Elliptic PDE learning is provably data-efficient

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Joint work with


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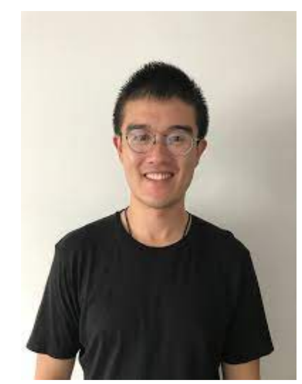
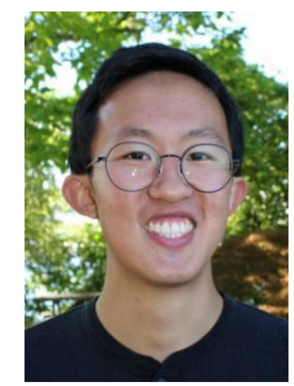

Tianyi Shi


Chris Wang

Related papers:

"Learning elliptic partial differential equations with randomized linear algebra" by Boullé and T. in FoCM, 2022

"Learning Green's functions associated with time-dependent partial differential equations" by Boullé, Kim, Shi, and T. in JMLR, 2022

"Elliptic PDE learning is provably data-efficient" by Boullé, Halikias and T. in PNAS, 2023

"Operator learning for hyperbolic partial differential equations" by Wang and T., on ArXiv, 2024

Operator learning in a nutshell

Operator between function spaces: $\mathscr{G} : \mathscr{X} \to \mathscr{Y}$

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$$\text{E.g., } \hat{\mathscr{G}}_\theta = \underbrace{\mathscr{Q}}_{\text{Decoder}} \circ \underbrace{\sigma}_{\text{Nonlinear activation function}}(\mathscr{K}_L) \circ \cdots \circ \sigma(\mathscr{K}_1) \circ \underbrace{\mathscr{P}}_{\text{Encoder}}$$

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Nonlinear activation function

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$$(\mathcal{K}_1 v)(x) = \int_{D_1} \kappa_1(x, y) v(y) dy + b_1(x)$$

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FNO, GNO [Li, Kovachki, Azizzadenesheli, Liu, Bhattacharya, Stuart, & Anandkumar, 20], MgNO [He, Liu, Xu 23], DeepGreen [Gin, Shea, Brunton & Kutz, 21], DeepONet [Lu, Jin & Karniadakis, 19] IAE-net [Ong, Shen, Yang, 2022], DIMON [Yin, Charon, Brody, Lu, Trayanova, Maggioni, 2024]

Neural operator learning

Usually, we collect input-output data $\{f_i, \mathcal{G}(f_i)\}_{i=1}^N$ and try to solve

$$\inf_\theta \frac{1}{N} \sum_{i=1}^{N} \|\mathcal{G}(f_i) - \hat{\mathcal{G}}_\theta(f_i)\|_{\mathcal{Y}}^2$$

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<u>Questions:</u>

What are the $\mathscr{G}$'s of interest?

How big does N need to be for a certain accuracy?

If N is big enough, then how do I generate the $f_i's$?

Solution operators associated with PDEs

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My focus for this talk:

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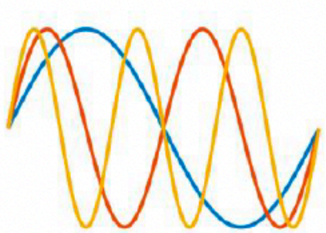
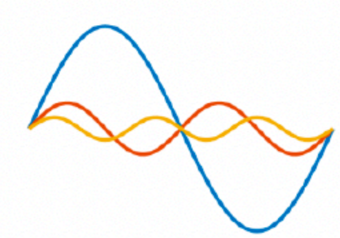


