DEEL
DEpendable & Explainable Learning

Towards instance-dependent approximation guarantees for scientific machine learning using Lipschitz neural networks

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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 ([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 strict 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 are so good as is…

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

Finding an uniform error bound for g

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

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

By finding bounds on

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

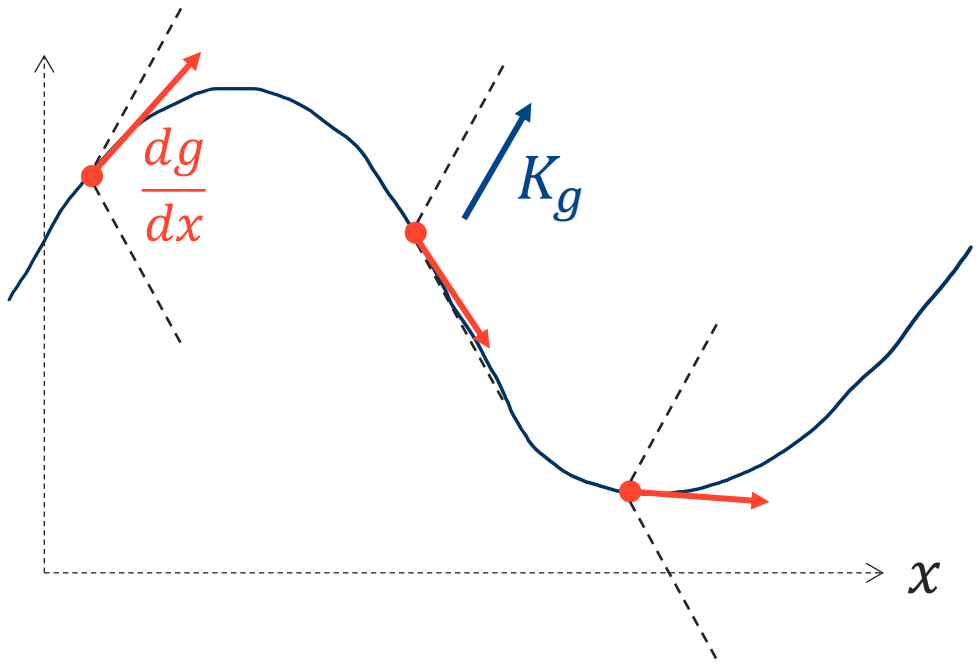
In the following, we try to bound $\|f - g\|_\infty$, the max. of the absolute error with a bound $\bar{J}_g$.
To that end, we will leverage the properties of Lipschitz neural networks

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

Lipschitz Neural Networks

Usual applications of Lipschitz neural networks:

- **Improved (and certified) robustness to adversarial attacks [11]**
- Better generalization for classification tasks [3]
- Better explainability [10]
- Perform well in Wasserstein distance estimation [3,11]

Original
(class: w/o)

Minimum adversarial perturbation
Classical neural net.
(class: w)

Minimum adversarial perturbation
Lipschitz neural net.
(class: w)

Adversarial perturbation on CelebA dataset
(binary classification of w vs w/o glasses

Lipschitz Neural Networks

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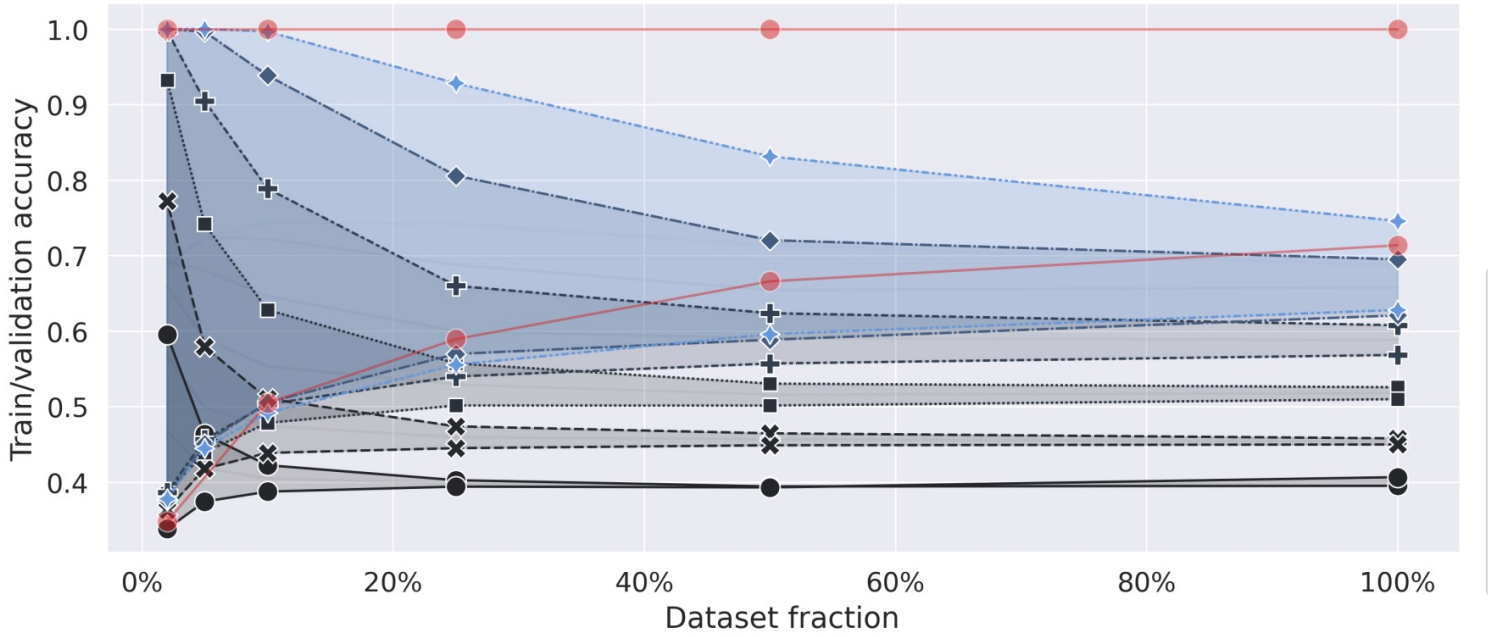

Generalization gap for Lipschitz NN with different K_g vs a classical neural network (in red)

Lipschitz Neural Networks

Usual applications of Lipschitz neural networks:

- Improved (and certified) robustness to adversarial attacks [11]
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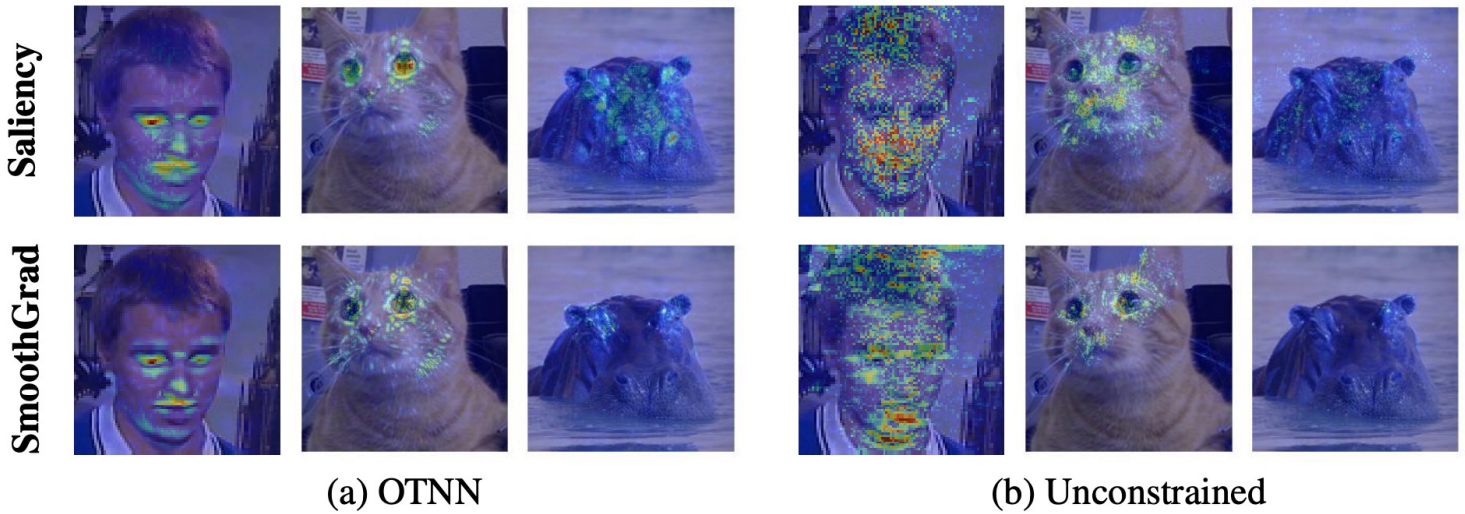
- **Better explainability [10]**
- Perform well in Wasserstein distance estimation [3,11]



Explanation maps for a Lipschitz network (OTNN) vs a classical network (Unconstrained)

Usual applications of Lipschitz neural networks:

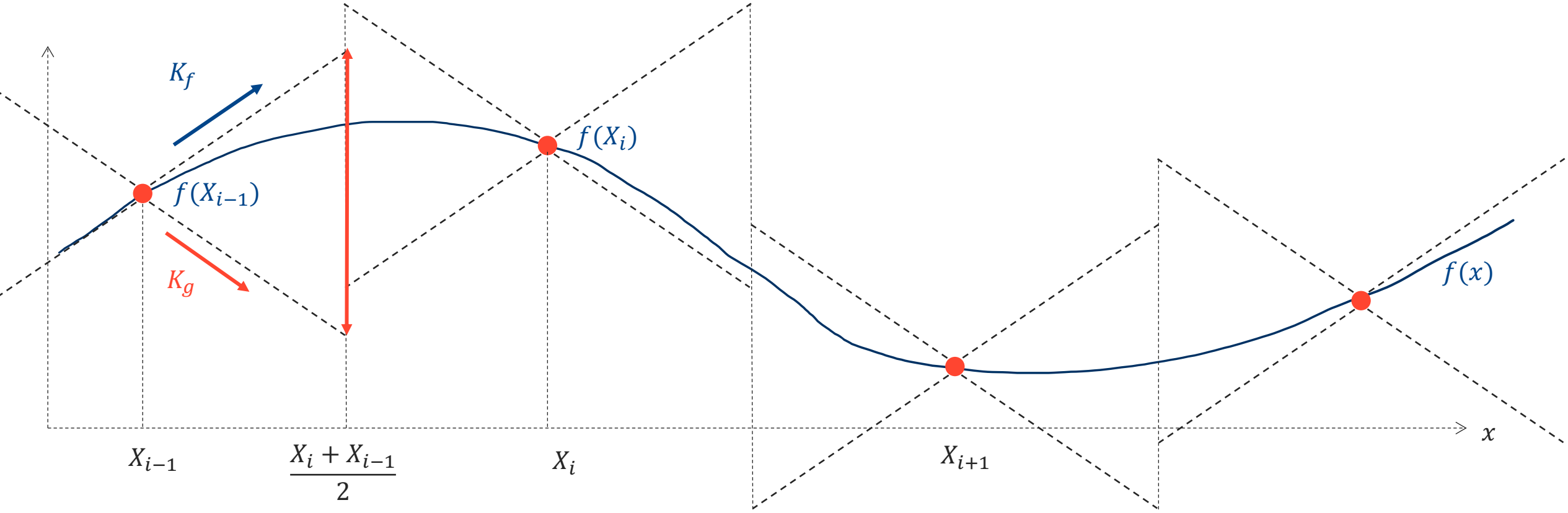
- Improved (and certified) robustness to adversarial attacks [11]
- Better generalization for classification tasks [3]
- Better explainability [10]
- **Perform well in Wasserstein distance estimation [3,11]**

