2$ . Centered at an edge point (left) and at an interior point (right).

## Example

## More Gaussians

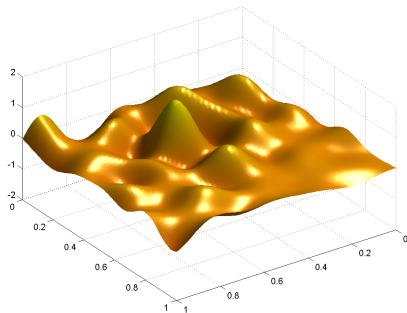
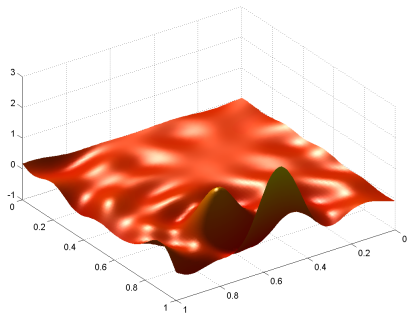


**Figure:** Cardinal functions for Gaussian interpolation (with  $\varepsilon = 5$ ) on 81 tensor-product Chebyshev points in  $[0, 1]^2$ . Centered at an edge point (left) and at an interior point (right).



## Example

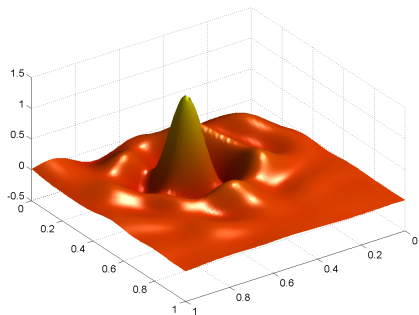
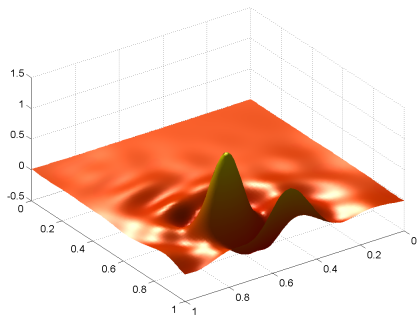
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**Figure:** Cardinal functions for Gaussian interpolation (with  $\varepsilon = 5$ ) on 81 Halton points in  $[0, 1]^2$ . Centered at an edge point (left) and at an interior point (right).

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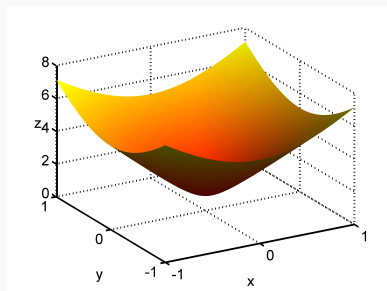
### Multiquadric Cardinal Functions



**Figure:** Cardinal functions for multiquadric interpolation (with  $\varepsilon = 5$ ) on 81 Halton points in  $[0, 1]^2$ . Centered at an edge point (left) and at an interior point (right).

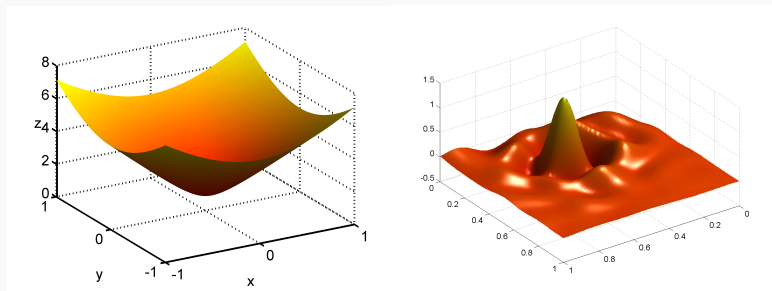
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The plot above shows that the associated cardinal functions are just as localized as those for the Gaussian basic functions, and thus the function space spanned by multiquadrics is a “good” local space.

## The Power Function

Another important ingredient needed for our error estimates is the so-called **power function**.

For any strictly positive definite kernel  $K \in C(\Omega \times \Omega)$ ,  $\Omega \subseteq \mathbb{R}^d$ , any set of distinct points  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subseteq \Omega$ , and an **arbitrary vector**  $\mathbf{u} \in \mathbb{R}^N$ , we define the quadratic form

$$Q(\mathbf{u}) = K(\mathbf{x}, \mathbf{x}) - 2 \sum_{j=1}^N u_j K(\mathbf{x}, \mathbf{x}_j) + \sum_{i=1}^N \sum_{j=1}^N u_i u_j K(\mathbf{x}_i, \mathbf{x}_j).$$



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Suppose  $\Omega \subseteq \mathbb{R}^d$  and  $K \in C(\Omega \times \Omega)$  is strictly positive definite. For any distinct points  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subseteq \Omega$  the **power function**  $P_{K, \mathcal{X}}$  is defined pointwise by

$$[P_{K, \mathcal{X}}(\mathbf{x})]^2 = Q(\dot{\mathbf{u}}(\mathbf{x})),$$

where  $\dot{\mathbf{u}}$  is the vector of cardinal functions studied above.

