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DEpendable & Explainable Learning

Towards instance-dependent approximation guarantees for Lipschitz approximators, application to Scientific ML.

P. Novello, IRT Saint Exupery
C. Gauchy, CEA
M. Dalery, Laboratoire de Mathématiques de Besançon
M. Peyron, CERFACS & EVIDEN
S. Saha, Indian Statistical Institute

IVADO · IRT Saint Exupéry · CRIAQ · ANITI Artificial & Natural Intelligence Toulouse Institute · Institut intelligence et données

Challenges of SciML

Scientific Machine Learning is thriving [2] ...

- Extends traditional surrogate modeling and function approximation to larger scale problems (mesh data) [5,7].
- Encompasses new techniques like Physics informed learning, neural operators ([5,6]., this workshop) to refine the quality of the approximation and foster practitioner's trust in those models.

...but surrogate models and numerical schemes are not considered equals

- Such models are data driven and lack guarantees as seen classical numerical schemes
- Some workaround to leverage ML without affecting the guarantees:
  - ML-driven preconditioning [9], Mesh initialization [13],...

Still, the performances of next gen surrogate models can be so good as is...

...Couldn't we provide strict **approximation guarantees for SciML models**?

Finding an error bound for g

We approximated a function $f: \mathcal{X} \in \mathbb{R}^d \to \mathbb{R}$ using a neural network g and a set of learning points $\left(X_1, Y_1 = f(X_1)\right), \dots, \left(X_n, Y_n = f(X_n)\right)$

Now, **can we provide approximation guarantees after the training using g and $\left(X_1, Y_1 = f(X_1)\right), \dots, \left(X_n, Y_n = f(X_n)\right)$ only?**

By finding bounds on

$$J_g = \|f - g\|_\infty = \max_{x \in \mathcal{X}} |f(x) - g_\theta(x)|$$

In the following, we try to bound the norm $\|f - g\|_\infty$, with a bound $\bar{J}_g$.

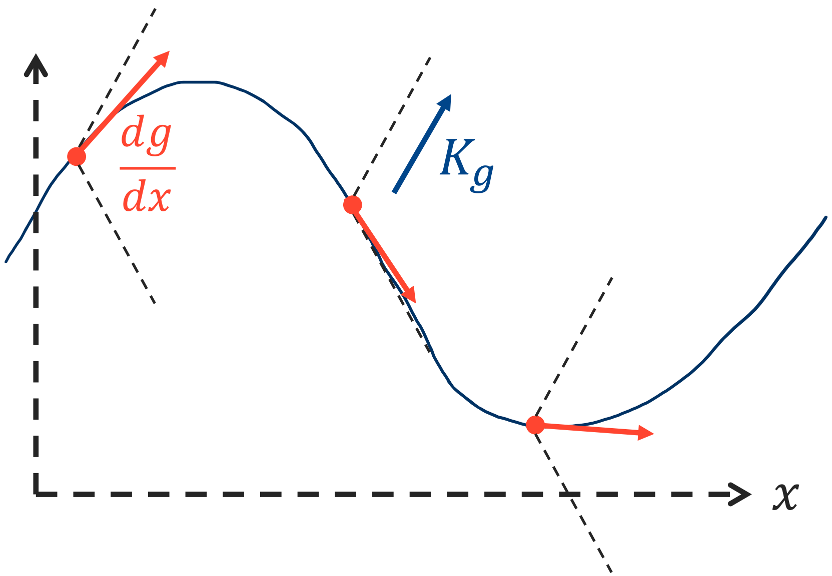
To that end, we will leverage the properties of Lipschitz neural networks

Lipschitz Neural Networks

A function f is said Lipschitz continuous, of constant K_f if :

$$\forall x, y \in \mathbb{R}^d, |f(x) - f(y)| \leq K_f \times \|x - y\|$$

A neural network g is said K_g-Lipschitz when it satisfies the above property.



Its rate of change is bounded by K_g

Motivation: Error bound in 1D

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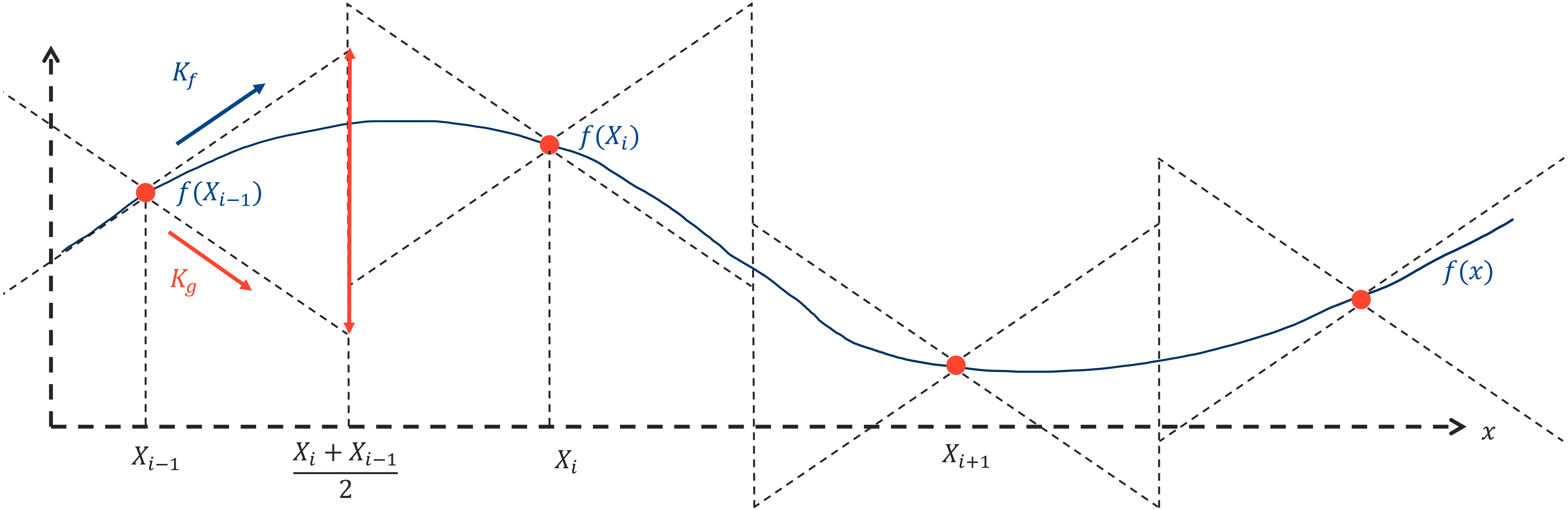
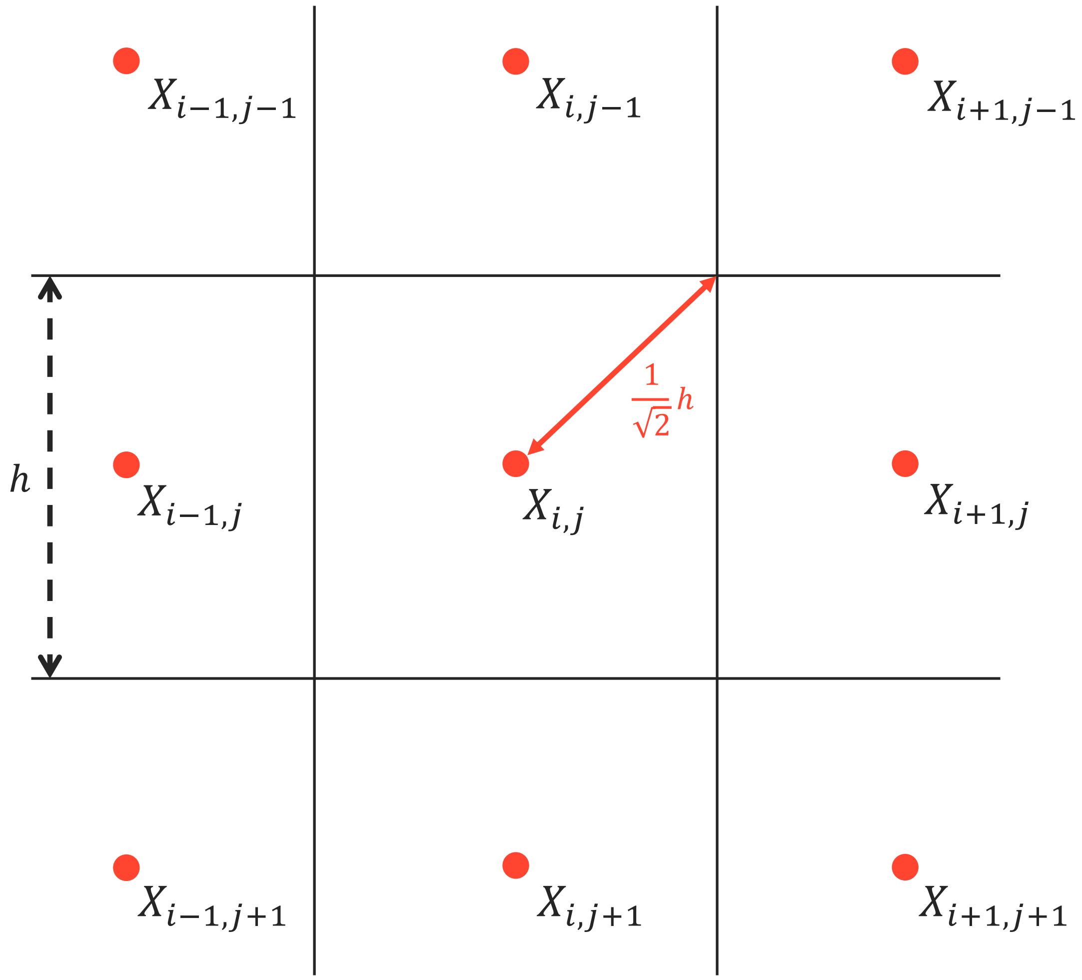


Take the difference between maximum variation of f and g on each subdivision:

$$J_g \leq \max_{i \in \{1,\dots,n\}} \frac{1}{2}\left(K_g + K_f\right)\|X_i - X_{i-1}\| + \boxed{|f(X_i) - g(X_i)|}$$

$=$ 0 in this example

Motivation: Error bound in 2D (and beyond)



Bound in 2D ($d = 2$):

- Consider n^2 learning points $\{X_{i,j}\}_{i,j\in\{1,\ldots n\}^\wedge 2}$ at the center of a grid with cells of edge size h.