Wasserstein-1 distance:

$$W_1(\mu,\eta) = \max_{f \in L_1} \int f(x) d(\mu - \eta)(x)$$

Can be found by approximating the set of 1-Lipschitz functions with 1-Lipschitz neural nets and perform the optimization

Motivation: Error bound in 1D

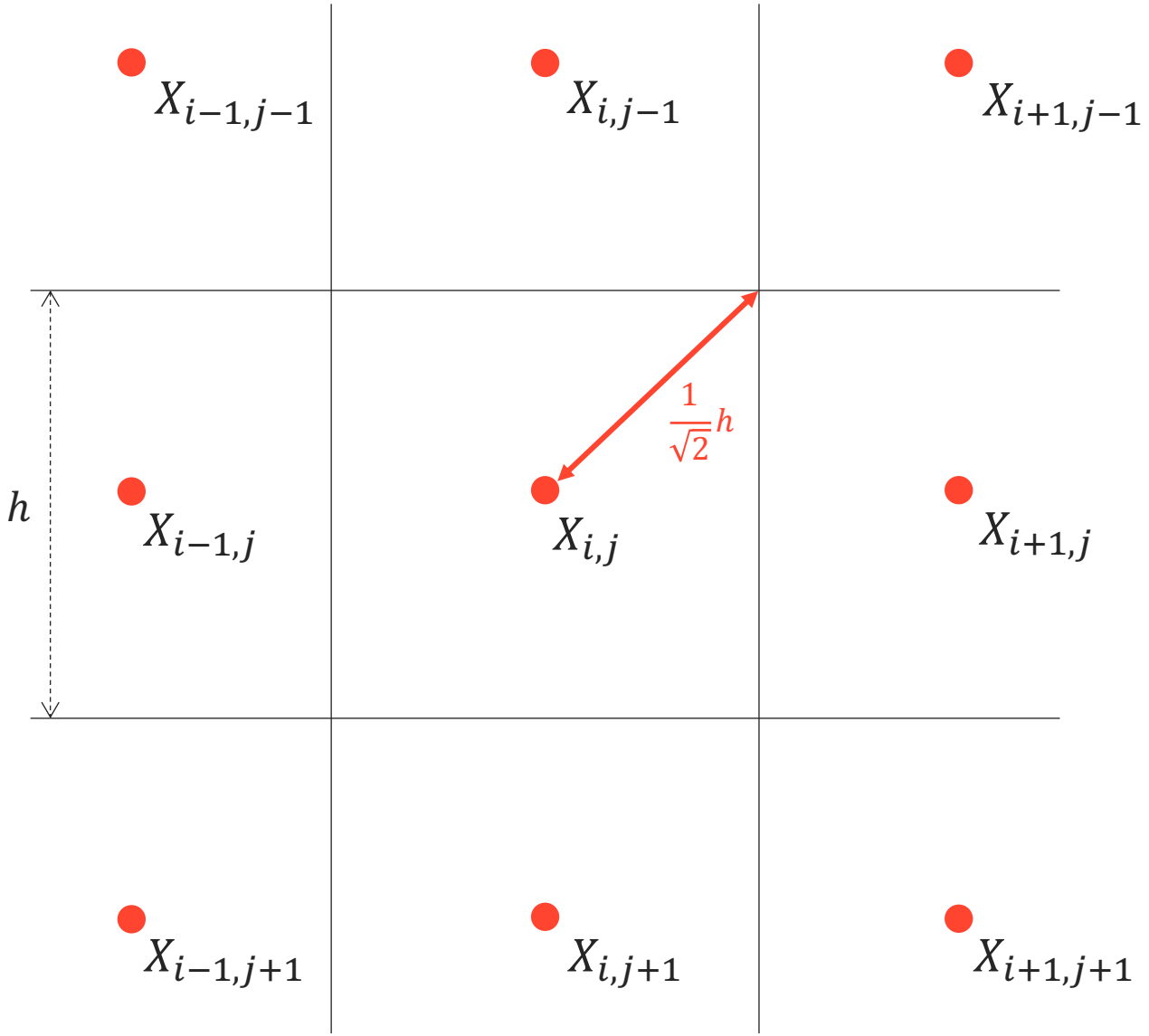


Take the difference between maximum variation of f and g on each subdivision:

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

$= 0$ in this example

Motivation: Error bound in 2D (and beyond)



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

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

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

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

Bound in ND ($d = N$):

In the k-th cell of center X_p:

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

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:

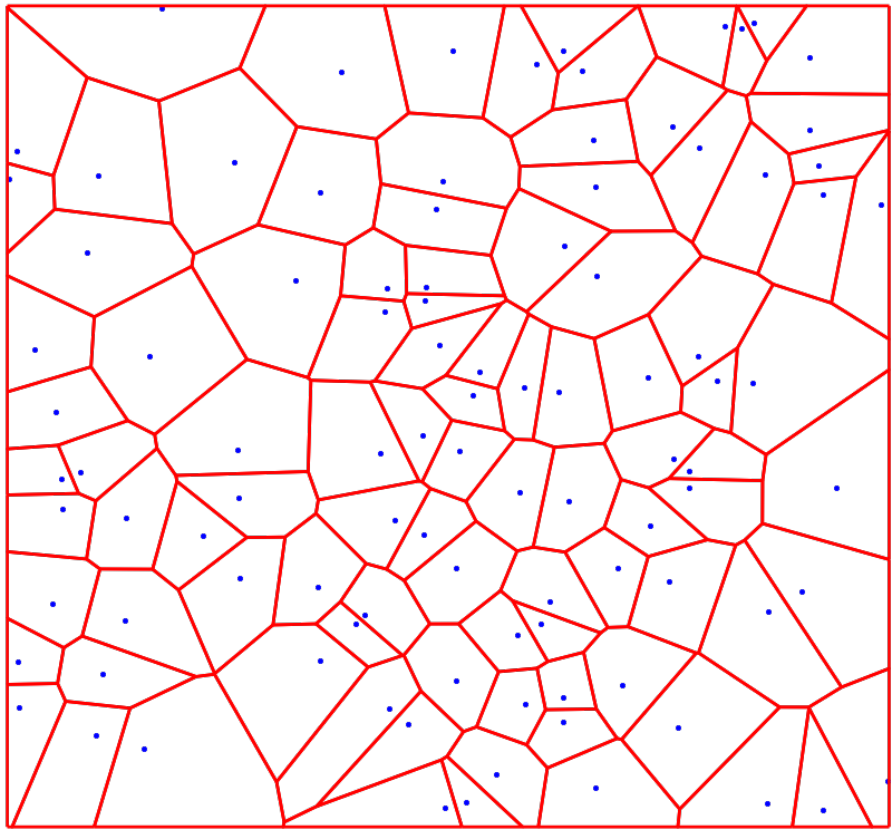
- The DOE should be defined in advance and we could not add points sequentially
- Grids suffer from the curse of dimensionality, the number of f evaluations would grow exponentially with d
- Monte Carlo is convenient

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

Outline

- Introduction
- **Error bound with Voronoï diagrams**
- Overcoming Voronoï diagrams complexity
- Conclusion & Takeaway

Definition of a Voronoï diagram (and some notations)



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

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

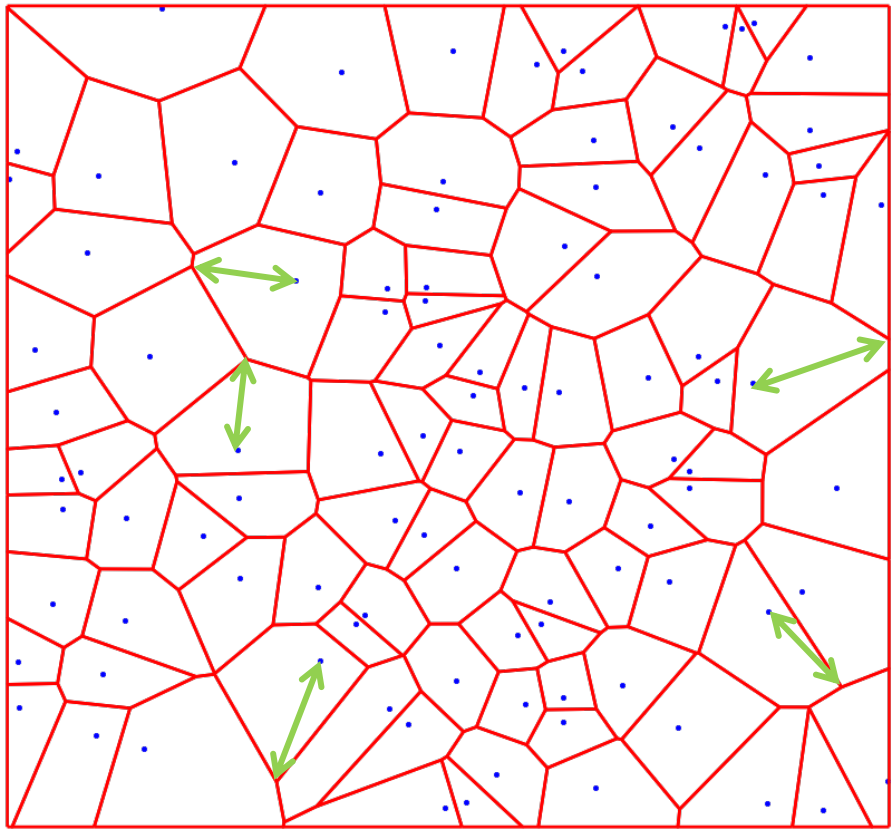
$$\mathcal{V}^d(X_i) = \{x \in \mathcal{X} | \forall j \in \{1, \dots, n\}, \|x - X_i\| \leq \|x - X_j\|\}$$

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

We have that $\mathcal{X} = \mathrm{U}_{i \in \{1,\dots,n\}} \mathcal{V}^d(X_i)$, 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



Let $N: x \to \underset{X_i \in \mathbf{X}}{argmin} \|x - X_i\|$ (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