Using the definition of the native space norm from Chapter 2 we can rewrite the quadratic form  $Q(\mathbf{u})$  as

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- In the paper [WS93] the power function was referred to as *kriging function*. However, as we saw in Chapter 4, the *power function* corresponds to the square root of the kriging variance.



Using the linear system notation employed earlier, i.e.,  $K_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ ,  $i, j = 1, \dots, N$ ,  $\mathbf{u} = (u_1, \dots, u_N)^T$ , and  $\mathbf{k}(\mathbf{x}) = (K(\mathbf{x}, \mathbf{x}_1), \dots, K(\mathbf{x}, \mathbf{x}_N))^T$ , we note that we can also rewrite the quadratic form  $Q(\mathbf{u})$  as

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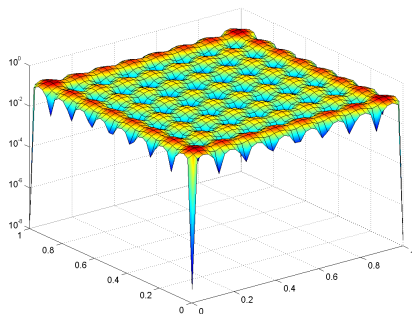
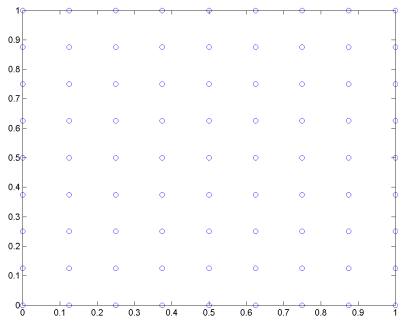
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## Example

## Gaussian Power Function

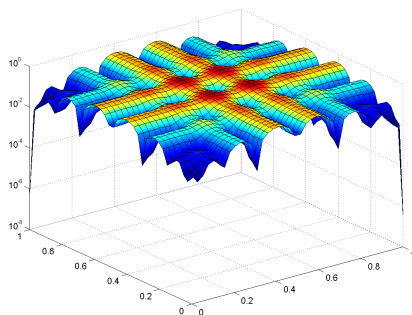
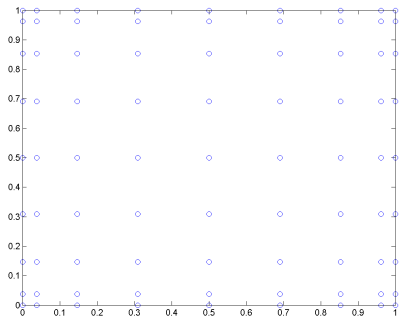


**Figure:** Data sites and power function for Gaussian interpolant with  $\varepsilon = 6$  based on  $N = 81$  uniformly gridded points in  $[0, 1]^2$ .



## Example

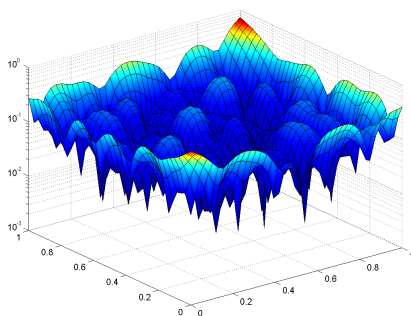
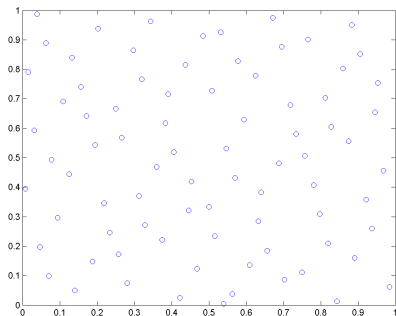
### More Gaussian Power Function



**Figure:** Data sites and power function for Gaussian interpolant with  $\varepsilon = 6$  based on  $N = 81$  tensor-product Chebyshev points in  $[0, 1]^2$ .

## Example

## More Gaussian Power Function



**Figure:** Data sites and power function for Gaussian interpolant with  $\varepsilon = 6$  based on  $N = 81$  Halton points in  $[0, 1]^2$ .