Forcing functions



PDE solutions

Solution operators associated with PDEs

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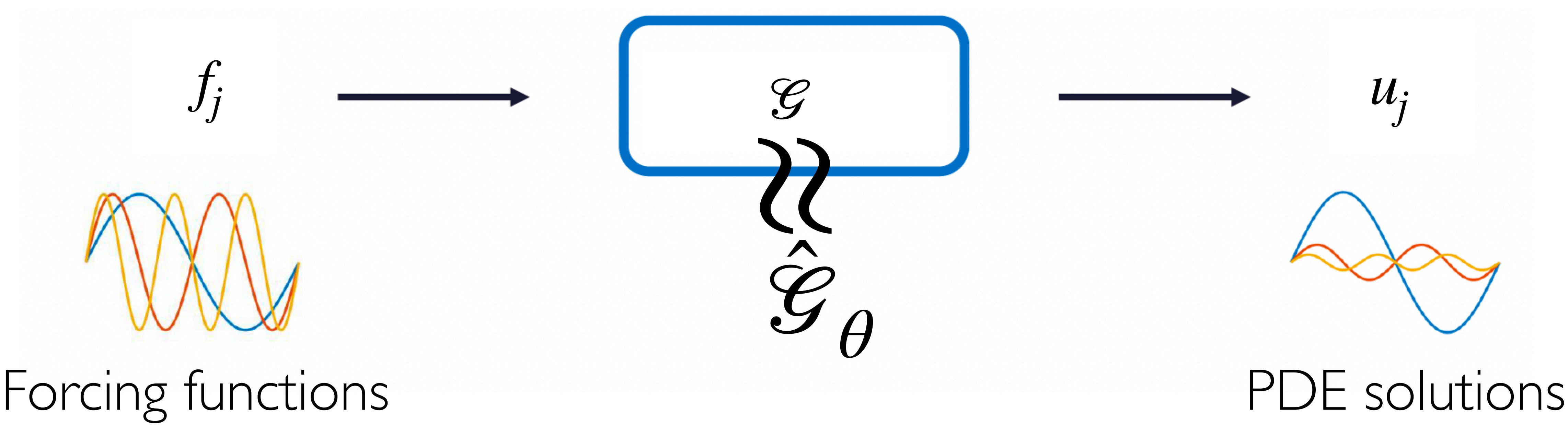
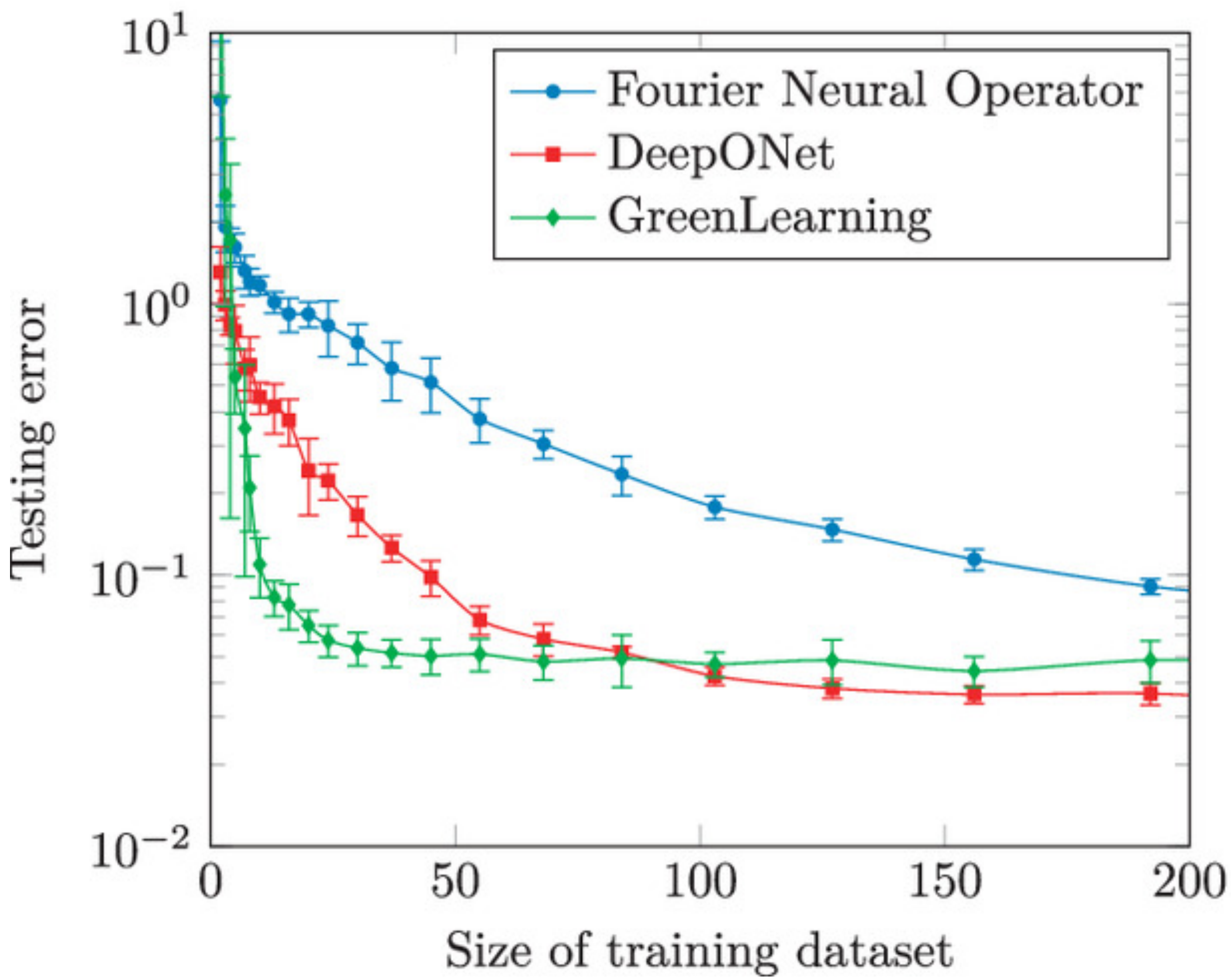