In the k-th cell of center $X_{i,j}$:

$$J_g^k \leq |f(X_{i,j}) - g(X_{i,j})| + \frac{1}{\sqrt{2}}(K_f + K_g)h = \bar{J}_g^k$$

Bound in ND ($d = N$):

In the k-th cell of center X_p:

$$J_g^k \leq |f(X_p) - g(X_p)| + \frac{\sqrt{N}}{2}(K_f + K_g)h = \bar{J}_g^k$$

Then,

$$J_g \leq \max_k \bar{J}_g^k$$

Breaking free from grids

Main problem: Learning points are rarely structured as a grid

What about learning in the context of Scientific ML?

~~We control the design of experiment so we could build it as a grid~~

~~**Very constraining:**~~

- ~~The DOE should be defined in advance and we could not add points sequentially~~
- ~~Grids suffer from the curse of dimensionality, the number of f evaluations would grow exponentially with d~~
- ~~Monte Carlo is convenient~~

Aim of this work: find ways to build upper bounds for J_g when $\left(X_1, Y_1 = f(X_1)\right), \dots, \left(X_n, Y_n = f(X_n)\right)$ is not structured as a grid

Outline

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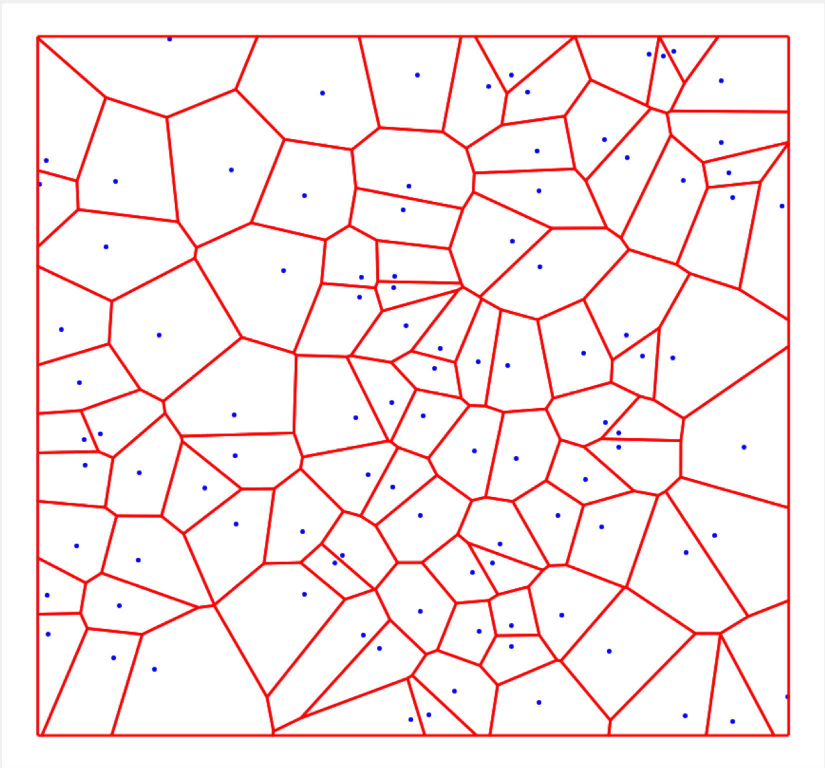
- Introduction
- **Error bound with Voronoï diagrams**
- Bounding with certified Deterministic Optimistic Optimization
- Conclusion & Takeaway

Definition of a Voronoï diagram (and some notations)



A Voronoï diagram $\mathcal{V}^d$ is built on a set of points $\mathbf{X} = \{X_1, \dots, X_n\}, X_i \in \mathcal{X} \subset \mathbb{R}^d$.

Each point is called a site, and the diagram is defined by its cells $\{\mathcal{V}^d(X_1), \dots, \mathcal{V}^d(X_n)\}$ themselves defined by

$$\mathcal{V}^d(X_i) = \{x \in \mathcal{X} \mid \forall j \in \{1, \dots, n\}, \|x - X_i\| \leq \|x - X_j\|\}$$

If $x \in \mathcal{V}^d(X_i)$, then X_i is the nearest neighbor of x

We have that $\mathcal{X} = \bigcup_{i \in \{1,\dots,n\}} \mathcal{V}^d(X_i)$, so to obtain $\bar{J}_g$, it is enough finding $\bar{J}_g^i$, an upper bound for

$$J_g^i = \max_{x \in \mathcal{V}^d(X_i)} |f(x) - g(x)|$$

Error bound using Voronoï diagram

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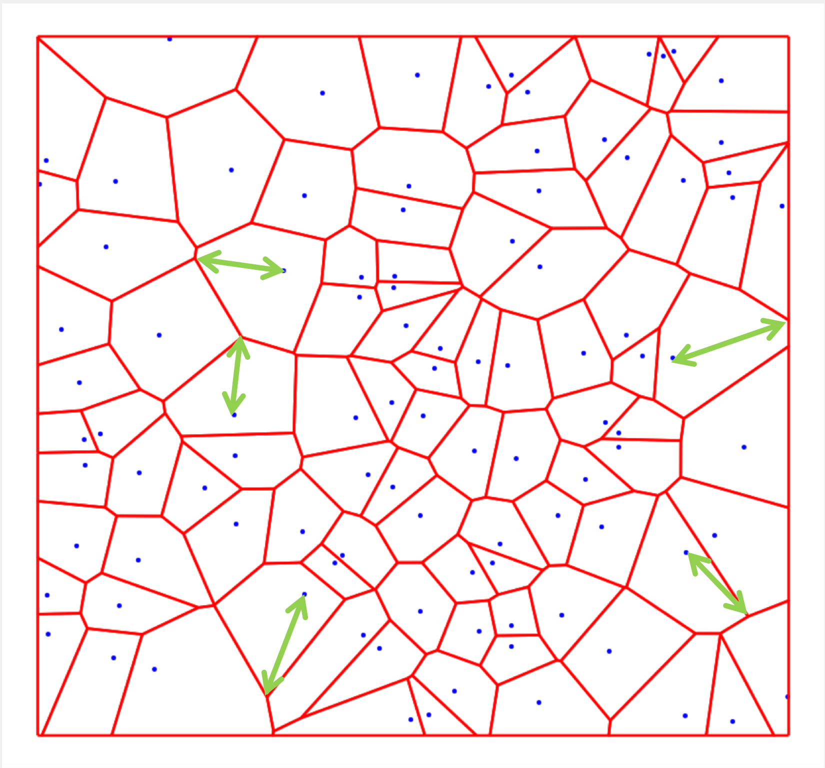


Let $\color{red}{N}: x \rightarrow \underset{X_i \in \mathbf{X}}{argmin} \|x - X_i\|$ (nearest neighbor map)

Then by the Lipschitz property of g and f, we have that $\forall x \in \mathcal{X}$,

$$|f(x) - g(x)| \leq (K_f + K_g)\|x - N(x)\| + |f(N(x)) - g(N(x))|$$

Lemma 1

Goes well with Voronoï diag!