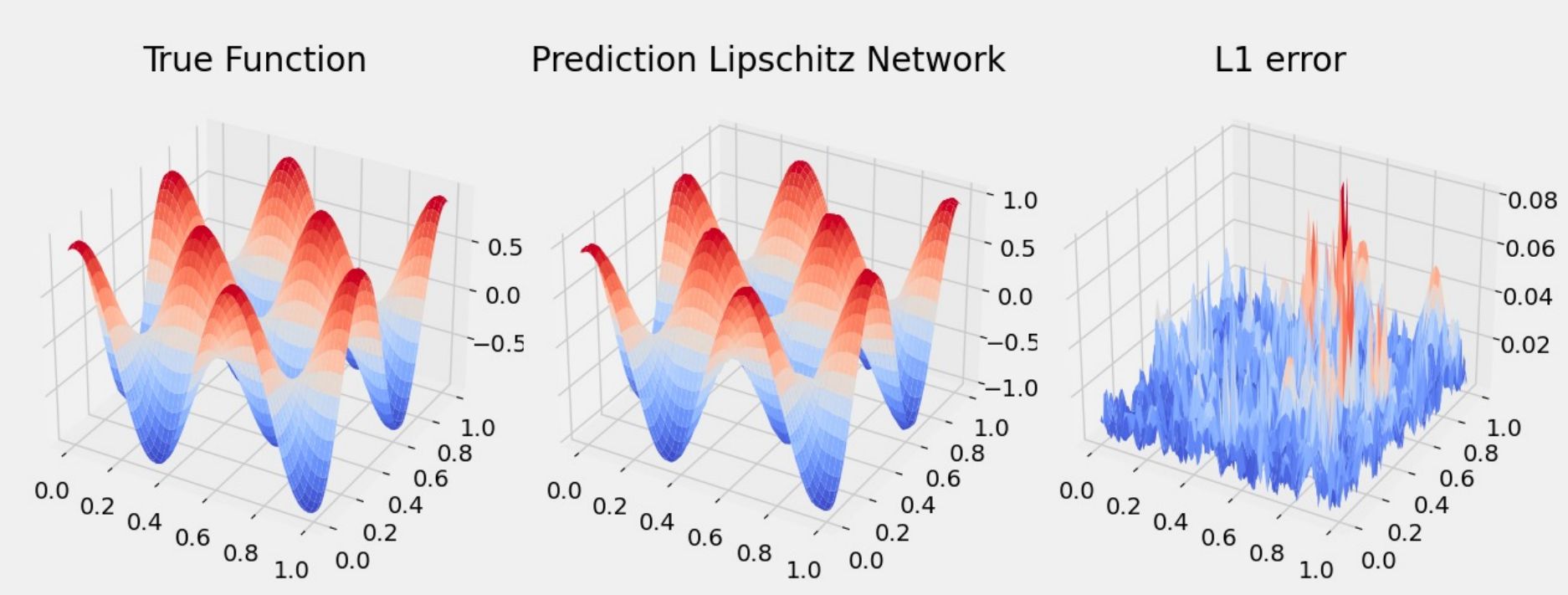
$$J_g^i \leq |f(X_i) - g(X_i)| + (K_f + K_g) r(X_i)$$

Hence,

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

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

Experiments on toy functions

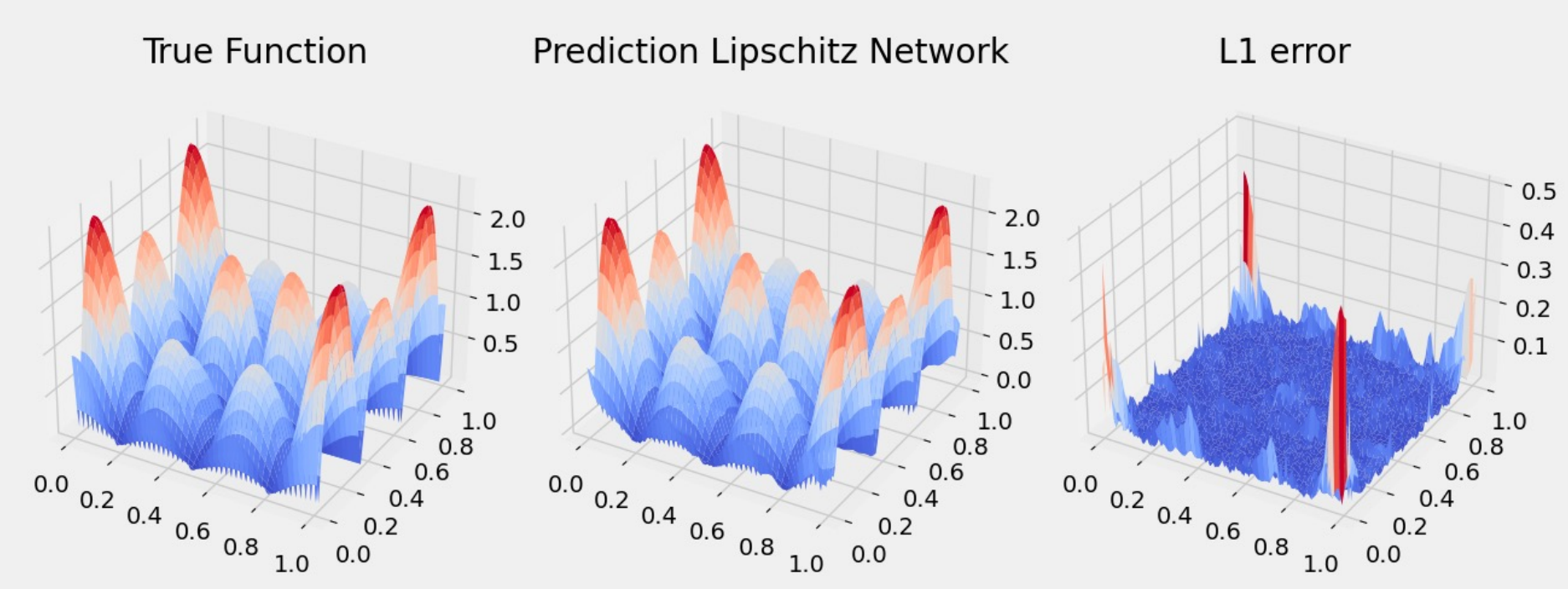


Sinus function

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

10000 training points

Experiments on toy functions



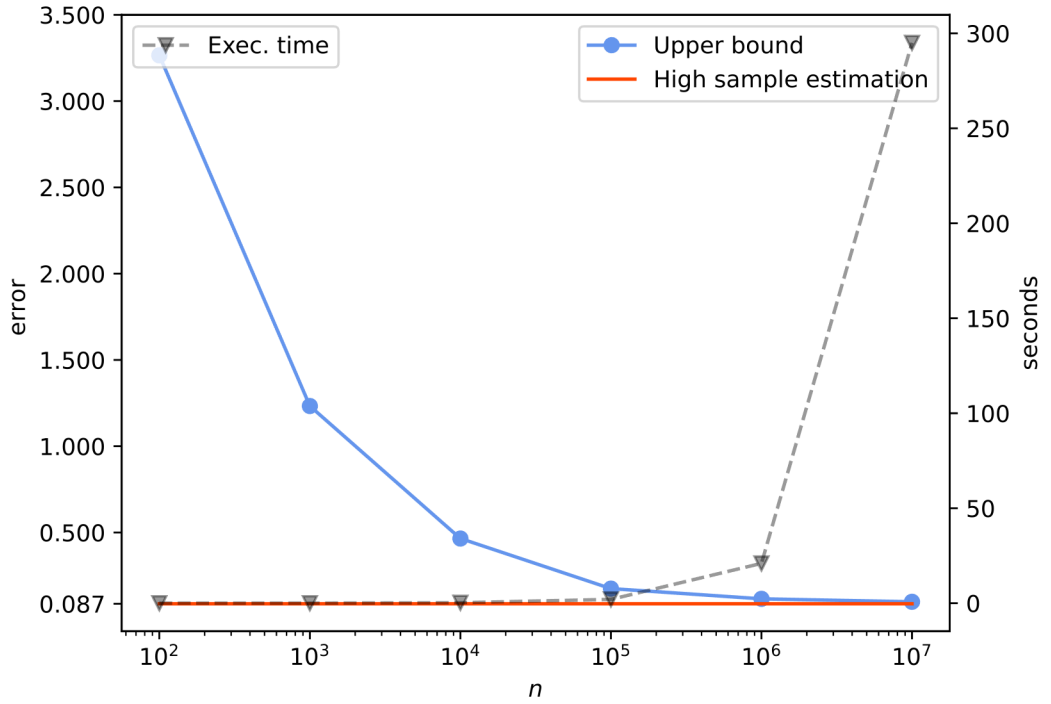
Holder table function

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

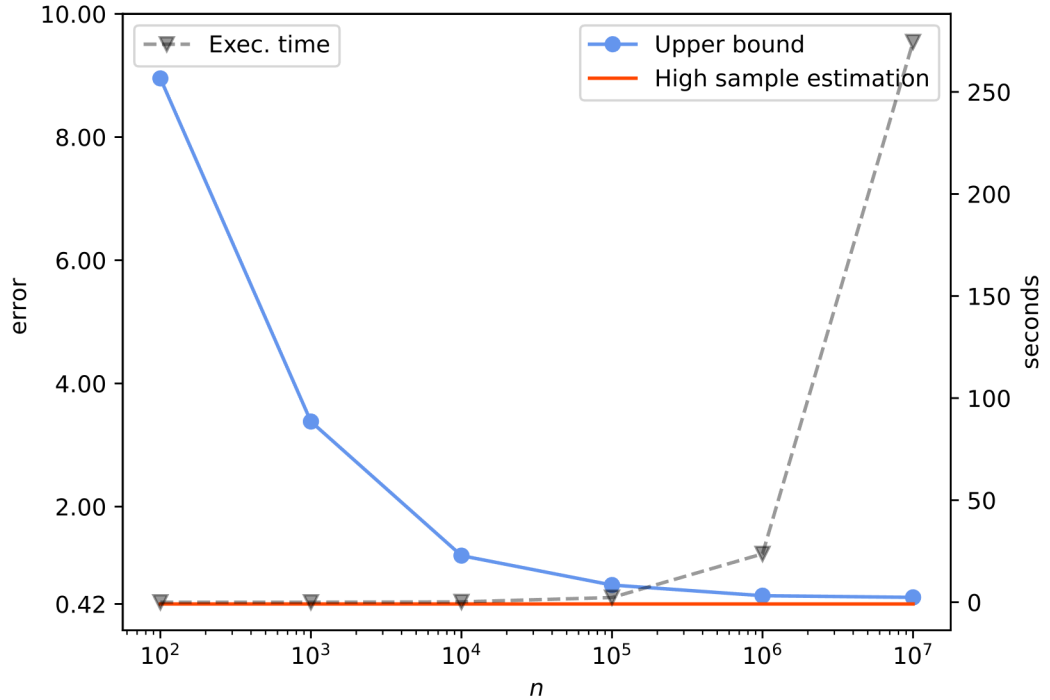
10000 training points

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?

Learning heat diffusion

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:

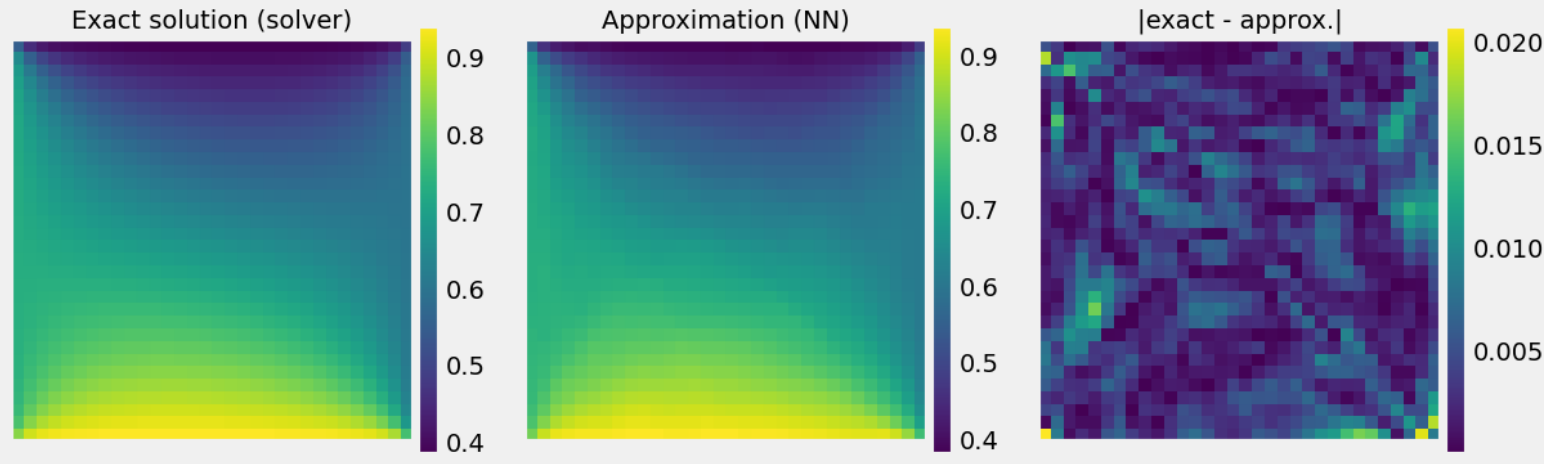
- Sample $n = 5000$ boundary conditions $\{(a_i, b_i, c_i, d_i)\}_{i\in\{1,\dots,n\}}$ uniformly on $[0,1]^4$.
- Conduct n simulations on a $p\times p$ grid ($p = 32$), yielding a temperature field $\{T_{jk}\}_{j,k\in\{1,\dots,p\}^2}$.