Data-efficient solution operator learning

2D Poisson equation

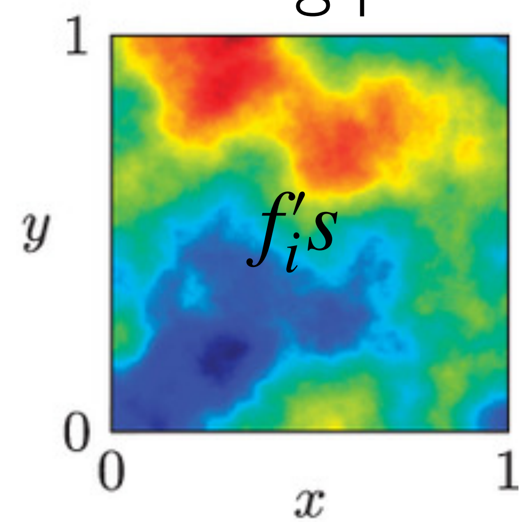
$$\nabla^2 u = f, \qquad u|_{[0,1]^2} = 0$$

Accuracy of the approx. solution operator

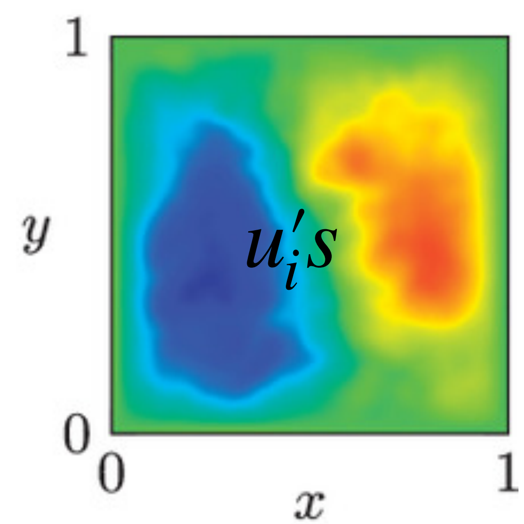


N

Training pairs



Forcing term



Solution

Green's function associated with linear PDEs

Linear PDE

$$\mathscr{L}u = f \text{ on } \Omega \subseteq \mathbb{R}^d$$

$$u|_{\partial\Omega} = 0$$

$\longrightarrow$

Solution operator

$$u(x) = \underbrace{\int_{\Omega} G(x,y) f(y) dy}_{=(\mathscr{G}f)(x)}$$

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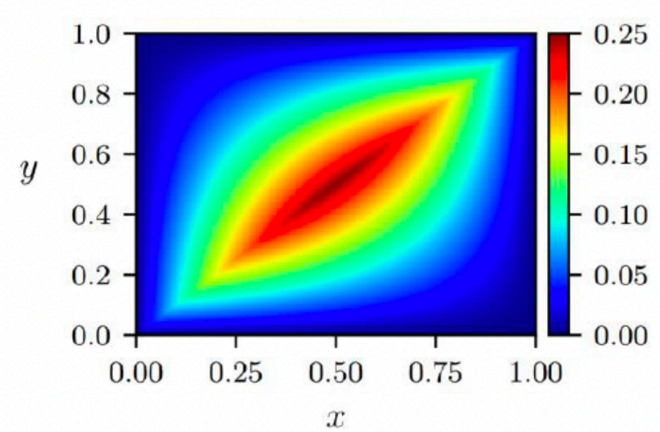
Poisson equation

$$-\nabla^2 u = f$$

$$u(0) = u(1) = 0$$



Green's function for PDEs in $d > 1$ are unbounded functions

Green's function recovery

Theorem: [Boullé & T., 2021], [Boullé, Kim, Tianyi & T., 2022], [Boullé, Hailikas & T., 2023] [Wang & T., 2024]
There is a randomized algorithm that, for any $\epsilon > 0$, can construct an approx. G of $\hat{G}$ for PDE class with $\boxed{??}$ input-output pairs (f_j, u_j) such that

$$\|G - \hat{G}\|_{L^p} \leq \epsilon \|G\|_{L^p}$$

with high probability.

PDE class	$\boxed{??}$	p

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uniformly self-adjoint hyperbolic in $d = 1$	$\mathcal{O}(\epsilon^{-(6+1/r)}\log^{3}(1/\epsilon)/\Gamma_\epsilon)$	2

Recovering a matrix with matrix-vector products

We can recover a symmetric low-rank matrix with matrix-vector products $v \mapsto Av$:

Randomized SVD:

[Halko, Martinsson, & Tropp, 2011], [Martinsson & Tropp, 2020]

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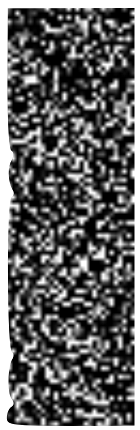
$Y =$ 