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### Theorem

*Let  $\Omega \subseteq \mathbb{R}^d$ ,  $K \in C(\Omega \times \Omega)$  be strictly positive definite, and suppose that the points  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  are distinct. Denote the interpolant to  $f \in \mathcal{H}_K(\Omega)$  on  $\mathcal{X}$  by  $s$ . Then for every  $\mathbf{x} \in \Omega$*

$$|f(\mathbf{x}) - s(\mathbf{x})| \leq P_{K,\mathcal{X}}(\mathbf{x}) \|f\|_{\mathcal{H}_K(\Omega)}.$$



**Proof.**

Since  $f$  is assumed to lie in the native space of  $K$  the reproducing property of  $K$  yields

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Now all that remains to be done is to **combine the two formulas** just derived and **apply the Cauchy-Schwarz inequality**. Thus,



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 &= \|f\|_{\mathcal{H}_K(\Omega)} P_{K, \mathcal{X}}(\mathbf{x}),
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where we have used the representation (2) of the quadratic form  $Q(\hat{\mathbf{u}}(\mathbf{x}))$  and the definition of the power function.  $\square$



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One of the main benefits of the above theorem is that we are now able to **estimate the interpolation error by considering two independent phenomena**:

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- and the **distribution of the data** (measured in terms of the power function — independent of the actual data values).



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### Remark

- *This is analogous to the standard error estimate for polynomial interpolation cited in most numerical analysis texts.*
- *Effects due to the use of any specific kernel  $K$  (or basic function in the translation invariant or radial case) are felt in both terms since the native space norm of  $f$  also varies with  $K$ .*
  - *In particular, changing a possible shape parameter  $\varepsilon$  will have an effect on both terms in the error bound.*

# Outline

- 1 Introduction
- 2 The Connection to Optimal Recovery
- 3 Orthogonality in Reproducing Kernel Hilbert Spaces
- 4 Optimality Theorems
- 5 The Basic Power Function Error Estimate
- 6 Sampling Inequalities**



# Error Bounds via Sampling Inequalities

We now use so-called **sampling inequalities** to obtain error bounds. Sometimes this technique is referred to as a **zeros lemma**.

The basic idea for sampling inequalities seems to have **originated in the French school** with the work of Duchon, Arcangéli and Atteia [Duc78, Arc74]. Another early paper is [MP85].

The paper [NWW05] started a long string of recent activity such as [ALdST07, ALdST09, ALdST12, GRZ13, HNW10, HNSW11, Mad06, NWW06, Rie08, RSZ10, RZ08, RZ14, WR05, ZS13].





# How sampling inequalities lead to error bounds

A sampling inequality formalizes in a rigorous way the following very general — and also intuitively convincing — idea:

It's impossible for a smooth function  $u$  to become uncontrollably large on its domain  $\Omega$  provided

- 1 samples of  $u$  obtained on a sufficiently dense discrete subset  $\mathcal{X}$  of  $\Omega$  are small enough (or zero), and
- 2 the derivatives of  $u$  are bounded on  $\Omega$ .



A **typical sampling inequality** looks like this:

$$|u|_{W_q^m(\Omega)} \leq C \left( h^{k-m-d\left(\frac{1}{p}-\frac{1}{q}\right)_+} |u|_{W_p^k(\Omega)} + h^{-m} \|\mathbf{u}\|_{\ell_\infty} \right), \quad (5)$$

i.e., the **weak semi-norm**  $|\cdot|_{W_q^m(\Omega)}$  is bounded by

- a **strong semi-norm**  $|\cdot|_{W_p^k(\Omega)}$  (defined in terms of  $m \geq 0$  and  $k > m + \frac{d}{p}$ ), and
- a **discrete norm**  $\|\cdot\|_{\ell_\infty}$  of the values  $\mathbf{u} = (u(\mathbf{x}_1), \dots, u(\mathbf{x}_N))^T$  of  $u$  on the set  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  with fill distance  $h$ .



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Note that

- $|u|_{W_p^k(\Omega)}$  is multiplied by a positive power of  $h$  (i.e., its contribution decreases as  $h$  gets small),
- while  $\|\mathbf{u}\|_{\ell_\infty}$  is multiplied by a non-positive power of  $h$  (i.e., its contribution increases as  $h$  gets small).



In order to get a useful error bound we apply our sampling inequalities in the case where the function  $u$  is interpreted as the residual  $f - s$  between the function  $f$  and its approximation  $s$ .

Then, for any successful approximation method, the samples of the residual will be small and will (hopefully) outweigh the  $h^{-m}$  factor.