Let $r(X_i)$ be the radius of $\mathcal{V}^d(X_i)$ defined by

$$r(X_i) = \max_{x \in \mathcal{V}^d(X_i)} \|x - X_i\|$$

Then, it holds that

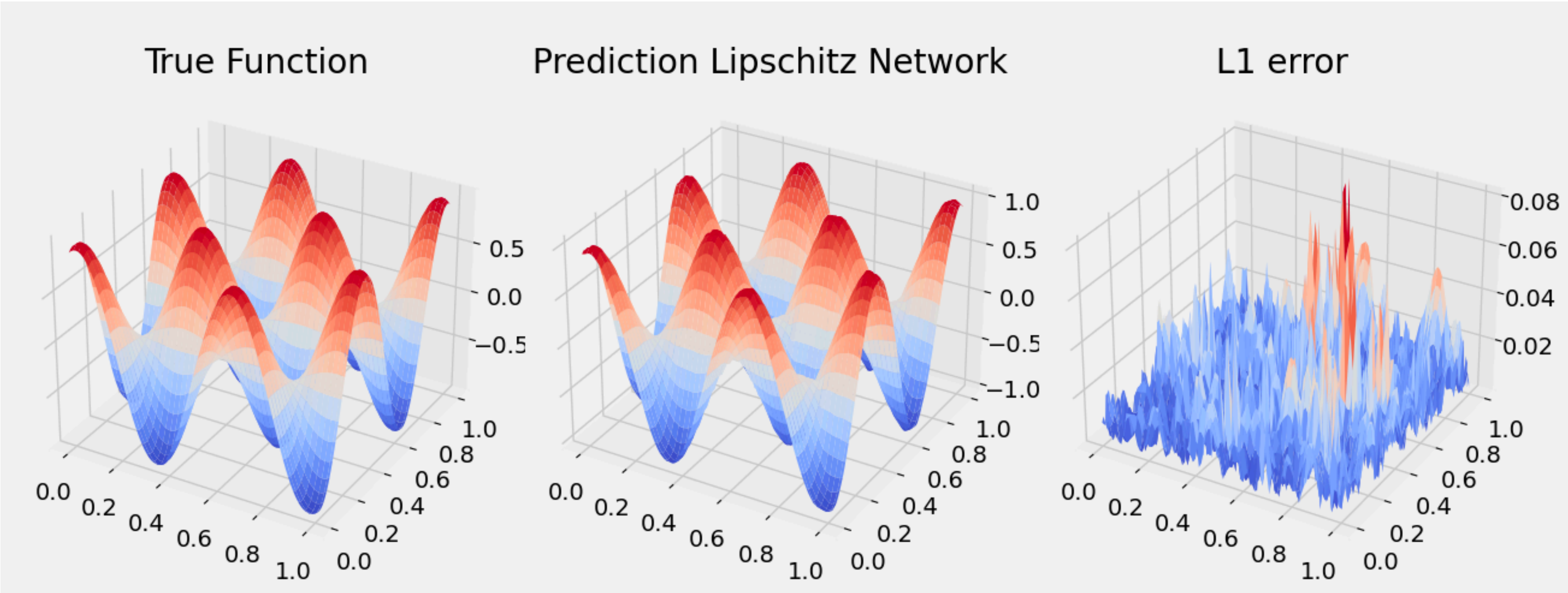
$$J_g^i \leq |f(X_i) - g(X_i)| + (K_f + K_g) r(X_i)$$

Hence,

$$J_g \leq \max_{i \in \{1,\ldots,n\}} |f(X_i) - g(X_i)| + (K_f + K_g) r(X_i)$$

- All we need is to compute $r(X_i)$

Experiments on toy functions

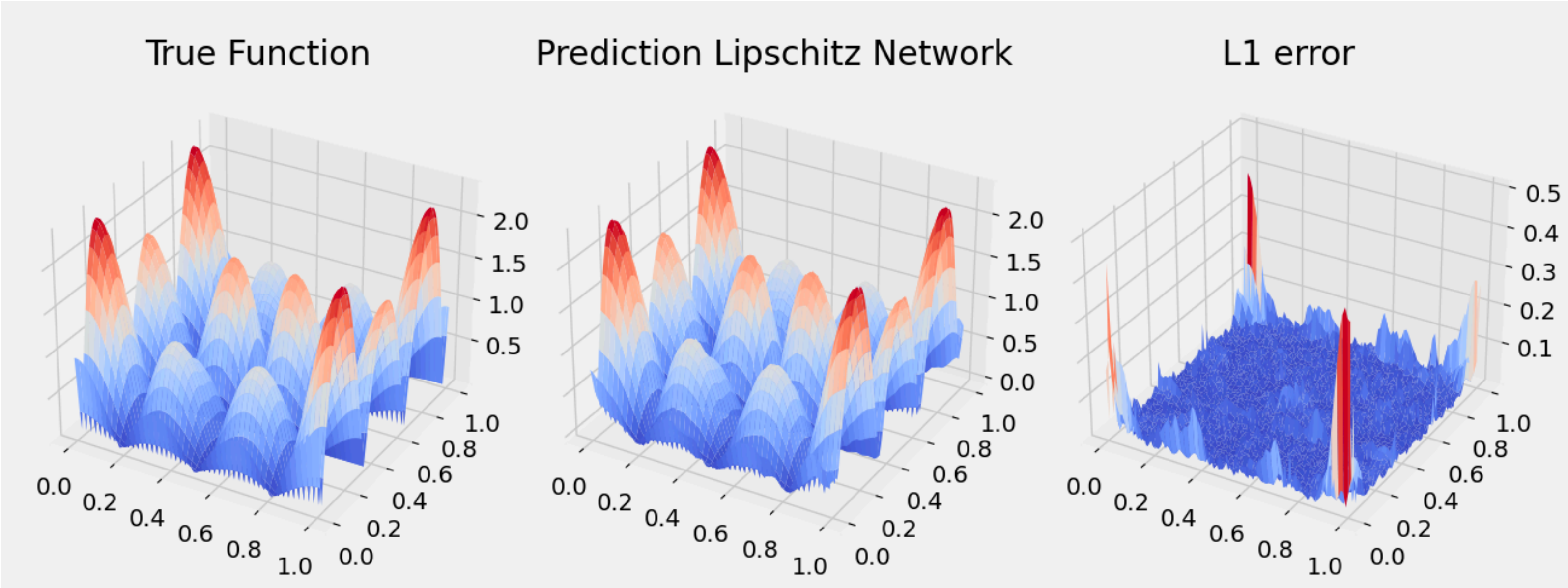


Sinus function

$$f: x, y \to \sin(x) \times \sin(y)$$

10000 training points

Experiments on toy functions



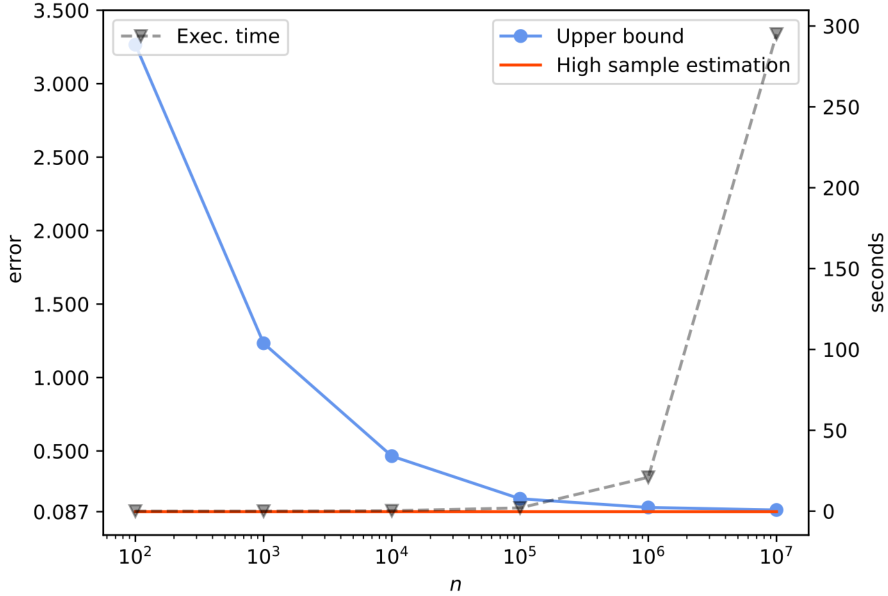
Holder table function

$$f: x, y \to \left| \sin(x) \cos(y) \exp\left(\left| 1 - \frac{\sqrt{x^2 + y^2}}{\pi} \right| \right) \right|$$

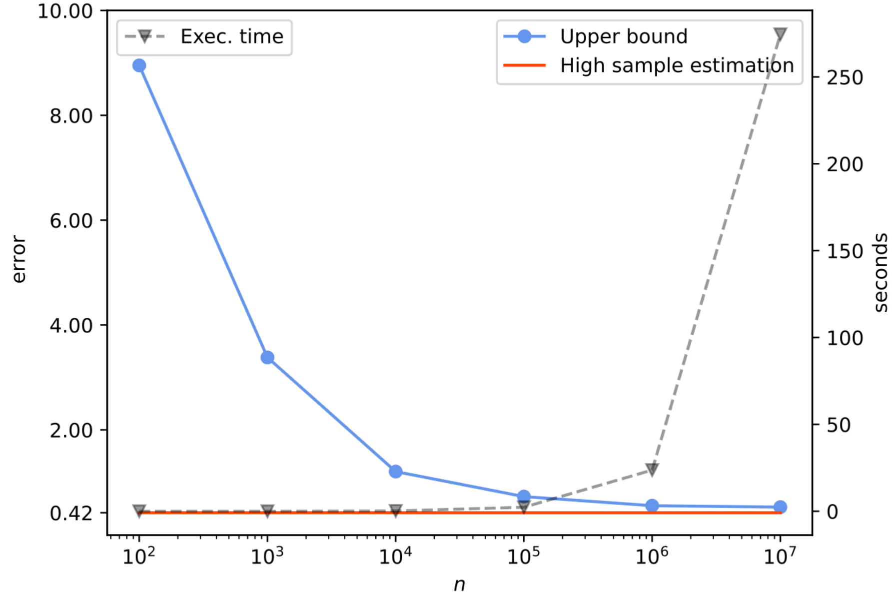
10000 training points

Complexity of Voronoï diagrams

Upper bound of L_∞ error with computation time for Sinus function (left) and Holder table function (right)



Best upper bound: 0.098
High sample estimation: 0.087



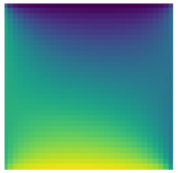
Best upper bound: 0.53
High sample estimation: 0.42

Problem: Voronoï diagram's complexity is exponential**…**

… what about higher d and n?