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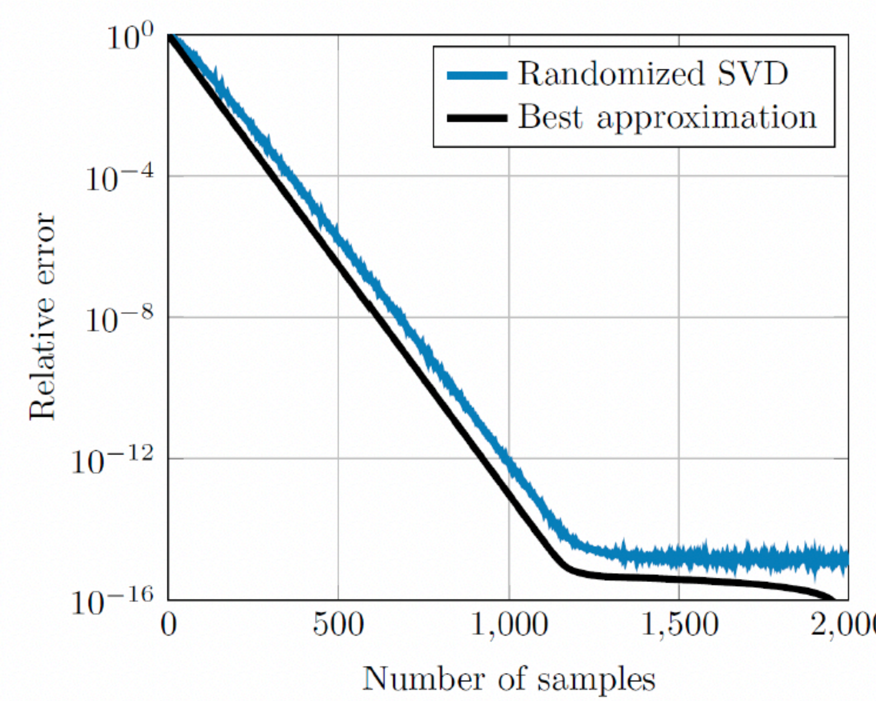
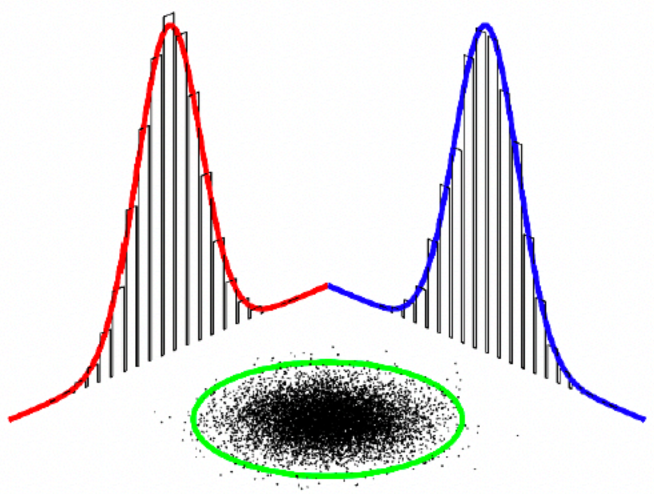
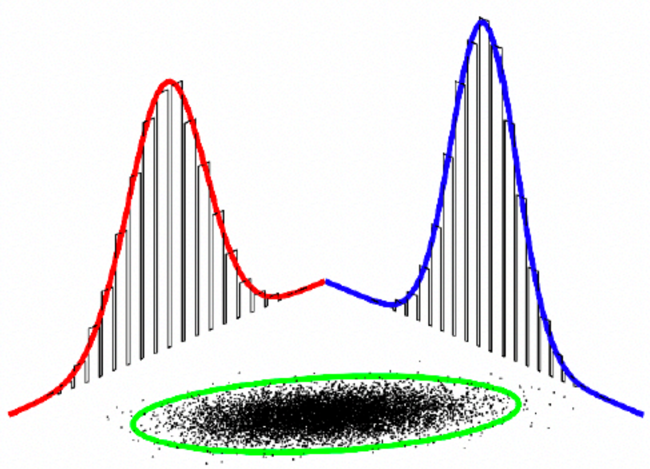


Generalization of the randomized SVD