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In particular, if  $s$  is obtained by interpolation on  $\mathcal{X}$ , then the residual vector  $\|\mathbf{u}\|_{\ell_\infty} = 0$ , and we get

$$|f - s|_{W_q^m(\Omega)} \leq Ch^{k-m-d\left(\frac{1}{p}-\frac{1}{q}\right)_+} |f - s|_{W_p^k(\Omega)}.$$



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### Remark

*This bound does not quite look like an error bound yet since it involves the residual  $f - s$  also on the right-hand side.*

Therefore, an important assumption needs to be made:

**We assume that our approximation satisfies the “energy split” (Pythagorean) lemma from above, i.e.,**

$$|f|_{W_p^k(\Omega)}^2 = |f - s|_{W_p^k(\Omega)}^2 + |s|_{W_p^k(\Omega)}^2,$$

which implies, in particular, that

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This is certainly true if the native space  $\mathcal{H}_K(\Omega)$  is equivalent to the Sobolev space  $W_p^k(\Omega)$ . Then we end up with the error bound

$$|f - s|_{W_q^m(\Omega)} \leq Ch^{k-m-d\left(\frac{1}{p}-\frac{1}{q}\right)_+} |f|_{W_p^k(\Omega)}.$$





To make this bound look a bit more familiar we consider

- $\Omega = [a, b]$ ,
- set  $m = 0$  (no simultaneous approximation of derivatives),
- let  $p = q = 2$  and
- convert the Sobolev (semi-)norm on the right-hand side to an  $L_2$ -norm of derivatives.



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Then we get for any  $f, s \in C^k([a, b])$

$$\|f - s\|_{L_2([a,b])} \leq Ch^k \|f^{(k)}\|_{L_2([a,b])}.$$



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### Remark

*This is, e.g., the kind of error bound that is typical for piecewise polynomial spline interpolation.*



# Sampling Inequalities for Kernel-based Approximation

We now look at error bounds for kernel-based interpolation methods obtained via sampling inequalities.

Sampling inequalities in 1D are relatively easy to understand and to obtain. So we first **consider the univariate case in detail**. This will cover, e.g., our **iterated Brownian bridge kernels**.

Then we **outline the important steps for the much more complicated multivariate case**.



We consider a **univariate kernel-based interpolation to data**  $\{x_i, f(x_i)\}_{i=1}^N$  at  $N$  distinct points  $\mathcal{X} = \{x_1, \dots, x_N\} \subset \Omega = [a, b]$  with **fill distance**  $h$  in the domain  $\Omega$ , i.e.,

$$h = \sup_{\mathbf{x} \in \Omega} \min_{\mathbf{x}_j \in \mathcal{X}} \|\mathbf{x} - \mathbf{x}_j\|.$$



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As discussed above, we must **first obtain a sampling inequality for a generic function**  $u$  of the same smoothness class as the kernel of interest.

Here **we assume that**  $u \in C^k(\Omega)$  for some non-negative integer  $k$ .



We begin by constructing a *local* polynomial interpolant of order  $k$  (i.e., degree  $k - 1$ ) to the generic function  $u \in C^k(\Omega)$  at the points  $\mathcal{X}_x = \{t_1, \dots, t_k\} \subset \mathcal{X}$ .

### Remark

For convenience we *denote the local points with  $t_j, j = 1, \dots, k$ , instead of picking appropriate subsets of indices for the original points in  $\mathcal{X}$ .*



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We pick the local interpolation points in dependence on the point of evaluation  $x$ , i.e.,  $\mathcal{X}_x$  consists of the  $k$  nearest neighbors of  $x$  from the set of global interpolation points  $\mathcal{X}$ ; this implies that we need  $N \geq k$ .





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This ensure that the local interpolation points are chosen as “symmetrical” as possible around  $x$ .



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This ensure that the local interpolation points are chosen as “symmetrical” as possible around  $x$ .

Furthermore, we define the interval  $I_x$  as the smallest closed interval which contains the points  $\mathcal{X}_x$ .



The **uniqueness of univariate polynomial interpolation** ensures that there exists a constant  $C$  such that for any polynomial  $p$  of degree at most  $k - 1$  we have

$$\sup_{x \in I_x} |p(x)| \leq C \sup_{t_j \in \mathcal{X}_x} |p(t_j)|, \quad (6)$$

i.e., the polynomial  $p$  is *determined* by its values on the set  $\mathcal{X}_x$ .



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### Remark

- A consequence of this property is that

$$p(t_j) = 0 \text{ for all } t_j \in \mathcal{X}_x \implies p \equiv 0 \text{ on } I_x,$$

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- In the univariate setting this is straightforward, but *in the multivariate setting this causes a first difficulty*, calling for the introduction of so-called *norming sets*.

A useful exact error formula for polynomial interpolation (known as Kowalewski's exact remainder formula, see [Dav63, Eqn. (3.7.10)], [Mad06]) can be obtained starting from a Taylor expansion of  $u$ .

We give the derivation of this formula since it sheds some light on the procedure recommended for the multivariate setting.