Diffusion in 2D:

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$



- We simulate heat diffusion on a homogeneous surface , with 4 Dirichlet boundary conditions and observe the field at convergence.
- The final heat field depends on the boundary conditions, but not on the initial state nor the diffusivity.

Design of experiment:

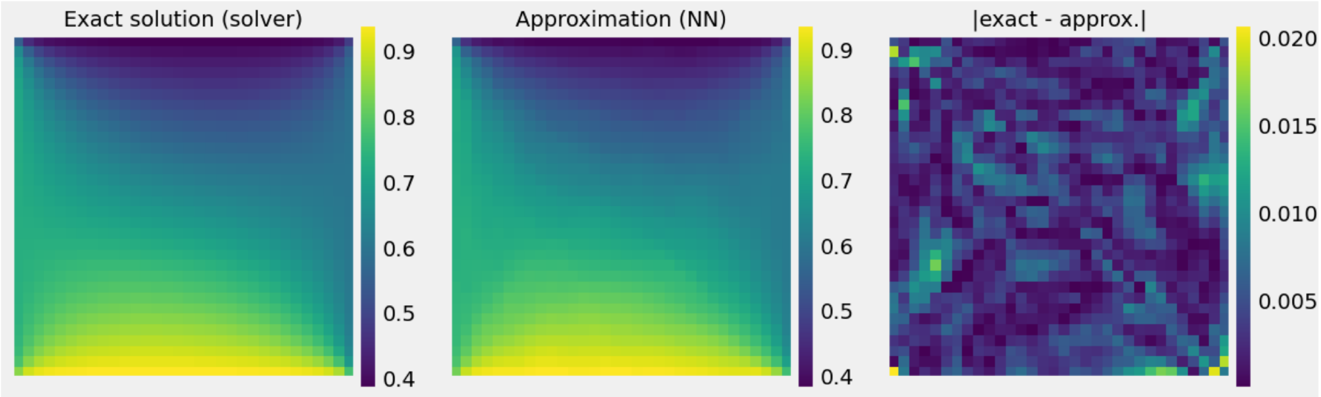
- Sample $n = 5000$ boundary conditions $\{(a_i, b_i, c_i, d_i)\}_{i\in\{1,\ldots,n\}}$ uniformly on $[0,1]^4$.
- Conduct n simulations on a $p\times p$ grid ($p = 32$), yielding a temperature field $\{T_{jk}\}_{j,k\in\{1,\ldots,p\}^2}$.

Training dataset:

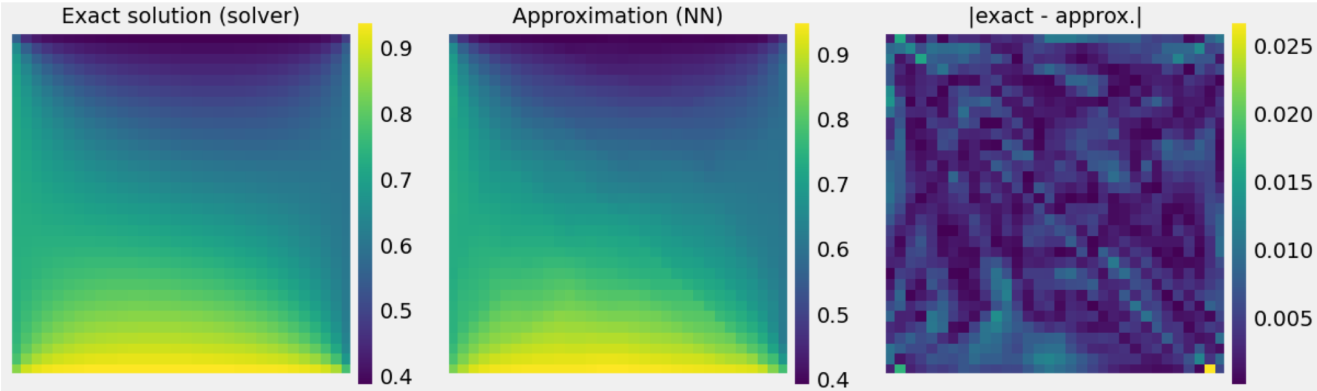
- A subset of $n\times p\times p/10 = 512{,}000$ points $\{(a_i, b_i, c_i, d_i, x_j, x_k), T_{j,k}\}_{i\in\{1,\ldots,n\},j,k\in\{1,\ldots,p\}^2}$

Neural implicit representation approach!

Approximation results



Lipschitz network, MSE=6.3×10^{-5}



Standard fully connected, MSE=4.1×10^{-5}

How to handle unknown K_f?

Two ways:

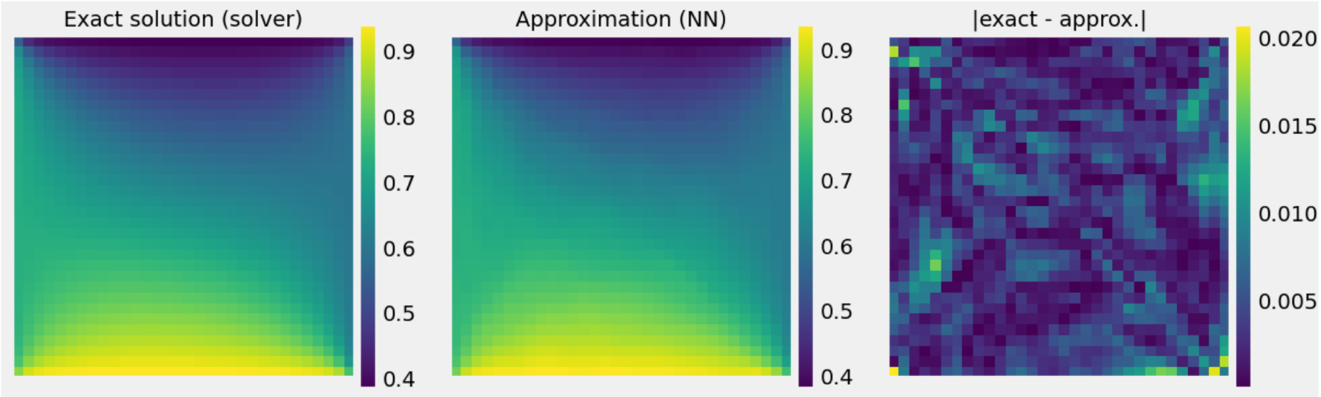
1. Empirical estimation of Lipschitz constant using:

$$\widehat{K_f} = \max_{i \in \{1,\dots,n\}} \left(\max_{X \in \mathcal{N}_k(X_i)} \frac{|f(X) - f(X_i)|}{\|X - X_i\|} \right)$$

   Where $\mathcal{N}_k(X_i)$ is the set of the k-th nearest neighbors of X_i.

2. Hypotheses of f:
   - In [8], the authors compute the Lipschitz constant of f when it is a Gaussian Process interpolating the data.
   - Could apply to polynomial regression
   - We might find the Lipschitz constant by studying the physics [4]

Error bound



Lipschitz network, MSE=6.3×10^{-5}

- Maximum empirical L_1error: $\mathbf{0.17}$

Voronoï diagram with a subset of 20000 points. Takes $\approx$ 3000 seconds ($exponential$ complexity…)

- Error bound: **84**!! Not very appealing…
- We have to find workarounds to use all the $n\times p\times p$ = 5,120,000 points

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Mapping to grid

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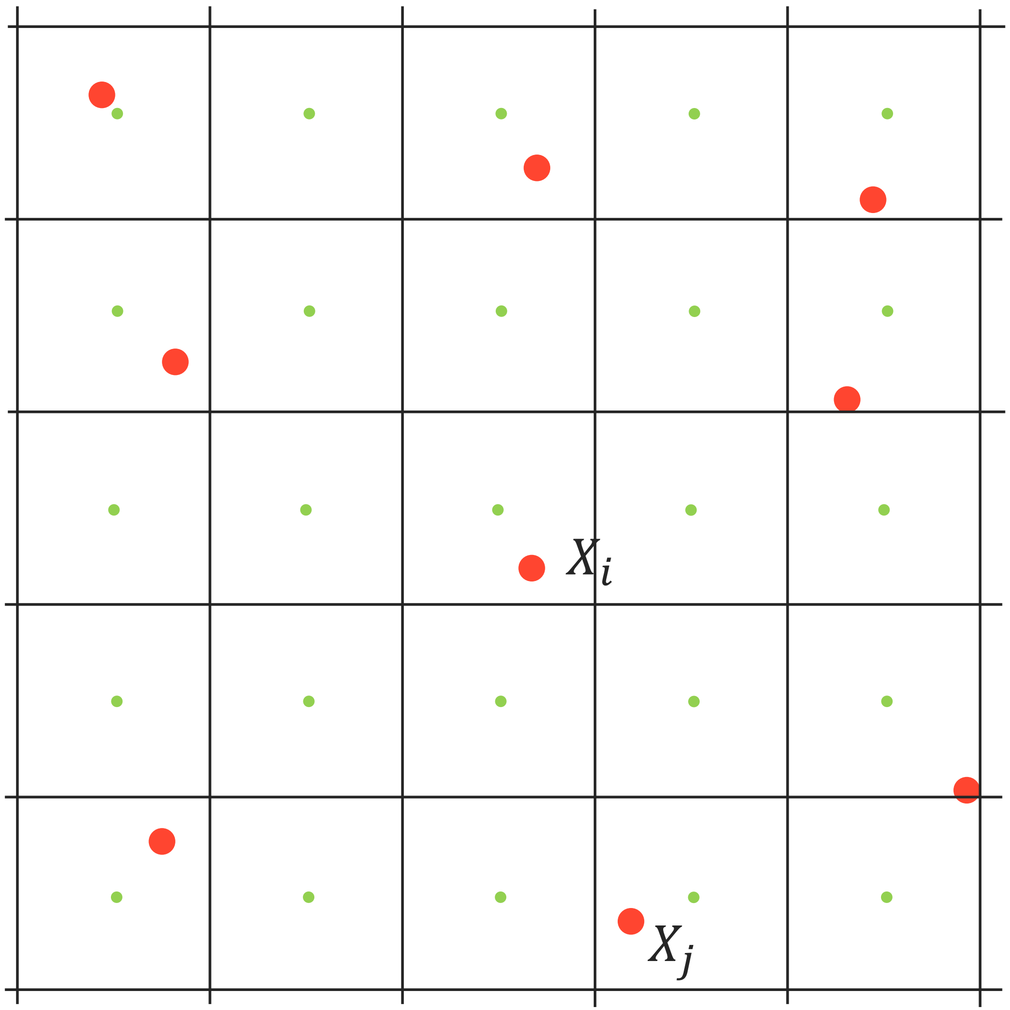


Let's consider $\mathbf{X} = \{X_1, \ldots, X_n\}$ uniformly distributed on $[0,1]^d$.