Training dataset:

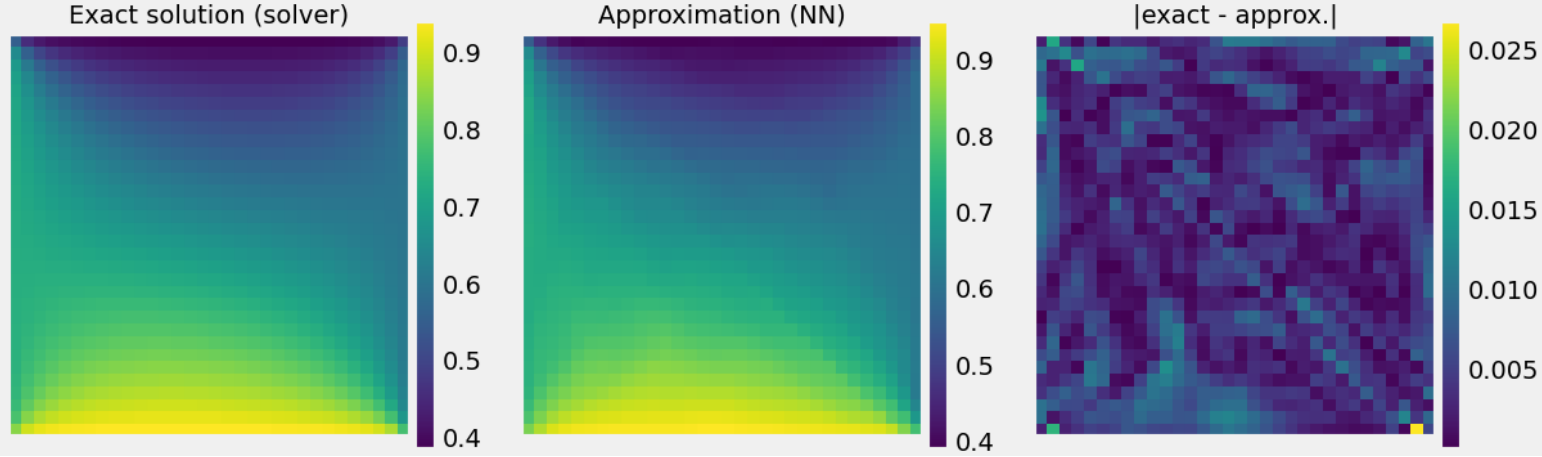
- A subset of $n\times p\times p/10 = 512{,}000$ points $\{(a_i, b_i, c_i, d_i, x_j, x_k), T_{j,k}\}_{i\in\{1,\dots,n\},j,k\in\{1,\dots,p\}^2}$

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:

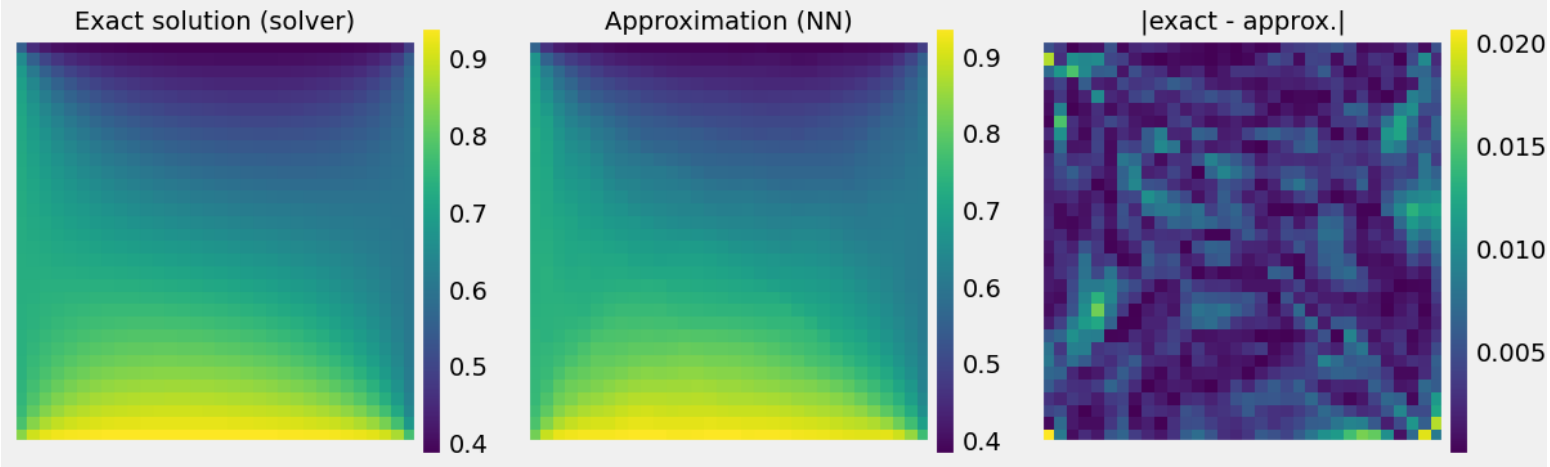
1. Empirical estimation of Lipschitz constant using:

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

   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_1 error: $\mathbf{0.17}$

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

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

Outline

- Introduction
- Error bound with Voronoï diagrams
- **Overcoming Voronoï diagrams complexity**
  - Mixed random and mesh datasets
  - Mapping to grid (for a tighter bound?)
- Conclusion & Takeaway

Mixed random and mesh datasets

Suppose that you have a set of points $\mathbf{X}^d = \{X_1^d, \dots, X_n^d\}$ uniformly sampled on a domain $[0,1]^d$.

Now consider a set of points $\{x_1, \dots, x_p\}$ evenly spaced on $[0,1]$.

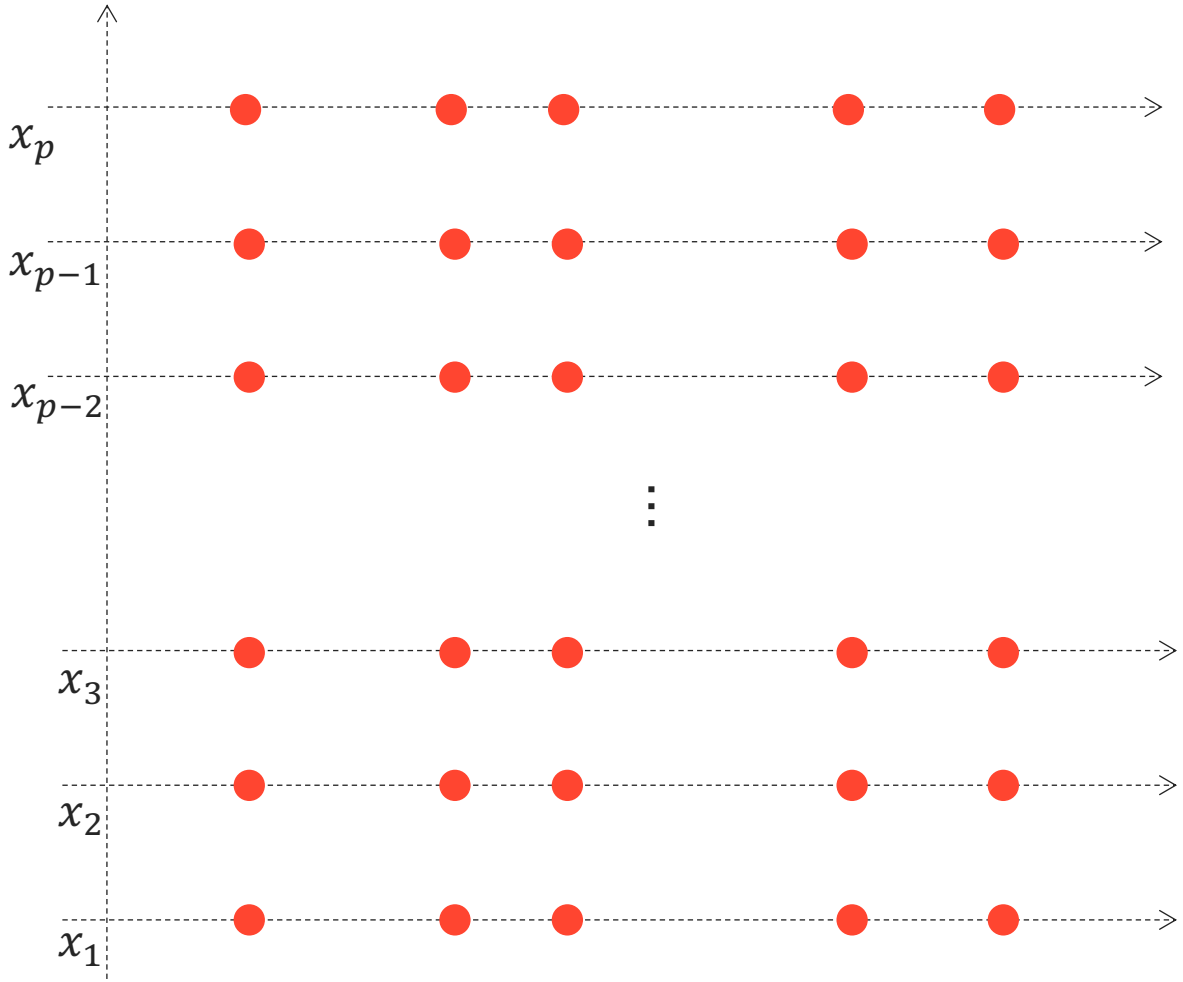
Then define the set of points

$$\mathbf{X}^{d+1} = \{X_{i,j}^{d+1}\}_{i \in \{1,\dots,n\}, j \in \{1,\dots,p\}}$$

such that

$$X_{i,j}^{d+1} = \left((X_i^d)_1, \dots, (X_i^d)_d, x_j \right),$$

where $X_i^d = \left((X_i^d)_1, \dots, (X_i^d)_d \right)$



Here, $d = 1$

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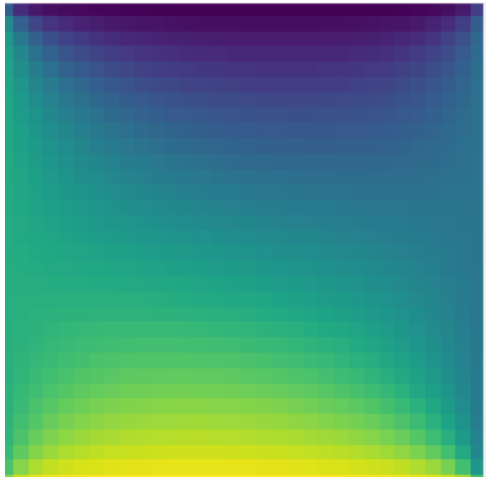
Example: numerical simulation