Standard Gaussian vectors



Correlated Gaussian vectors



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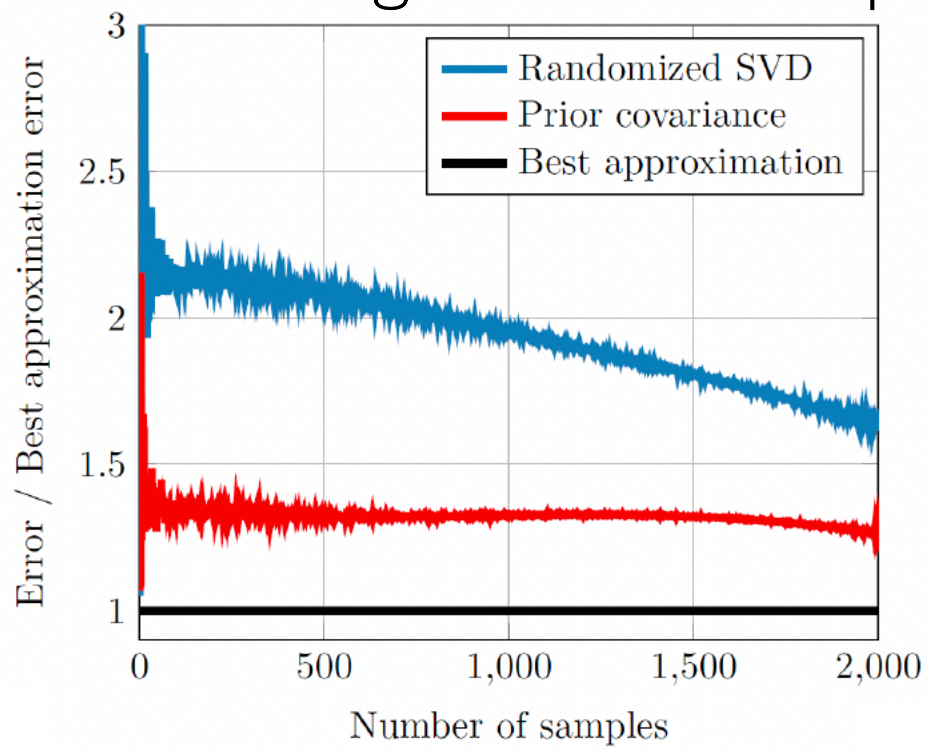
Generalization of the randomized SVD