We have that, $\forall x, i \in [0,1]^d \times \{1, \ldots, n\}$,

$$|f(x) - g(x)| \leq (K_f + K_g)\|x - X_i\| + |f(X_i) - g(X_i)|$$

We can do better because **we can evaluate $g(x)$**!

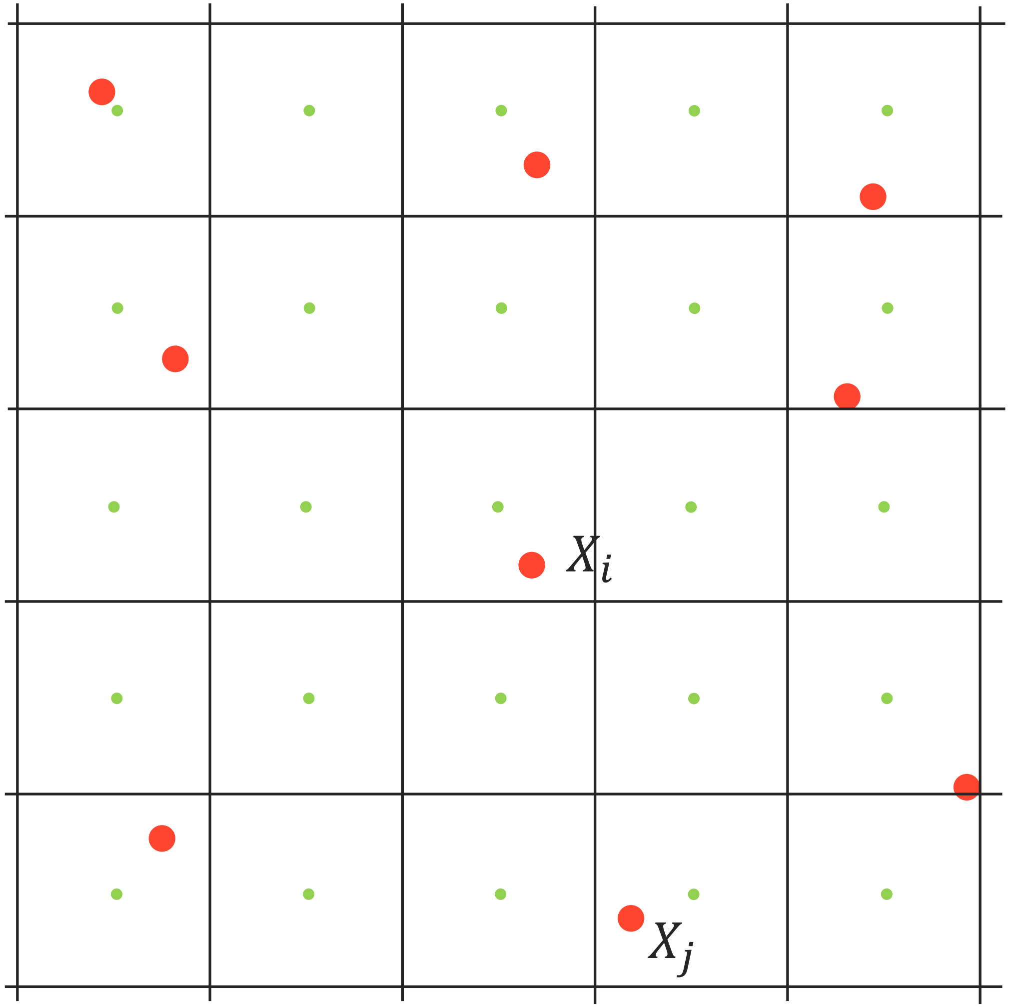
$\forall x, i \in [0,1]^d \times \{1, \ldots, n\}$,

$$|f(x) - g(x)| \leq K_f\|x - X_i\| + |f(X_i) - g(x)|$$

Lemma 2

Now, consider a grid of p^d cells with centers $\{c_1, \ldots, c_{p^d}\}$

Mapping to grid



Now, consider a grid of p^d cells $\{C_1, \ldots, C_{p^d}\}$ with centers $\{c_1, \ldots, c_{p^d}\}$

$\forall k \in \{1, \ldots, p^2\}$,

$$|f(c_k) - g(c_k)| \leq K_f \|c_k - X_i\| + |g(c_k) - f(X_i)|$$

Mapping to grid

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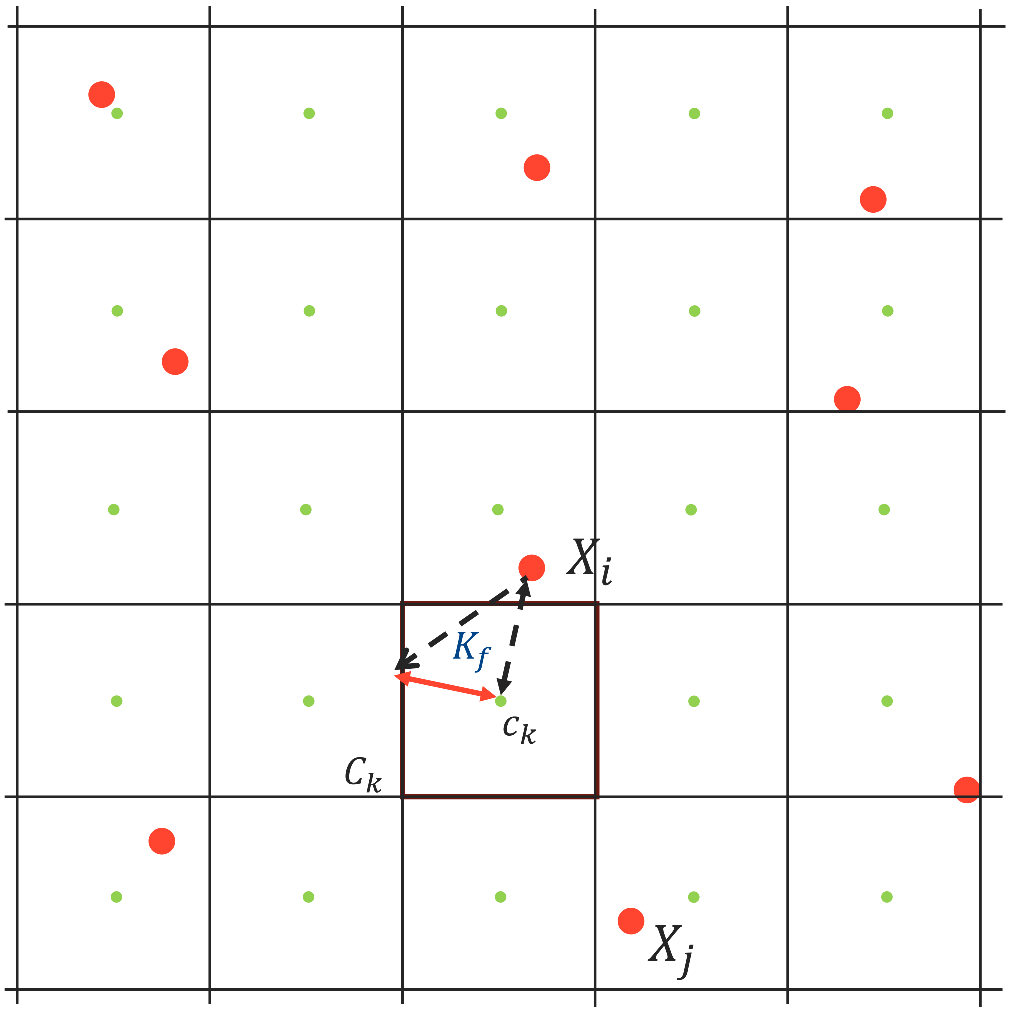