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**We give the derivation of this formula since it sheds some light on the procedure recommended for the multivariate setting.**

**Given  $u \in C^k(\Omega)$  and an arbitrary point  $t_j \in \mathcal{X}_x$ , we begin with [Mad06, Eqn. (2.2.1)]**

$$u(x) = u(t_j) - \sum_{i=1}^{k-1} \frac{u^{(i)}(x)}{i!} (t_j - x)^i + \int_{t_j}^x \frac{(t_j - t)^{k-1}}{(k-1)!} u^{(k)}(t) dt, \quad (7)$$

**which is obtained by swapping the roles of  $x$  and  $t_j$  in the usual version of Taylor's theorem with remainder.**



Now we consider the  $k^{\text{th}}$  order Lagrange polynomials for interpolation on  $\mathcal{X}_x$  which satisfy

- the cardinality conditions  $L_j(t_i) = \delta_{ij}$ ,  $i, j = 1, \dots, k$  and
- reproduce polynomials up to order  $k$ , i.e.,

$$\sum_{j=1}^k p(t_j) L_j(x) = p(x), \quad x \in I_x, \quad (8)$$





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In particular, we have

$$\sum_{j=1}^k L_j(x) \equiv 1.$$

This is known as a **partition of unity**.



Using this partition of unity property we can obtain a **weighted average of the Taylor formula** (7) for  $j = 1, \dots, k$ , i.e., we **multiply both sides of (7) by  $L_j(x)$**  and then **sum over  $j$  from 1 to  $k$**  resulting in

$$\begin{aligned}
 u(x) &= \sum_{j=1}^k L_j(x)u(t_j) - \sum_{j=1}^k L_j(x) \sum_{i=1}^{k-1} \frac{u^{(i)}(x)}{i!} (t_j - x)^i \\
 &\quad + \sum_{j=1}^k L_j(x) \int_{t_j}^x \frac{(t_j - t)^{k-1}}{(k-1)!} u^{(k)}(t) dt.
 \end{aligned} \tag{9}$$

- The **first sum** is nothing but  $p_k(x)$ , the **unique  $k^{\text{th}}$  order polynomial interpolating  $u$  on  $\mathcal{X}_x$** , since  $u(t_j) = p_k(t_j)$ ,  $j = 1, \dots, k$ , and  $p_k$  is defined by its Lagrange form  $p_k(x) = \sum_{j=1}^k L_j(x)p_k(t_j)$ .



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- The reproduction of polynomials up to degree  $k - 1$  (8) implies that the **double sum vanishes** since  $\sum_{j=1}^k L_j(x)(t_j - x)^i = 0$ ,  $i = 1, \dots, k - 1$ .



The result is **Kowalewski's exact remainder formula** as stated in [Mad06]:

$$u(x) = p_k(x) + \sum_{j=1}^k L_j(x) \int_{t_j}^x \frac{(t_j - t)^{k-1}}{(k-1)!} u^{(k)}(t) dt. \quad (10)$$



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By replacing  $p_k$  by its Lagrange form as in (9), and then **applying the triangle inequality to (10)** and **bounding the values of  $u$  in the first sum by their maximum** we get

$$|u(x)| \leq \Lambda_k \max_{t_j \in \mathcal{X}_x} |u(t_j)| + \sum_{j=1}^k |L_j(x)| \left| \int_{t_j}^x \frac{(t_j - t)^{k-1}}{(k-1)!} u^{(k)}(t) dt \right|, \quad (11)$$

where we have introduced the abbreviation

$$\Lambda_k = \max_{x \in I_x} \sum_{j=1}^k |L_j(x)|$$

to denote the **Lebesgue constant** for polynomial interpolation at the points  $t_1, \dots, t_k$ .



## Remark

*The Lebesgue constant depends on the distribution of interpolation points.*

- *It grows logarithmically in  $k$  for Chebyshev points (which is the minimal rate of growth, but not with optimal constant),*
- *while it grows exponentially in  $k$  for equally spaced points.*

*Note, however, that **this growth is not important for us since  $k$  is fixed here.***



In order to remove the Lagrange polynomials from the second term in (11) we make use of (6) so that

$$|L_j(x)| \leq C_j \max_{t_i \in \mathcal{X}_x} |L_j(t_i)| \leq C_j,$$

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This leaves us with

$$|u(x)| \leq \Lambda_k \max_{t_j \in \mathcal{X}_x} |u(t_j)| + C \sum_{j=1}^k \left| \int_{t_j}^x \frac{(t_j - t)^{k-1}}{(k-1)!} u^{(k)}(t) dt \right|,$$

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Now we bound the integral using the Cauchy–Schwarz inequality, i.e.,

$$\begin{aligned} \left| \int_{t_j}^x \frac{(t_j - t)^{k-1}}{(k-1)!} u^{(k)}(t) dt \right| &\leq \left| \int_{t_j}^x \frac{(t_j - t)^{2k-2}}{((k-1)!)^2} dt \right|^{1/2} \left| \int_{t_j}^x (u^{(k)}(t))^2 dt \right|^{1/2} \\ &= \frac{|t_j - x|^{k-1/2}}{\sqrt{2k-1}(k-1)!} \left| \int_{t_j}^x (u^{(k)}(t))^2 dt \right|^{1/2}. \end{aligned}$$