- Sample n different boundary conditions uniformly $\{\partial b_1, \dots, \partial b_n\}$
- compute the n simulations on a mesh of size $p\times p$

➢ $n\times p\times p$ learning points $\{(x_i, y_j, \partial b_k)\}_i$

mesh random unif

Mixed random and mesh datasets

Define the set of points

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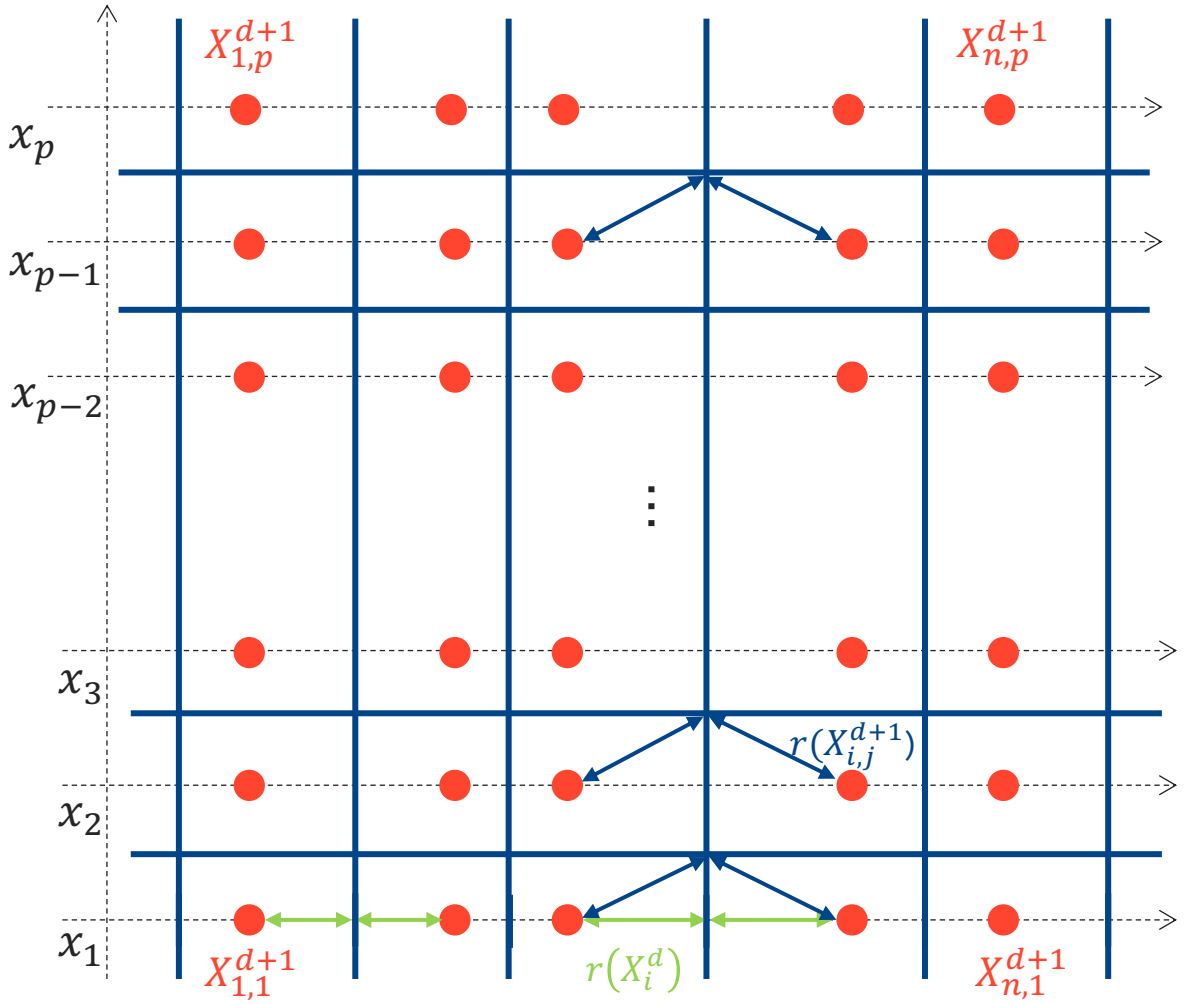
such that

$$X_{i,j}^{d+1} = \left(\left(X_i^d\right)_1, \dots, \left(X_i^d\right)_d, x_j\right),$$

Now, consider $\mathcal{V}^d$ the Voronoï diagram of $\{X_1^d, \dots, X_n^d\}$ and $r(X_i^d)$ the radius of $\mathcal{V}^d(\mathrm{X_i^d})$.

Then: $\forall i \in \{1, \dots, n\}, \forall j, k \in \{1, \dots, p\}^2$,

$$r(X_{i,j}^{d+1}) = r(X_{i,k}^{d+1}) = \sqrt{\frac{1}{4p^2} + r\left(X_i^d\right)^2}$$



Mixed random and mesh datasets

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In that case, we only need to compute the Voronoï diagram $\mathcal{V}^d$ for $\{X_i^d\}_{i\in\{1,\dots,n\}}$ to obtain $r(X_{i,j}^{d+1})$ and compute the bound!

Practical consequences:

- Compute a Voronoï diagram in dimension $d+1$ with $\mathrm{n}\times p$ points

Becomes

- Compute a Voronoï diagram in dimension d with n points

Mixed random and mesh datasets

Define the set of points

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Practical consequences:

Recursivity: For a 2D Grid

- Compute a Voronoï diagram in dimension $d+2$ with $\mathrm{n}\times p\times p$

Becomes

- Compute a Voronoï diagram in dimension d with n points

Mixed random and mesh datasets

Define the set of points

$$\mathbf{X}^{d+1} = \{X_{i,j}^{d+1}\}_{i\in\{1,\dots,n\},j\in\{1,\dots,p\}}$$

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In that case, we only need to compute the Voronoï diagram $\mathcal{V}^d$ for $\{X_i^d\}_{i\in\{1,\dots,n\}}$ to obtain $r(X_{i,j}^{d+1})$ and compute the bound!

Practical consequences:

Recursivity: For a 3D Grid

- Compute a Voronoï diagram in dimension $d+3$ with $\mathrm{n}\times p\times p\times p$

Becomes

- Compute a Voronoï diagram in dimension d with n points

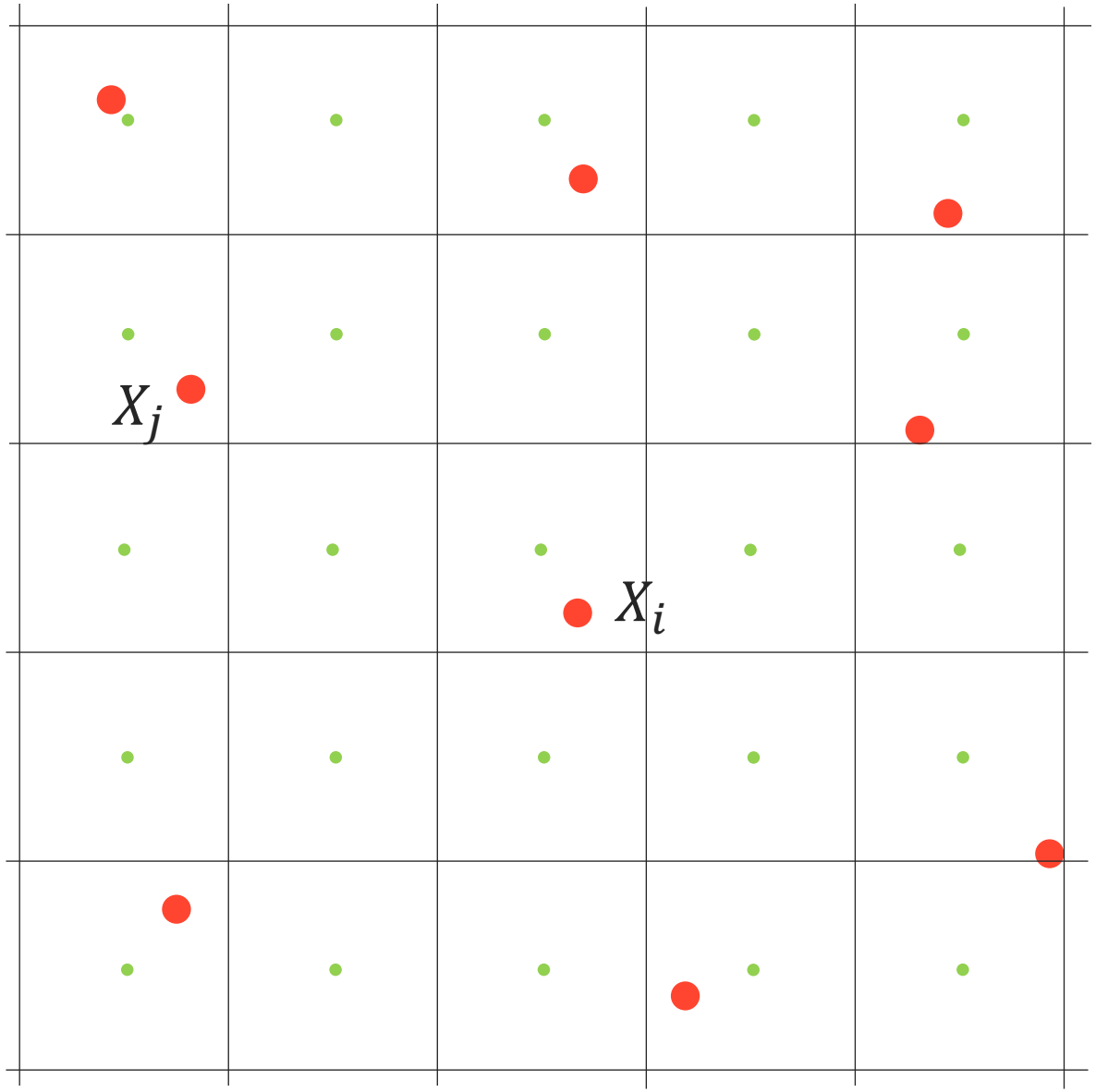
Results on Heat Diffusion

	Classical Voronoï	Mixed random/mesh
Nb points used	20×10^3	$\mathbf{512\times10^4}$
Total eval time (sec.)	> 3000	$\mathbf{1.72}$
Max L_1 error (est.)	0.1716	0.1716
Upper bound	84	$\mathbf{1.6320}$

Results of the different methods for computing $\bar{J}_g$

What if we cannot leverage a mixed grid-random dataset structure?