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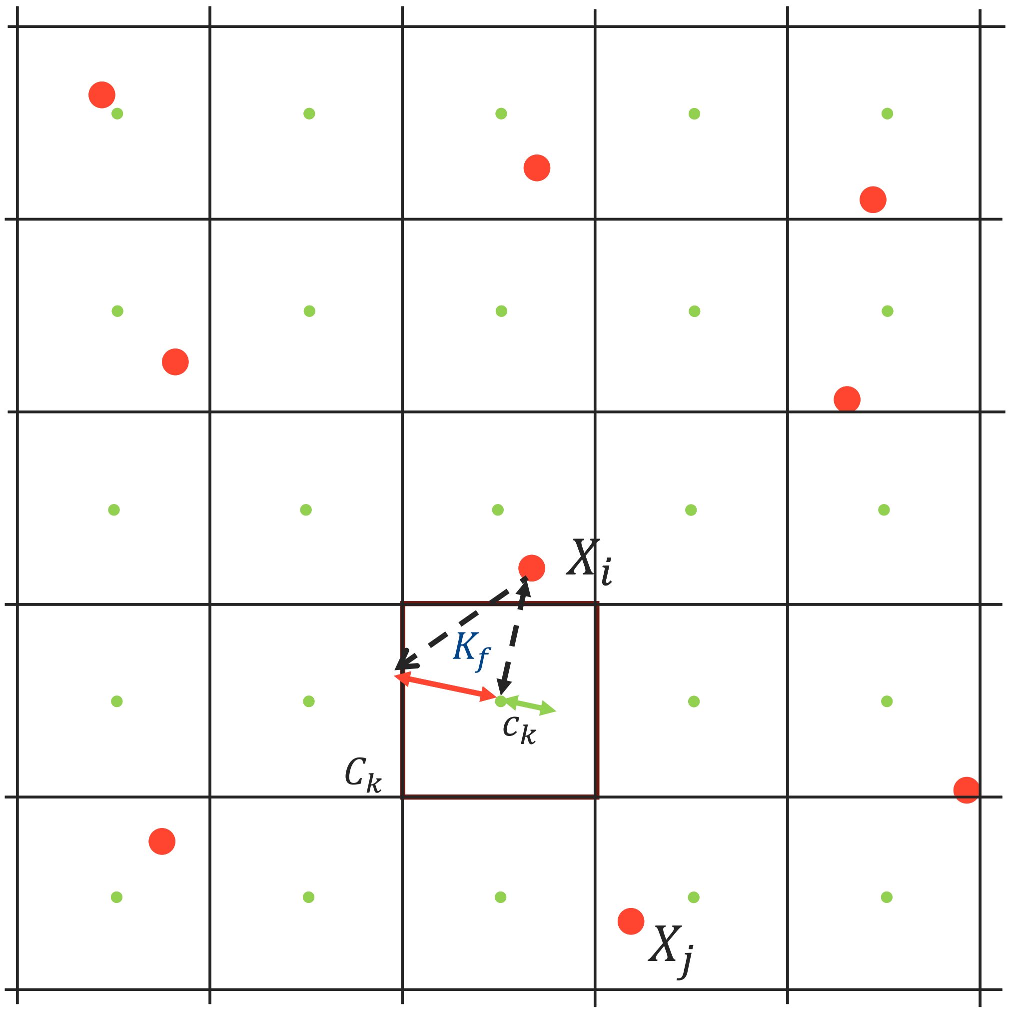

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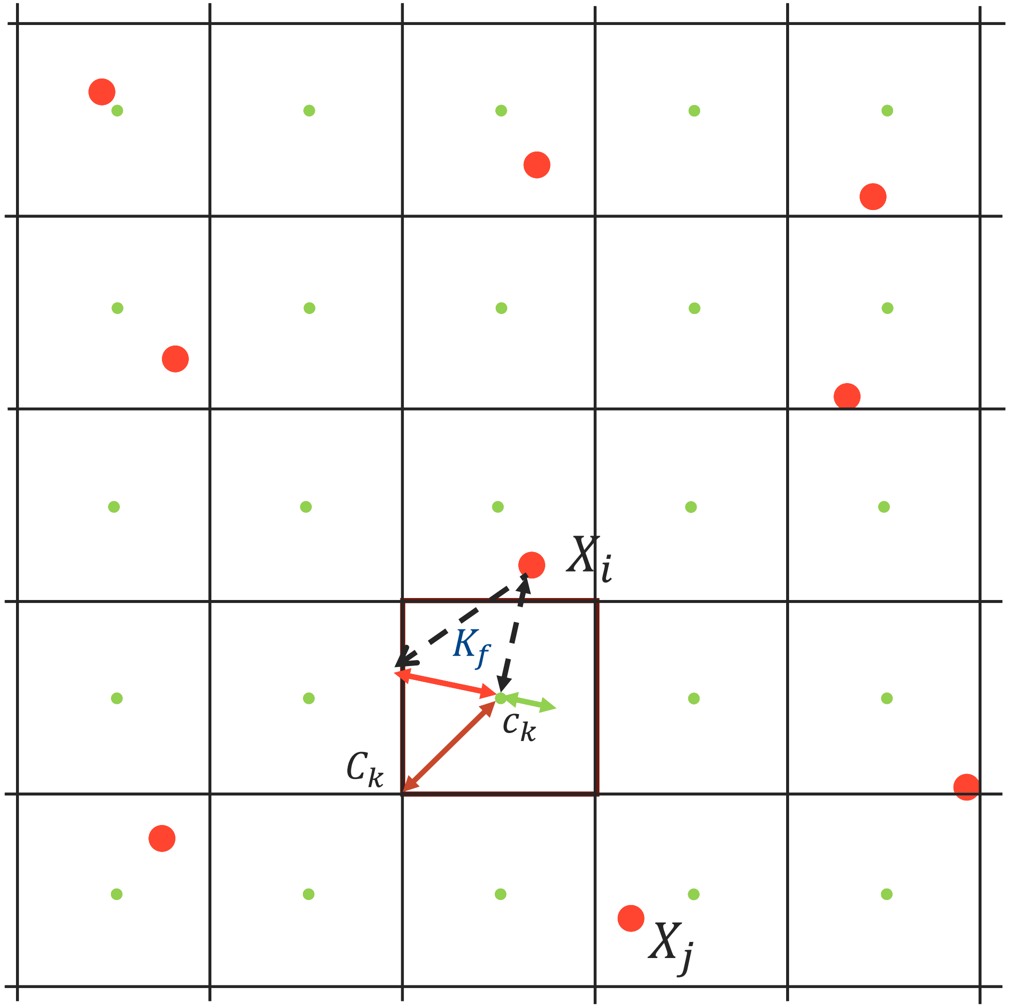

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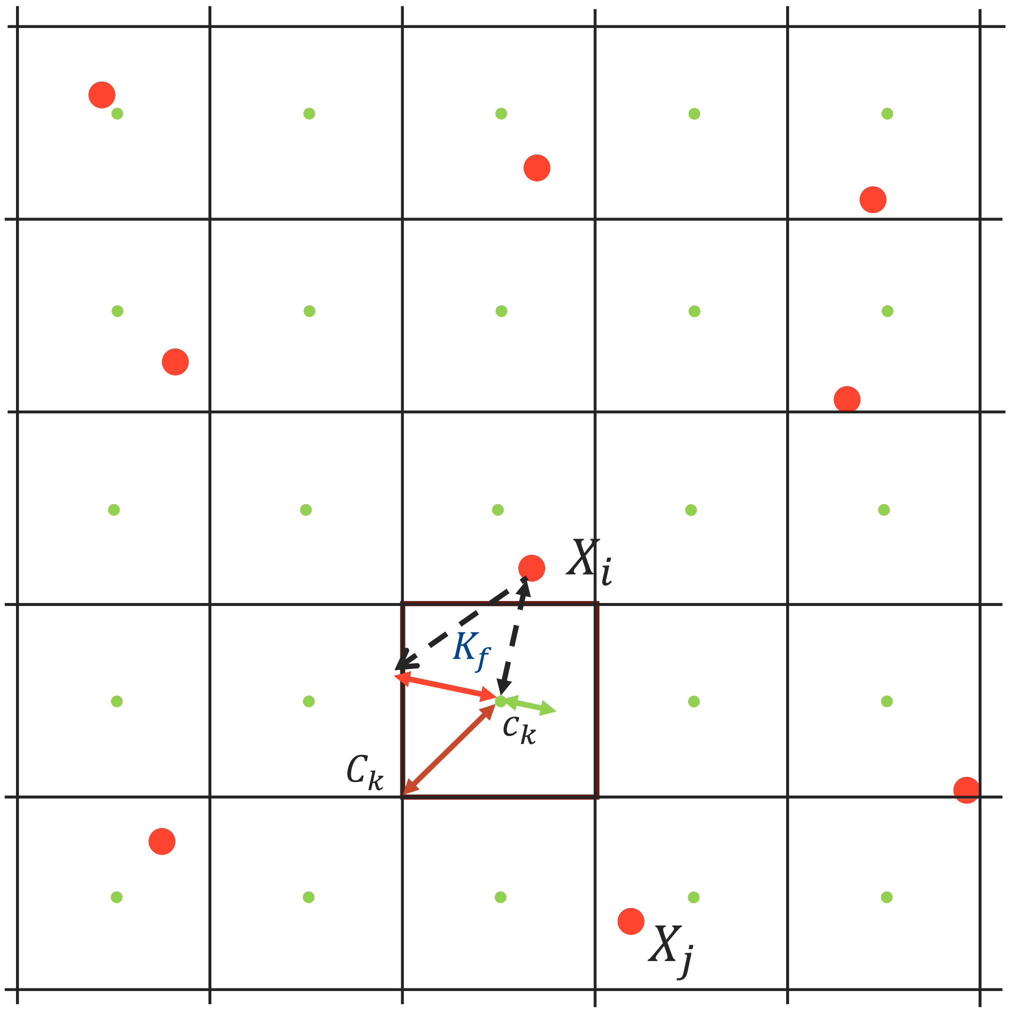
$\forall k \in \{1, \dots, p^2\}$,