Standard Gaussian vectors → **Correlated Gaussian vectors**

Prior knowledge about A helps:



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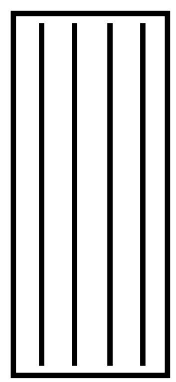
$Y =$ 

Cols are drawn from
Gaussian process $GP(0,C)$

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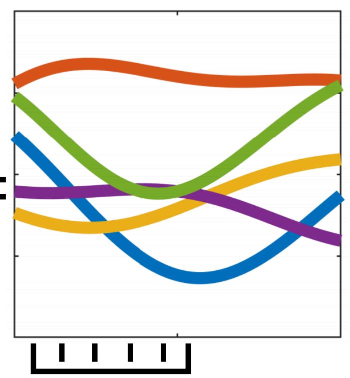
$Y =$ 

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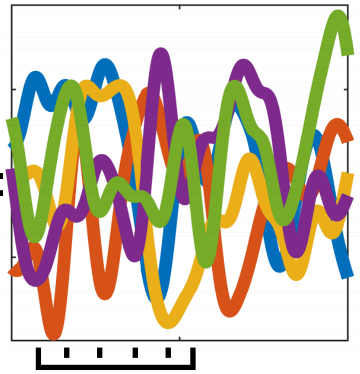
$Y =$ 

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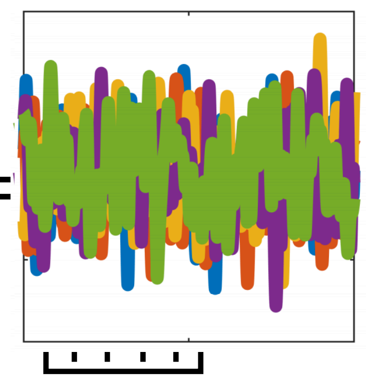
$Y =$ 

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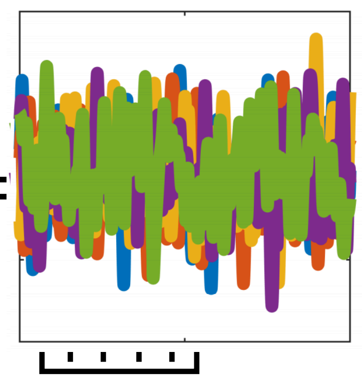
$Y =$ 

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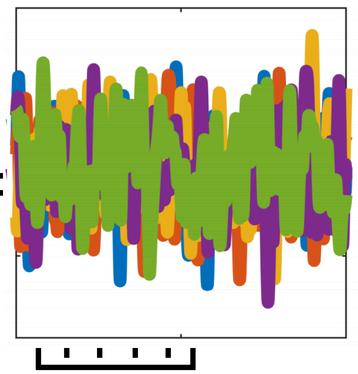
$Y =$ 

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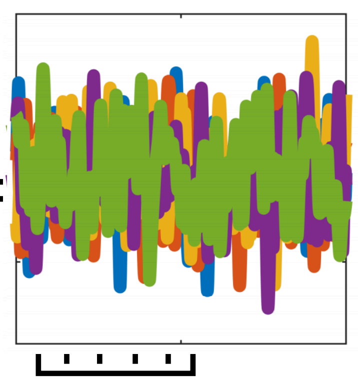
$Y =$ 

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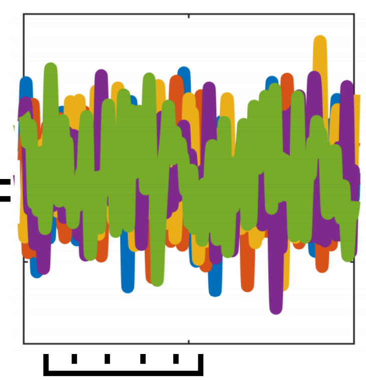
$Y =$ 