Mapping to grid



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

By **lemma 1**, $\forall x \in [0,1]^d$,

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

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

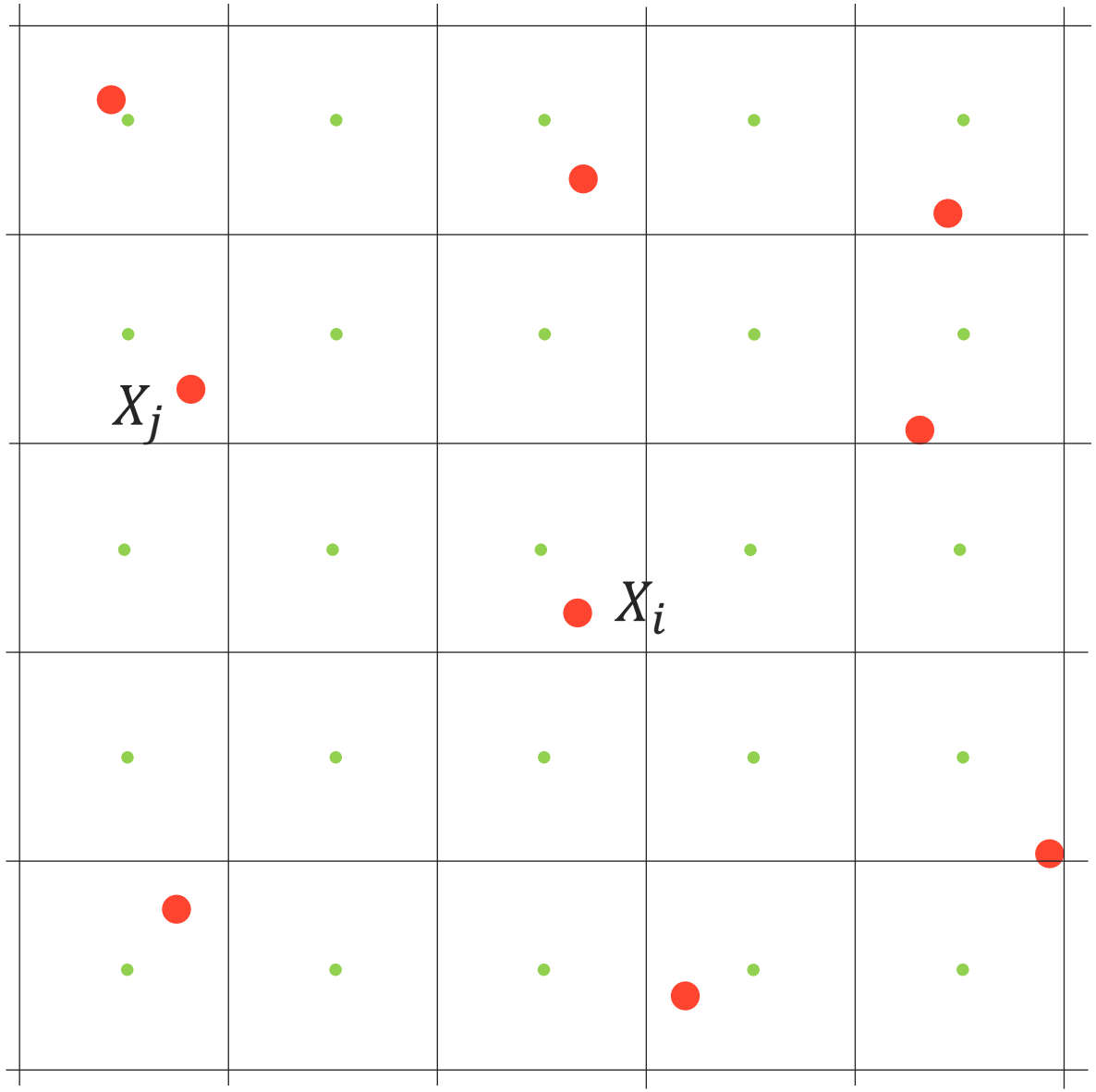
$\forall x \in [0,1]^d$,

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

Lemma 2

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

Mapping to grid

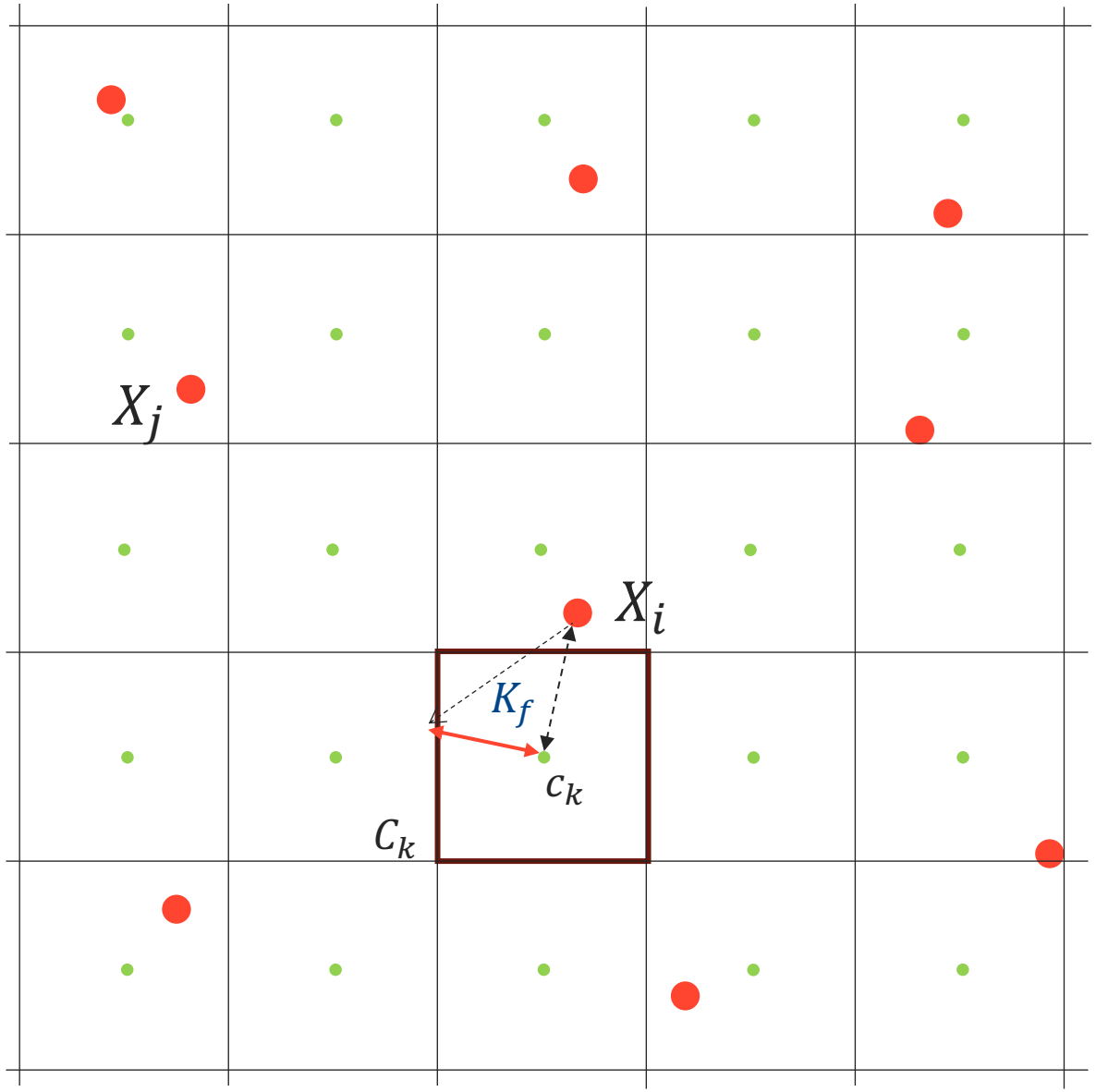


Now, consider a grid of p^d cells $\{C_1, \dots, C_{p^d}\}$ with centers $\{c_1, \dots, c_{p^d}\}$

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

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

Mapping to grid



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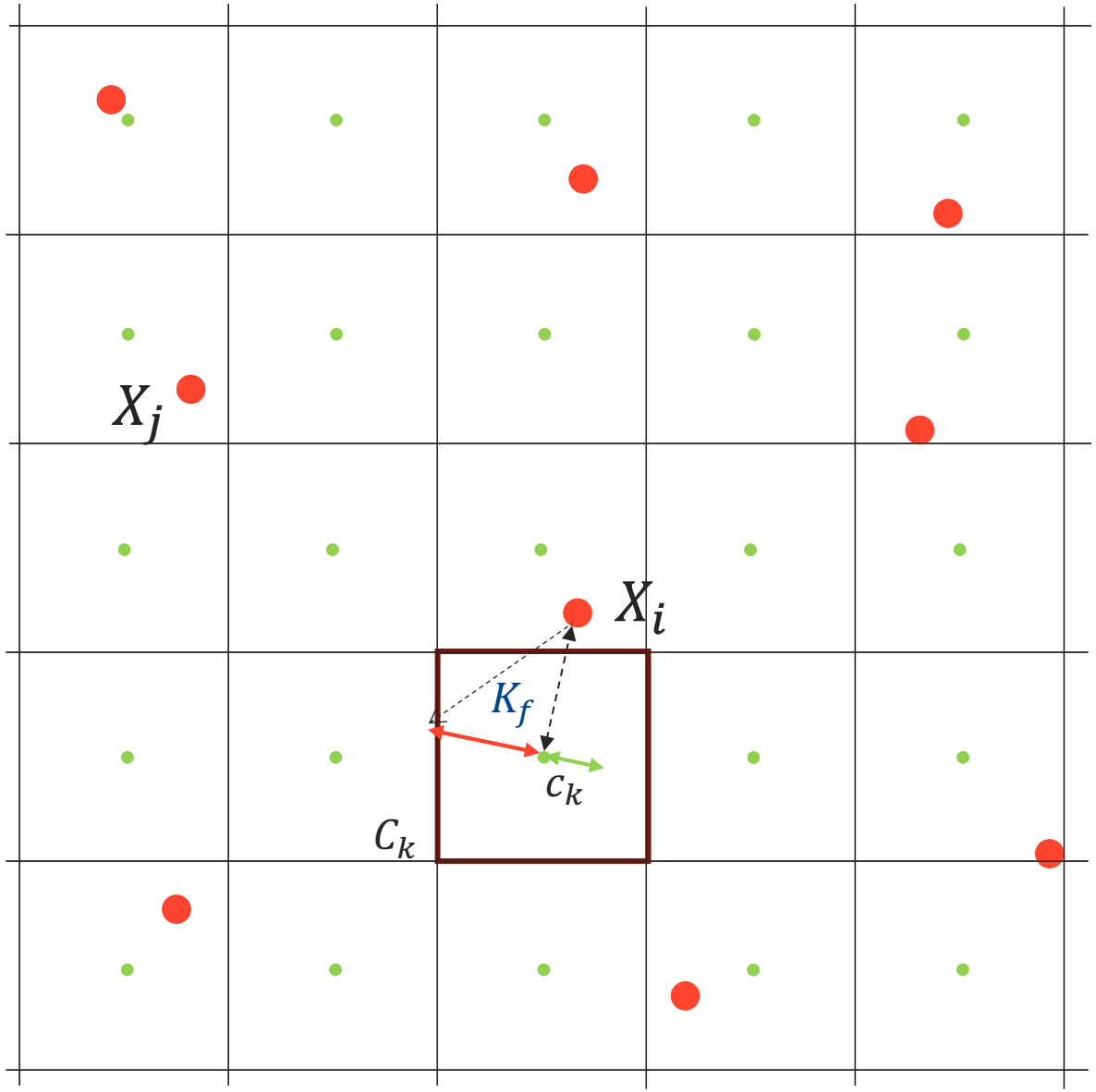