This results in

$$|u(x)| \leq \Lambda_k \max_{t_j \in \mathcal{X}_x} |u(t_j)| + C \sum_{j=1}^k \left\{ \frac{|t_j - x|^{k-1/2}}{\sqrt{2k-1}(k-1)!} \left| \int_{t_j}^x (u^{(k)}(t))^2 dt \right|^{1/2} \right\}.$$



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We will now aim for a sampling inequality in the  $L_2$ -norm.

Therefore we next square both sides of this inequality and apply the Cauchy–Schwarz estimates

$$(A + B)^2 \leq 2A^2 + 2B^2 \quad \text{and} \quad \left( \sum_{j=1}^k A_j \right)^2 \leq k \sum_{j=1}^k (A_j)^2$$

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This yields

$$|u(x)|^2 \leq 2\Lambda_k^2 \left( \max_{t_j \in \mathcal{X}_x} |u(t_j)| \right)^2 \tag{12}$$

$$+ \frac{2kC^2}{(2k-1)((k-1)!)^2} \sum_{j=1}^k |t_j - x|^{2k-1} \left| \int_{t_j}^x (u^{(k)}(t))^2 dt \right|.$$



To obtain an  $L_2$ -norm estimate on the local interval  $I_x$  we will have to integrate both sides over  $I_x = [\alpha, \beta]$  with appropriately chosen endpoints  $\alpha$  and  $\beta$ .



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We observe what happens if we integrate one of the summands on the right-hand side of (12) considering that  $t_j \in [\alpha, \beta]$ :

$$\begin{aligned} & \int_{\alpha}^{\beta} |t_j - x|^{2k-1} \left| \int_{t_j}^x (u^{(k)}(t))^2 dt \right| dx \\ &= \int_{\alpha}^{t_j} (u^{(k)}(t))^2 \int_t^{\alpha} |t_j - x|^{2k-1} dx dt + \int_{t_j}^{\beta} (u^{(k)}(t))^2 \int_t^{\beta} |t_j - x|^{2k-1} dx dt \end{aligned}$$



To obtain an  $L_2$ -norm estimate on the local interval  $I_x$  we will have to integrate both sides over  $I_x = [\alpha, \beta]$  with appropriately chosen endpoints  $\alpha$  and  $\beta$ .

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Since both  $|t_j - \alpha|$  and  $|t_j - \beta|$  are at most  $kh$  (because of the definition of fill distance) we get

$$\int_{\alpha}^{\beta} |t_j - x|^{2k-1} \left| \int_{t_j}^x (u^{(k)}(t))^2 dt \right| dx \leq \frac{(kh)^{2k}}{2k} \int_{\alpha}^{\beta} (u^{(k)}(t))^2 dt.$$





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We now plug this into the integrated version of (12) and use

$$\int_{\alpha}^{\beta} \left( u^{(k)}(t) \right)^2 dt = \|u^{(k)}\|_{L_2(I_x)}^2 \text{ to obtain}$$

$$\begin{aligned} \|u\|_{L_2(I_x)}^2 &\leq 2kh\Lambda_k^2 \left( \max_{t_j \in \mathcal{X}_x} |u(t_j)| \right)^2 + \frac{2kC^2}{(2k-1)((k-1)!)^2} \sum_{j=1}^k \frac{(kh)^{2k}}{2k} \|u^{(k)}\|_{L_2(I_x)}^2 \\ &= 2kh\Lambda_k^2 \left( \max_{t_j \in \mathcal{X}_x} |u(t_j)| \right)^2 + \frac{kC^2(kh)^{2k}}{(2k-1)((k-1)!)^2} \|u^{(k)}\|_{L_2(I_x)}^2. \end{aligned}$$



Note that we can rewrite

$$\|u\|_{L_2(I_x)}^2 \leq 2kh\Lambda_k^2 \left( \max_{t_j \in \mathcal{X}_x} |u(t_j)| \right)^2 + \frac{kC^2(kh)^{2k}}{(2k-1)((k-1)!)^2} \|u^{(k)}\|_{L_2(I_x)}^2.$$

as

$$\|u\|_{L_2(I_x)}^2 \leq C_1^2 h \left( \max_{t_j \in \mathcal{X}_x} |u(t_j)| \right)^2 + C_2^2 h^{2k} \|u^{(k)}\|_{L_2(I_x)}^2$$

provided the constants  $C_1$  and  $C_2$  (which depend on  $k$  and on the points in  $\mathcal{X}_x$ , but not on  $h$  or  $u$ ) are defined accordingly.