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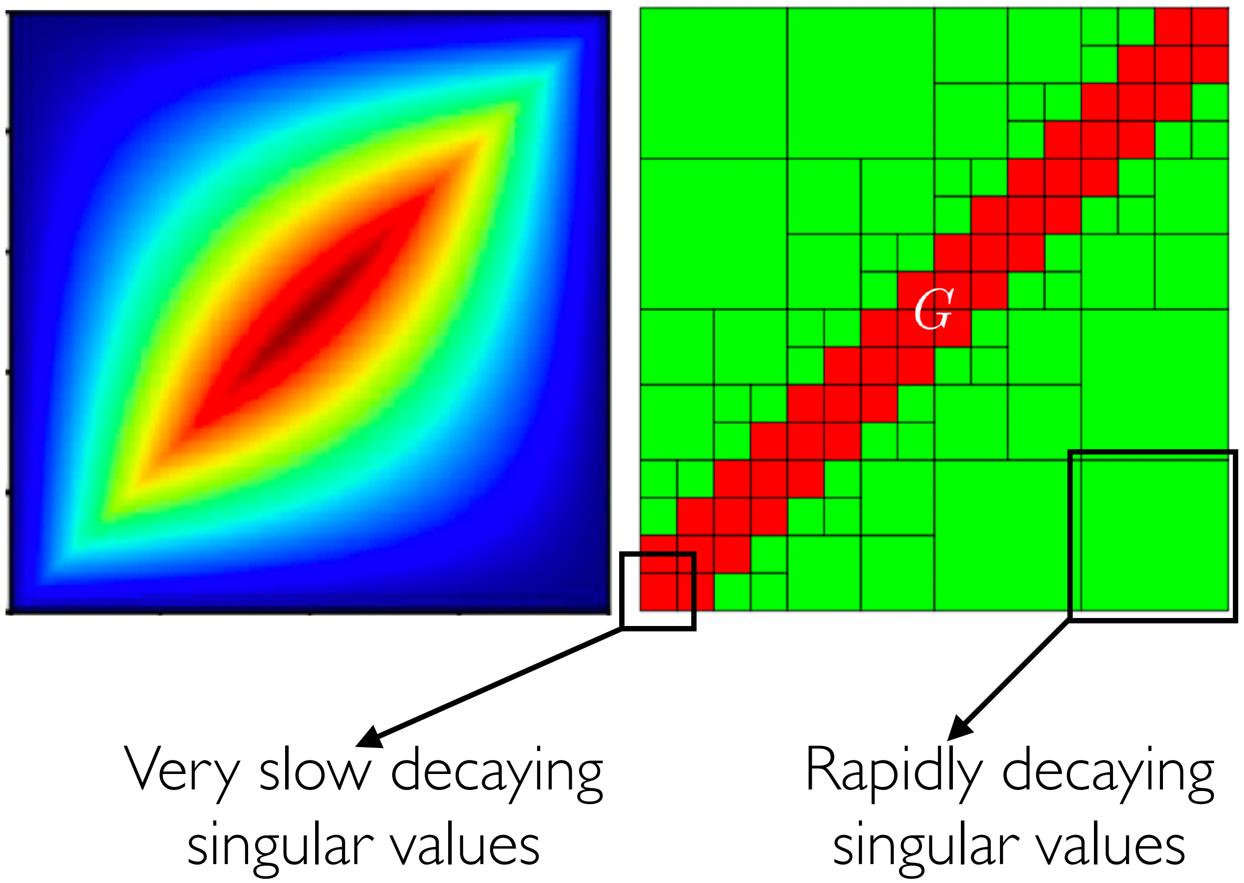
Problem:

Green's functions typically do not have rapidly decaying singular values.