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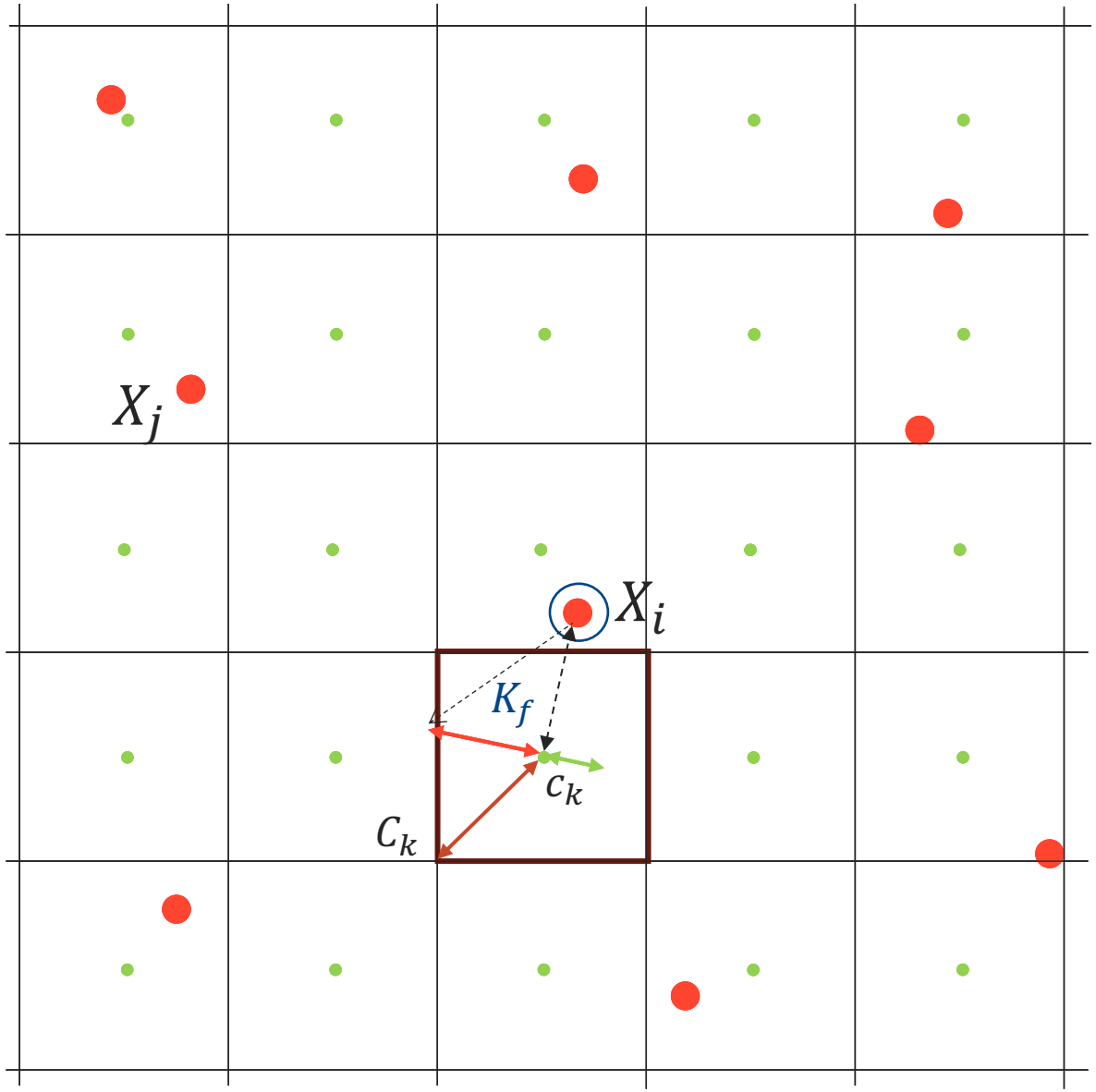

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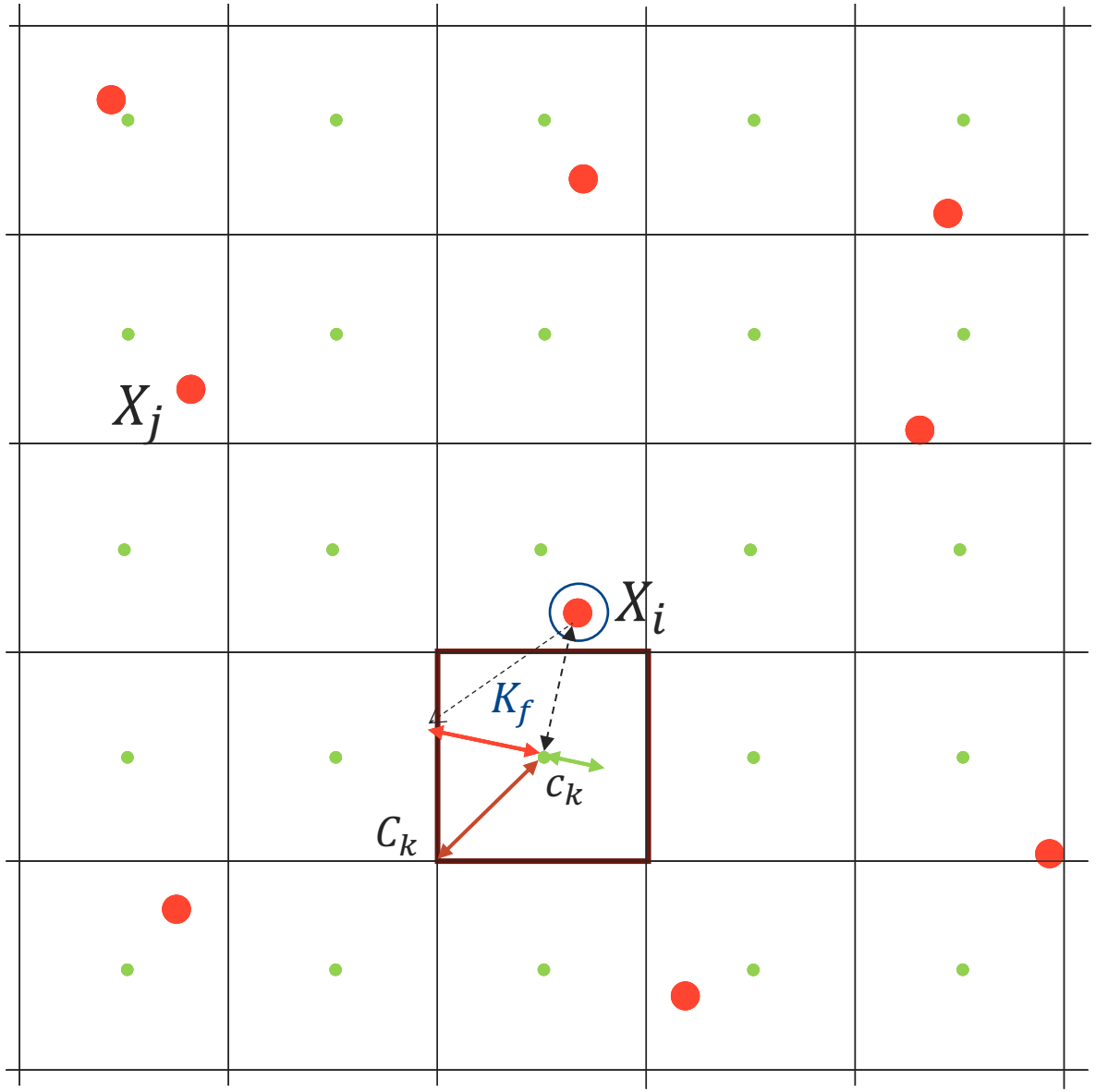
Since we know that $\forall x \in C_k$,

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

Mapping to grid



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

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

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

Mapping to grid

$\forall x \in C_k,$

$$|f(x) - g(x)| \leq \underbrace{K_f \|c_k - N(c_k)\|}_{\text{Requires calls to a nearest neighbor algorithm to find } N(c_k)} + \underbrace{|g(c_k) - g(N(c_k))|}_{\text{Requires evaluations of } g(c_k), \text{ which can be done in batch very efficiently}} + \underbrace{|f(N(c_k)) - g(N(c_k))|}_{\text{By definition, } N(c_k) \in \mathbf{X}. \text{ Error at each dataset point. Always evaluated for classical validation}} + \underbrace{\frac{\sqrt{d}}{2p}(K_f + K_g)}_{\text{free}}$$

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

Mapping to grid

$\forall x \in C_k$,

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

Computational efforts needed:

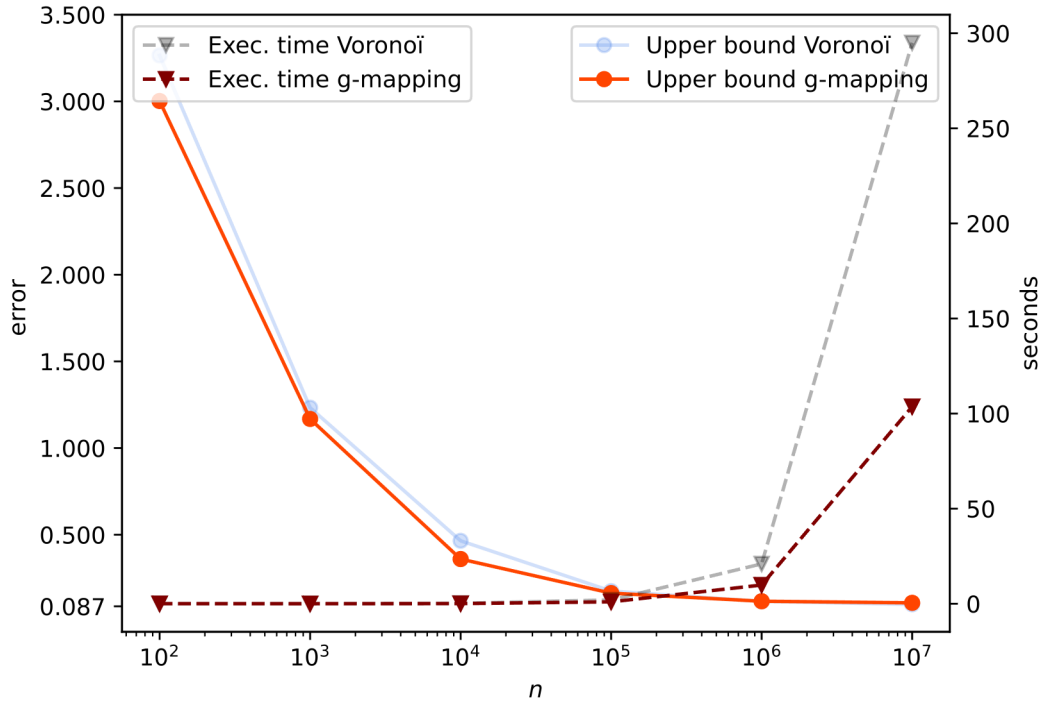
- Nearest neighbor algorithm
  - Many very efficient libraries (immensely cheaper than Voronoï diagram – complexity not exponential)
  - The bound is still valid with approximate nearest neighbors
- Evaluation of g
  - Very efficient on GPU

Beneficial side effect:

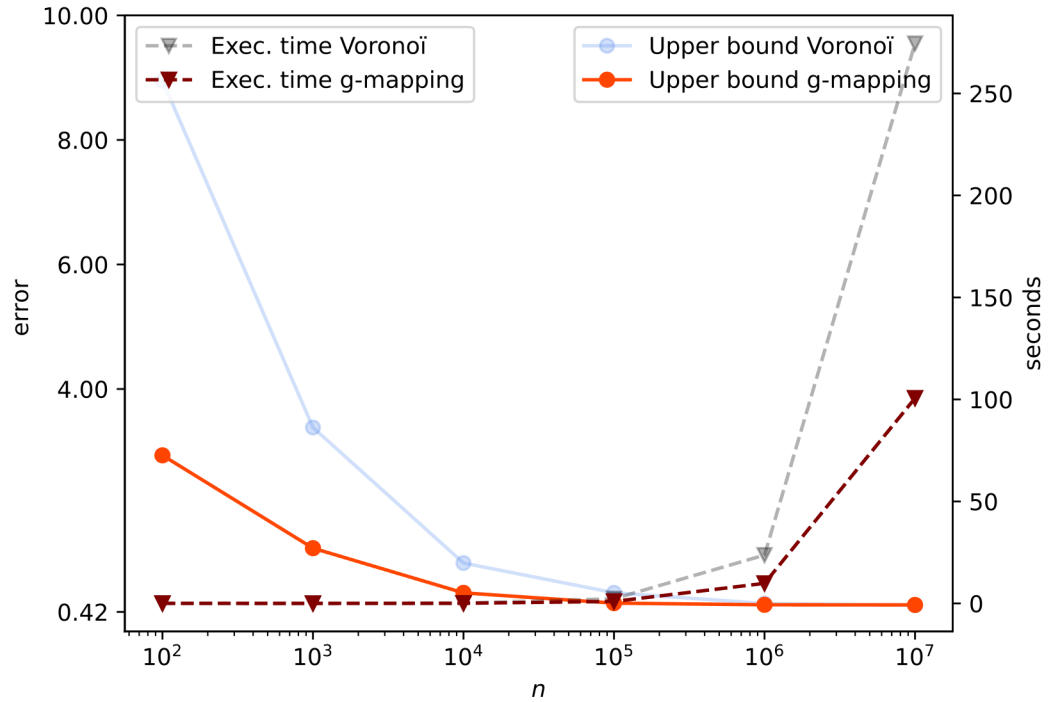
We were able to replace $K_g \|c_k - N(c_k)\|$ with $|g(c_k) - g(N(c_k))|$, which can make the bound tighter since by definition, $|g(c_k) - g(N(c_k))| \leq K_g \|c_k - N(c_k)\|$

Results on Toy functions

Upper bound of L_∞ error with computation time for Sinus function (left) and Holder table function (right).
The grid used is of size 1000×1000.



Best upper bound (Voronoï): 0.098
Best upper bound (grid mapping): 0.107
High sample estimation: 0.087



Best upper bound (Voronoï): 0.53
Best upper bound (grid mapping): 0.53
High sample estimation: 0.42

Results on Heat Diffusion

	Classical Voronoï	Mixed random/mesh	Grid mapping	Grid mapping
Nb points used	20×10^3	$\mathbf{512\times10^4}$	512×10^3	$\mathbf{512\times10^4}$
Total eval time (sec.)	> 3000	$\mathbf{1.72}$	$37 + 80$	$385 + 80$
Max L_1 error (est.)	0.1716	0.1716	0.1716	0.1716
Upper bound	84	1.6320	1.3014	$\mathbf{1.1953}$

Results of the different methods for computing $\bar{J}_g$ ($+80$ is the time for net predictions on the grid)

For Approx. Voronoï, we used a grid of size $p = 14$

- Computed nearest neighbors for 7,529,536 points
- Used faiss[1] library on GPU

1 https://github.com/facebookresearch/faiss

Takeaways - conclusions

We built algorithms to compute strict uniform upper bounds 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 building a **grid** and bounding each center's error.

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**.
- Estimation of K_f:
  - build **local estimators** to refine the bound, possibly using interpolators [8].
  - Could we find K_f by using underlying **PDEs knowledge** [4]?
- Goes well with the **Neural Implicit Representation** approach. Could be paired with **neural operator** learning by low dimension parametrization of boundary conditions/initialization.
- **Hybridization** between ML and classical solvers

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

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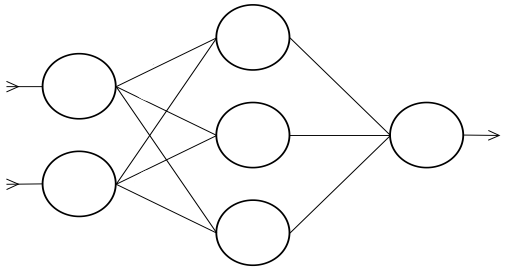
Construction of 1-Lipschitz neural networks

Classical fully connected neural network:



Construction of 1-Lipschitz neural networks

Classical fully connected neural network:

$$\begin{cases} g(x) = g_l \circ g_{l-1} \circ \cdots \circ g_1(x) \\ g_k(x) = \sigma_k(W_k \cdot x + b_k) \end{cases}$$

with (for layer k):

- Activation function σ_k
- Weights matrix W_k
- Bias vector b_k

How to make it 1-Lipschitz ?

- Ensure that **each g_k is 1-Lipschitz**
  - ✓ Most activation functions are 1-Lipschitz
  - ✓ Bias is a simple shift
  - ✓ What about the weights ?

The naïve way:

During training, set $\boldsymbol{W_k \leftarrow \frac{W_k}{\|W_k\|}}$, where $\|W_k\|$ is the spectral norm of W_k.

Construction of 1-Lipschitz neural networks

DEEL

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During training, set $\boldsymbol{W_k \leftarrow \frac{W_k}{\|W_k\|}}$, where $\|W_k\|$ is the spectral norm of W_k.

Problem: Eigenspaces of successive W_k may not be aligned:

- it might happen that $K_g \ll 1$

Construction of 1-Lipschitz neural networks

The orthogonal neural networks way:

During training, enforce orthonormality of each W_k [1].

- Implemented in **deel-torchlip**[1] using Bjork orthonormalization algorithm at each training iteration
- Use GroupSort [1] activation function, whose gradient is always 1
- In that case, $\boldsymbol{K_g = 1}$!!

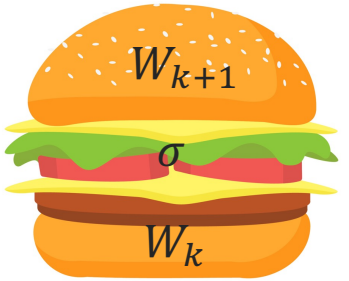
Problem: Enforcing orthonormality has an effect on the class of function g can approximate

- might hinder expressivity for regression tasks…
  - And orthonormalization is an iterative algorithm so prone to error if not converged
  - And it takes more time to train

1 https://github.com/deel-ai/deel-torchlip

Construction of 1-Lipschitz neural networks

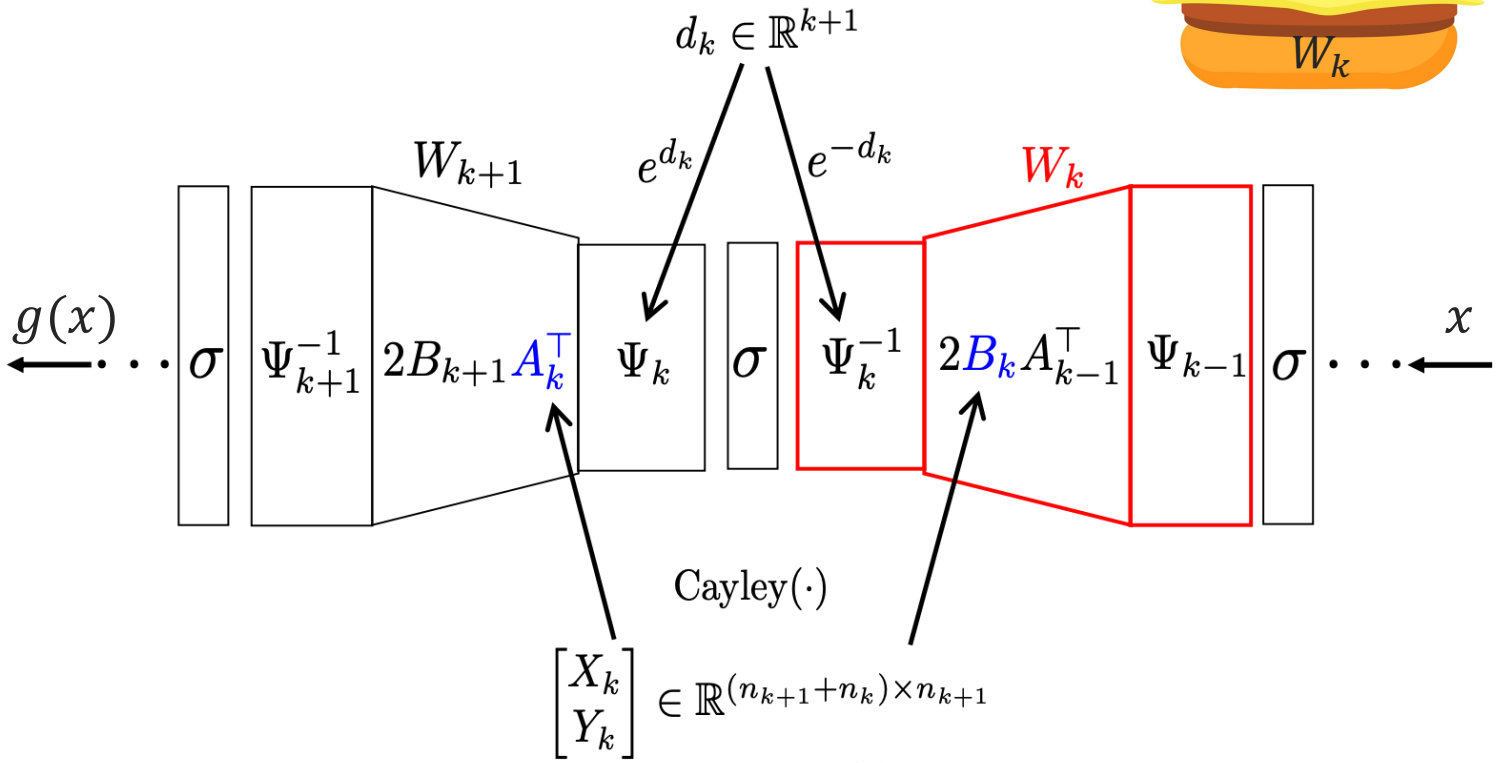
The « sandwich » layers way [12]:



Direct parametrization of W_k by trainable $\{X_k, Y_k, b_k, d_k\}$ such that the whole network g is K_g-Lipschitz.

- Each layer can be $> K_g$-Lipschitz, the whole network will still be K_g-Lipschitz.
- Very efficient, only involve matrix multiplication.
- The constraint is enforced by design (no approximation).

- … And each layer (kind of) looks like a sandwich.



A "sandwich" layer [12]

Construction of 1-Lipschitz neural networks

How to make it 1-Lipschitz ?

1. **The orthogonal neural networks way**
2. **The sandwich layers way**

How to make it K-Lipschitz ?

- Let each g_k be $\sqrt[l]{K}$-Lipschitz.
  Have to know in advance the desired value of K

- Let g_l be K-Lipschitz (by alleviating constraints on W_l)
  K can be learnt