$$|f(c_k) - g(c_k)| \le K_f \|c_k - X_i\| + |g(c_k) - f(X_i)|$$

Since we know that $\forall x \in C_k$,

$$|f(x) - g(x)| \le |f(c_k) - g(c_k)| + \frac{\sqrt{d}}{2p}(K_f + K_g)$$

Mapping to grid



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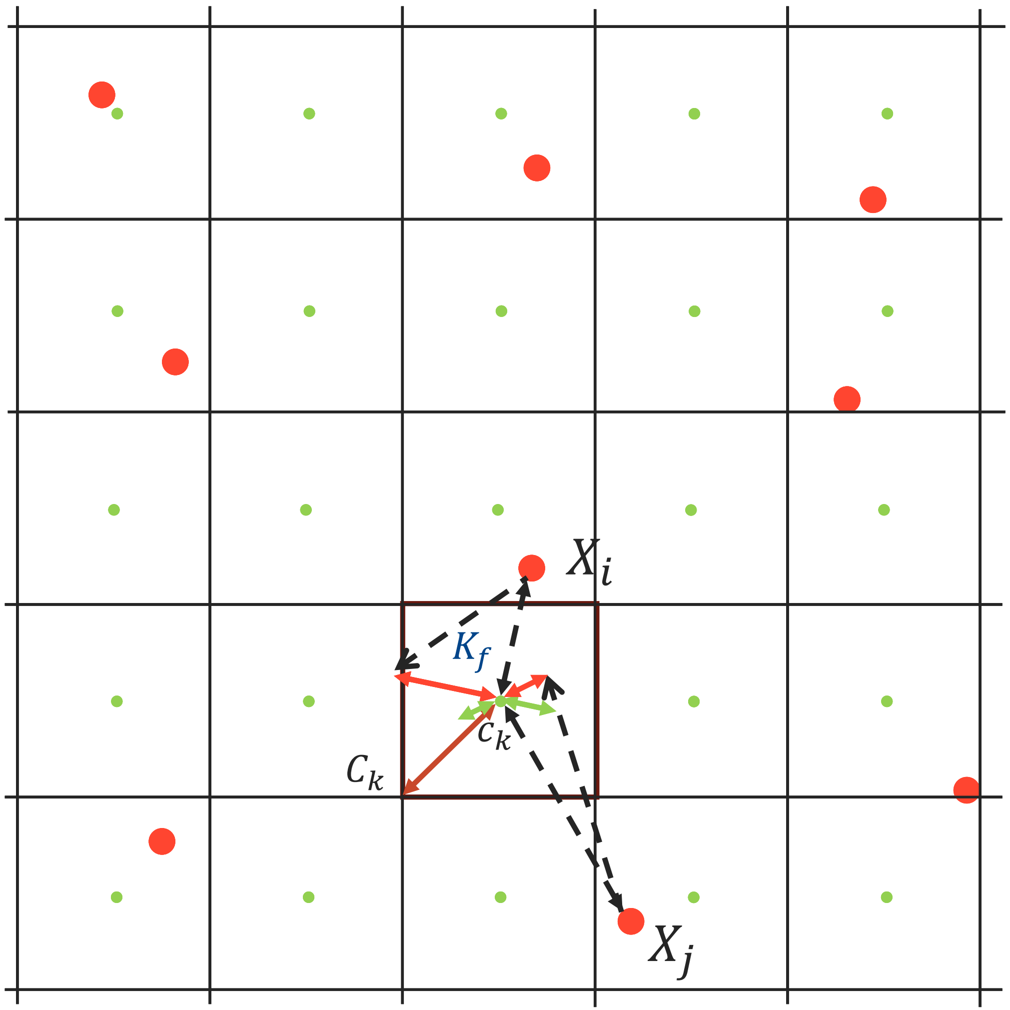
$\forall k \in \{1, \dots, p^2\}$,

$$|f(c_k) - g(c_k)| \leq K_f \|c_k - X_i\| + |g(c_k) - f(X_i)|$$

We have that $\forall x \in C_k$,

$$|f(x) - g(x)| \leq K_f \|c_k - X_i\| + |g(c_k) - f(X_i)| + \frac{\sqrt{d}}{2p}(K_f + K_g)$$

Mapping to grid



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$\forall k \in \{1, \dots, p^2\}$,

$$|f(c_k) - g(c_k)| \leq K_f \|c_k - X_i\| + |g(c_k) - f(X_i)|$$

We have that $\forall x \in C_k$,

$$|f(x) - g(x)| \leq \min_{i \in \{1,\dots,n\}} K_f \|c_k - X_i\| + |g(c_k) - f(X_i)| + \frac{\sqrt{d}}{2p}(K_f + K_g)$$

Mapping to grid

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$\forall x \in C_k,$

$$|f(x) - g(x)| \leq \underbrace{K_f \|c_k - X_i\|}_{\text{Requires calls to a nearest neighbor algorithm to find } N(c_k)} + \underbrace{|g(c_k) - f(X_i)|}_{\text{Requires evaluations of } g(c_k)\text{, which can be done in batch very efficiently}} + \underbrace{\frac{\sqrt{d}}{2p}(K_f + K_g)}_{\text{free}}$$

Requires calls to a nearest neighbor algorithm to find $N(c_k)$

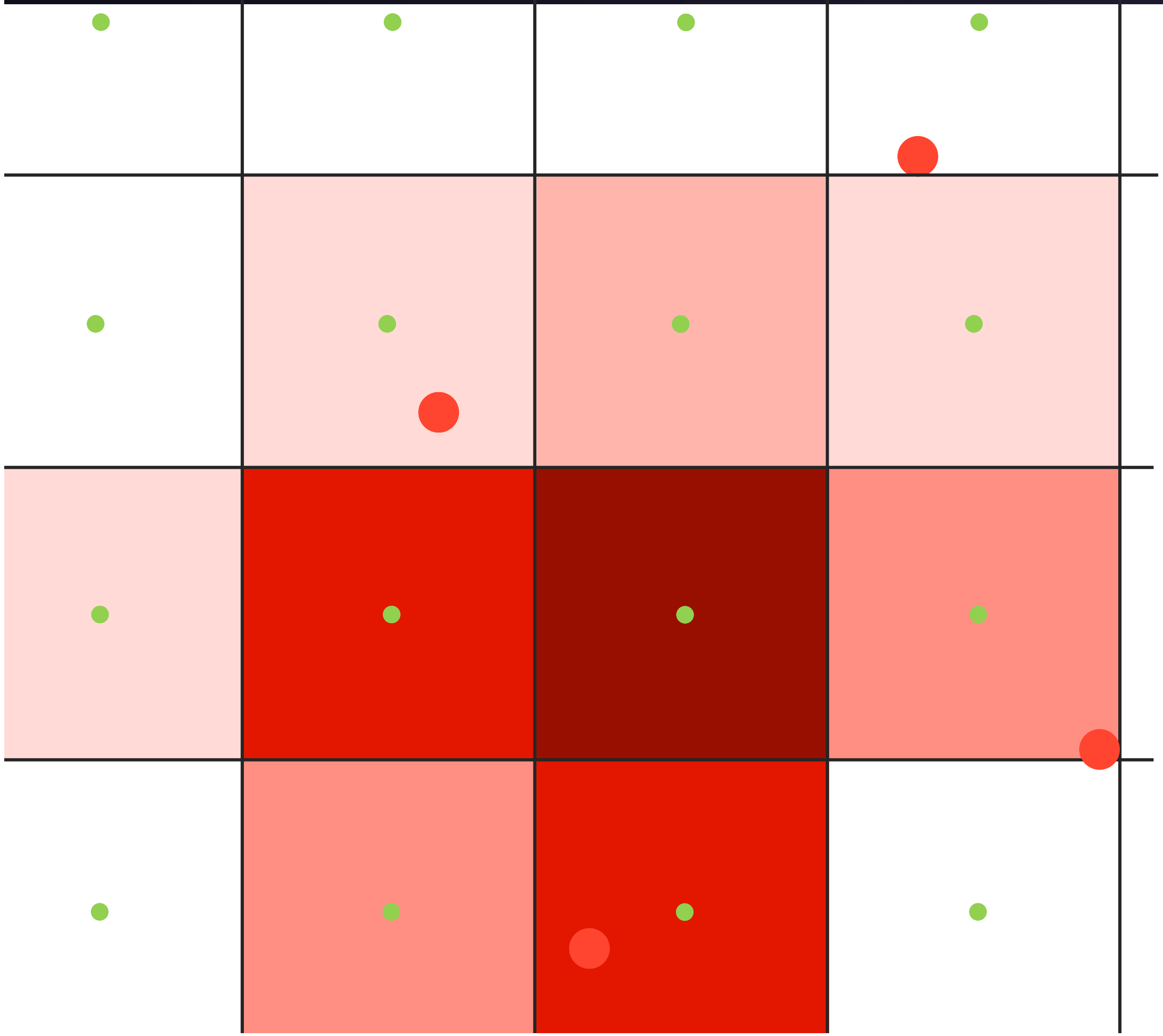
Requires evaluations of $g(c_k)$, which can be done in batch very efficiently

free

Computational efforts needed:

- Nearest neighbor algorithm
  - Many very efficient libraries (immensely cheaper than Voronoï diagram – complexity not exponential)
  - The bound is still valid with approximate nearest neighbors
- Evaluation of g
  - Very efficient on GPU

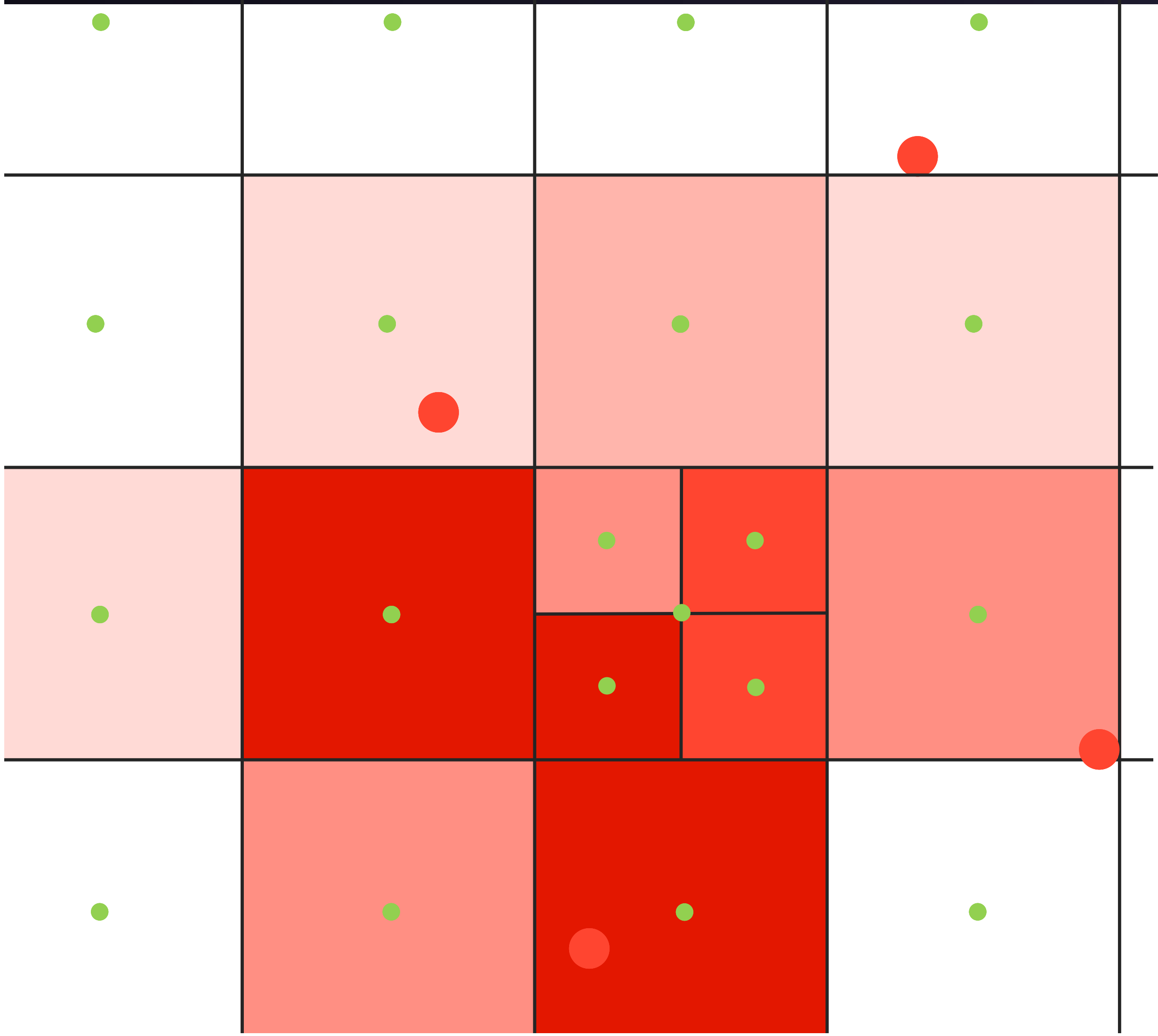
C-DOO



$\forall x \in C_k,$

$$|f(x) - g(x)| \leq \min_{i \in \{1,\dots,n\}} K_f \|c_k - X_i\| + |g(c_k) - f(X_i)| + \frac{\sqrt{d}}{2p}(K_f + K_g)$$

C-DOO



$\forall x \in C_k,$

$$|f(x) - g(x)| \leq \min_{i \in \{1,\ldots,n\}} K_f \|c_k - X_i\| + |g(c_k) - f(X_i)| + \frac{\sqrt{d}}{4p}(K_f + K_g)$$

Certified Deterministic Optimistic Optimization [14]

Split cells until convergence towards

$$\max_{x \in \mathcal{X}} \min_{i \in \{1,\ldots,n\}} K_f \|x - X_i\| + |g(x) - f(X_i)|$$

With a known certificate ϵ

Mapping to grid

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Certified Deterministic Optimistic Optimization [14]
Finds x^* and ϵ^* such that $\forall x \in \mathcal{X}$

$$\min_{i\in\{1,\ldots,n\}} K_f \|x - X_i\| + |g(x) - f(X_i)| \leq \epsilon^* + \min_{i\in\{1,\ldots,n\}} K_f \|x^* - X_i\| + |g(x^*) - f(X_i)|$$

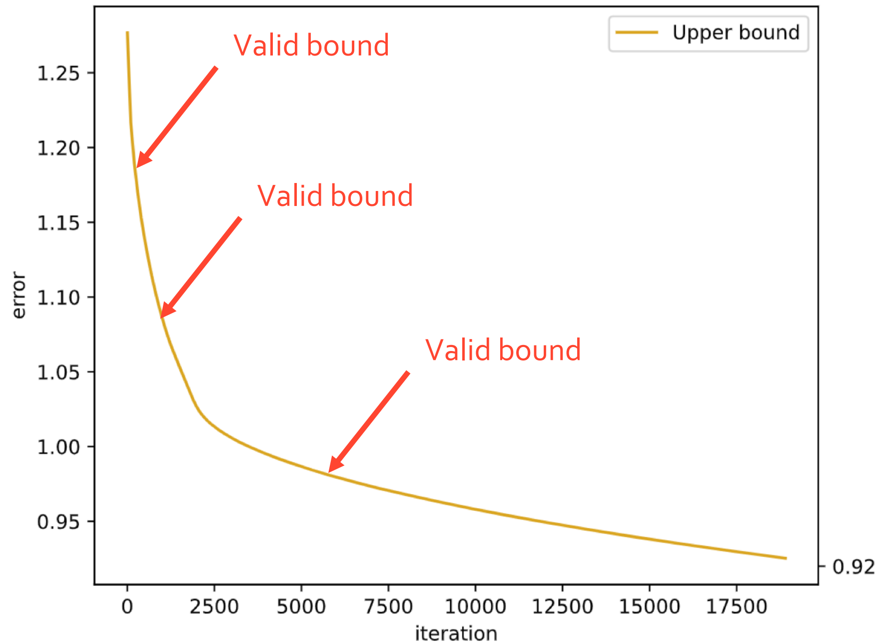
Hence, $\forall x \in \mathcal{X}$

$$|f(x) - g(x)| \leq \epsilon^* + \min_{i\in\{1,\ldots,n\}} K_f \|x^* - X_i\| + |g(x^*) - f(X_i)|$$

New bound !

Results on Heat Diffusion

	Classical Voronoï	Mixed random/mesh	C-DOO
Nb points used	20×10^3	$\mathbf{512\times10^4}$	$\mathbf{512\times10^4}$
Total eval time (sec.)	> 3000	$\mathbf{1.72}$	4,87 per iteration (see graph)
Max L_1 error (est.)	0.17	0.17	0.17
Upper bound	84	1.87	**0, 92**



Can be very long, but can stop anytime to obtain a bound

Beyond SciML: Braking Distance Estimation

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Braking Distance Estimation for plane landing

	C-DOO
Nb points used	$\mathbf{512 \times 10^4}$
Total eval time (sec.)	7.89
Max L_1 error (est. in meters)	763
Upper bound (in meters)	**1097**

In that case, fast convergence

The bound is not far from the worst error obtained in the training dataset with a Lipschitz neural network.
=> It is practically useful!

Takeaways - conclusions

We built algorithms to compute strict upper bound for $||f - g||_\infty$, where g is a Lipschitz neural net approximating for f. Can be very tight for low dimension.

- Voronoï based, **very costly** because of Voronoï diagram's **exponential complexity**.
- Can be made **way cheaper** by leveraging the **mesh structure** of some data dimensions.
- Can be **relaxed** by casting bounding into an optimization problem and using **C-DOO.**

Perspectives:

- The method is applicable to **any K-lip model** like Gaussian Processes [8] or Polynomial interpolation.
- The algorithms make it possible **to locate the error**, which could be useful for **active learning** (we could provably reduce the error bound) or **sequential optimization**.
- Goes well with the **Neural Implicit Representation** approach (including PINNs).
- **Hybridization** between ML and classical solvers
- The work will continue in ANITI's integrative programs:

DEEL (2) AI4SAVE

Check out "Accelerating hypersonic reentry simulations using deep learning-based hybridization (with guarantees)" Novello et al, Journal of Computational Physics!

Preprint version: available soon. Reach me out to know more and stay up to date.

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