Note that we can **rewrite**

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Applying the inequality  $\sqrt{A^2 + B^2} \leq A + B$  (for  $A, B > 0$ ) we have the **final form of the local sampling inequality**

$$\|u\|_{L_2(I_x)} \leq C_1 \sqrt{h} \max_{t_j \in \mathcal{X}_x} |u(t_j)| + C_2 h^k \|u^{(k)}\|_{L_2(I_x)}.$$



To finally obtain a *global* sampling inequality we use a technique introduced in [Duc78].

For this covering argument to apply we note that we can cover the interval  $\Omega = [a, b]$  with a family of subintervals  $I_x$  as discussed above.

In fact,

- each of these subintervals has length at most  $kh$  and
- each point  $x \in \Omega$  is covered by at most  $k \leq N$  subintervals.



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In fact,

- each of these subintervals has length at most  $kh$  and
- each point  $x \in \Omega$  is covered by at most  $k \leq N$  subintervals.

This allows us to sum up all the local estimates to arrive at

$$\|u\|_{L_2(\Omega)} \leq C_3 \sqrt{b-a} \max_{x_j \in \mathcal{X}} |u(x_j)| + C_4 h^k \|u^{(k)}\|_{L_2(\Omega)}, \quad (13)$$

where the constants  $C_3$  and  $C_4$  depend on  $k$ ,  $N$ , and the distribution of the points in  $\mathcal{X}$ , but not on  $h$  and  $u$ .



Note that

$$\|u\|_{L_2(\Omega)} \leq C_3 \sqrt{b-a} \max_{x_j \in \mathcal{X}} |u(x_j)| + C_4 h^k \|u^{(k)}\|_{L_2(\Omega)},$$

looks like our typical sampling inequality (5) with

- $\Omega = [a, b]$ ,
- $C = \max\{C_3 \sqrt{b-a}, C_4\}$ ,
- $m = 0$ , and
- $p = q = 2$ .



The sampling inequality (13) says that the continuous  $L_2$ -norm of  $u$  is bounded by

- the  $k^{\text{th}}$  power of the fill distance times the stronger  $H^k$ -norm of  $u$  and
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This estimate holds for any function  $u \in C^k(\Omega)$ .

In particular, it provides an error bound for any method that generates an interpolant  $s \in C^k(\Omega)$  to a function  $f \in C^k(\Omega)$  at the points in  $\mathcal{X}$ . In this case we have

$$\|f - s\|_{L_2(\Omega)} \leq Ch^k \|(f - s)^{(k)}\|_{L_2(\Omega)}$$

as outlined above.





In order to get the upper bound to depend only on the input data, i.e.,  $f$  and  $\mathcal{X}$  (or its fill distance  $h$ ) we use the triangle inequality so that

$$\|f - s\|_{L_2(\Omega)} \leq Ch^k \left( \|f^{(k)}\|_{L_2(\Omega)} + \|s^{(k)}\|_{L_2(\Omega)} \right).$$



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If we are working in a setting in which the interpolant is also a minimum norm interpolant (such as in a reproducing kernel Hilbert space  $\mathcal{H}_K(\Omega)$ ) then

$$\|s^{(k)}\|_{L_2(\Omega)} \leq \|f^{(k)}\|_{L_2(\Omega)},$$

provided  $\mathcal{H}_K(\Omega)$  is equivalent to the Sobolev space  $H^k(\Omega)$ , and we obtain the error bound

$$\|f - s\|_{L_2(\Omega)} \leq 2Ch^k \|f\|_{H^k(\Omega)}.$$



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- *In order to “double” the orders one needs to take into account additional properties of the native Hilbert space.*
- *In particular, incorporating the boundary behavior of  $f$  and  $s$  is important to achieve those higher orders. We already saw this experimentally in Chapter 6.*



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- This approach *can also be extended to other settings, such as (least squares) approximation or PDE error estimates* — both in *strong form and weak form*.



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- This approach *can also be extended to other settings*, such as (least squares) *approximation* or *PDE error estimates* — both in strong form and weak form.
- Details on more advanced versions of error bounds based on sampling inequalities are available in the original literature listed above.





# Sampling inequalities in higher dimensions

The main problem in higher dimensions is the misbehavior of polynomial interpolation:

- depending on the points in  $\mathcal{X}$ , the interpolating polynomial may not be unique, or it may not even exist (see, e.g., [GS00]).

Therefore, one usually resorts to

- **oversampling** and
- an **approximation in terms of local (moving) least squares polynomials**.

This approach then also calls for so-called **norming sets** as defined in [JSW99] (or as **determining sets** in [Mad06]).



A **norming set**  $\Lambda$  of a normed linear space  $\mathcal{F}$  is a finite set of linear functionals (such as point evaluation functionals  $\lambda_i(f) = f(\mathbf{x}_i)$ ,  $i = 1, \dots, N$ ) defined on the dual of  $\mathcal{F}$ .

It **provides a bound of the continuous  $\mathcal{F}$ -norm of  $f$  by only discrete samples, i.e.,**

$$\|f\|_{\mathcal{F}} \leq C \sup_{\lambda_i \in \Lambda, \|\lambda_i\|=1} |\lambda_i(f)| \quad \text{for all } f \in \mathcal{F} \quad (14)$$

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We saw an **example for the case of univariate polynomials and point evaluation functionals** earlier:

$$\sup_{x \in I_x} |p(x)| \leq C \sup_{t_j \in \mathcal{X}_x} |p(t_j)|.$$



Following [RSZ10], we now sketch a **standard way to prove a typical sampling inequality** of the form

$$\|D^\alpha u\|_{L_q(\Omega)} \leq C \left( h^{k-|\alpha|-d\left(\frac{1}{p}-\frac{1}{q}\right)_+} \|u\|_{W_p^k(\Omega)} + h^{-|\alpha|} \|S_{\mathcal{X}} u\|_{\ell_\infty} \right).$$

Here  $S_{\mathcal{X}}$  is a **sampling operator** on  $\mathcal{X}$  and  $\alpha$  is a multi-index so that  $D^\alpha$  denotes a **standard multivariate derivative operator of order  $|\alpha|$** .



For some domain  $\mathcal{D}$ , star-shaped with respect to a ball<sup>1</sup>, let  $\{a_j^{(\alpha)}, j = 1, \dots, N\}$  be a **local polynomial reproduction of degree  $k$**  with respect to a discrete set  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathcal{D}$ , i.e.,

$$D^\alpha q(\mathbf{x}) = \sum_{j=1}^N a_j^{(\alpha)}(\mathbf{x}) q(\mathbf{x}_j)$$

holds for every multi-index  $\alpha$  with  $|\alpha| \leq k$ , all  $\mathbf{x} \in \mathcal{D}$  and all  $q \in \Pi_k^d(\mathcal{D})$ , where  $\Pi_k^d$  denotes the space of all  $d$ -variate polynomials of degree at most  $k$ .

---

<sup>1</sup> $\mathcal{D}$  is called *star-shaped with respect to a ball  $B$*  if, for all  $\mathbf{x} \in \mathcal{D}$ , the closed convex hull of  $\{\mathbf{x}\} \cup B$  is a subset of  $\mathcal{D}$  (see, e.g., [BS94, (4.2.2) Definition]).



Then we have

$$|D^\alpha u(\mathbf{x})| \leq \|D^\alpha(u-p)\|_{L_\infty(\mathcal{D})} + \sum_{j=1}^N \left| a_j^{(\alpha)}(\mathbf{x}) \right| (\|u-p\|_{L_\infty(\mathcal{D})} + \|S_{\mathcal{X}}u\|_{\ell_\infty})$$

for arbitrary  $u \in W_p^k(\mathcal{D})$  and any polynomial  $p \in \Pi_d^k(\mathcal{D})$ .

Using a **polynomial reproduction argument based on norming sets**, the **Lebesgue constant can be bounded** by  $\sum_{j=1}^N \left| a_j^{(\alpha)}(\mathbf{x}) \right| \leq 2$ , if **some moderate oversampling is allowed**.



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### Remark

*As a local polynomial approximation one usually chooses the averaged Taylor polynomials of degree  $k$  (see [BS94, Section 4.1].*

*In contrast to the averaging process we used in the one-dimensional setting, the multivariate average needs to be constructed with an appropriately defined measure which reproduces polynomials.*

Doing all of this leads to a **local sampling inequality** of the form

$$\|D^\alpha u\|_{L^\infty(\mathcal{D})} \leq \frac{C}{(k - |\alpha|)!} \delta_{\mathcal{D}}^{k-d/p} \left( \delta_{\mathcal{D}}^{-|\alpha|} + h^{-|\alpha|} \right) \|u\|_{W_p^k(\mathcal{D})} + 2h^{-|\alpha|} \|S_{\mathcal{X}} u\|_{\ell_\infty}$$

where  $\delta_{\mathcal{D}}$  denotes the diameter of  $\mathcal{D}$ .





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To derive **sampling inequalities on a global Lipschitz domain  $\Omega$**  satisfying an interior cone condition, we cover  $\Omega$  by domains  $\mathcal{D}$  which are star-shaped with respect to a ball, satisfying  $\delta_{\mathcal{D}} \approx h$  (see [Duc78] for details on such coverings).



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**Global estimates are obtained by summation or maximization over the local estimates** (see, e.g., [Wen05, Theorem 11.32]) similar to what was done in the one-dimensional setting.



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