ϵ_k decays very slowly with k

Green's functions are low rank on separated blocks

One dimension



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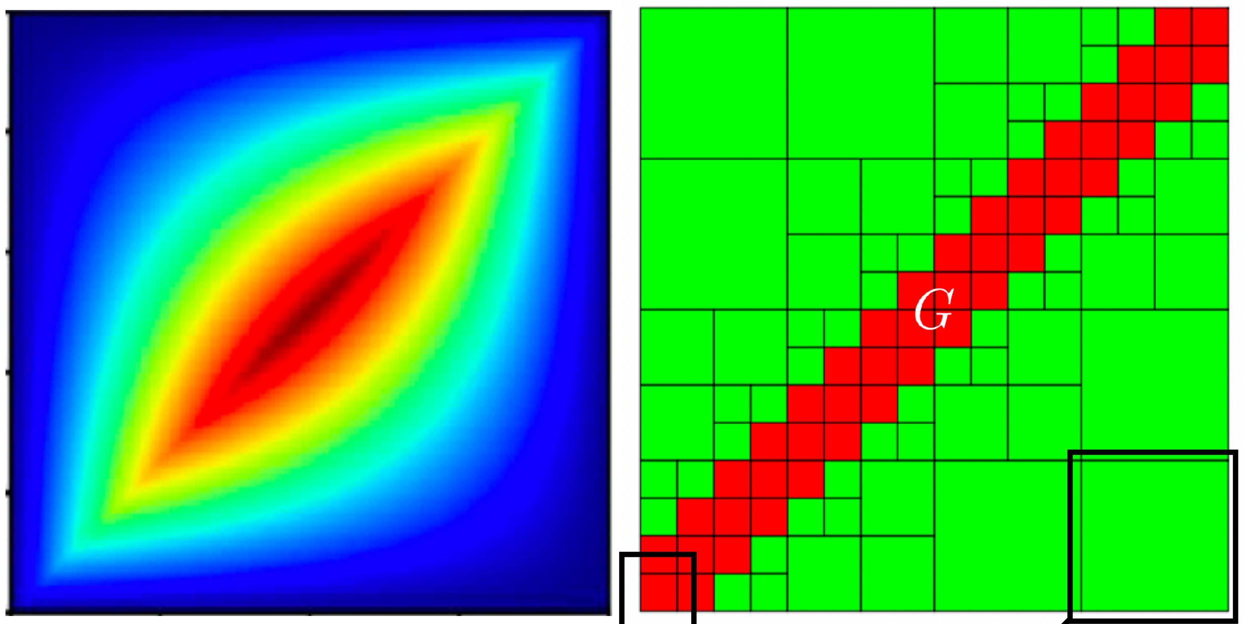
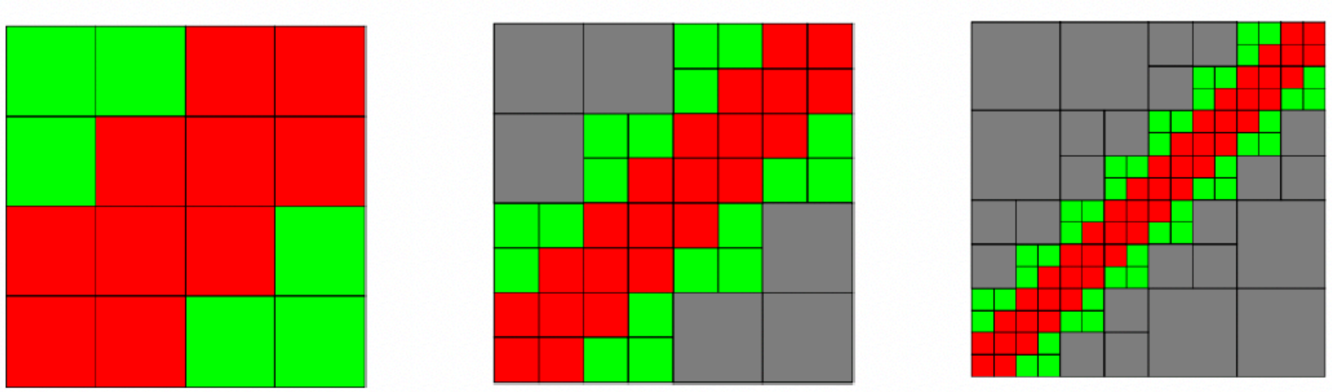


Very slow decaying singular values

Rapidly decaying singular values

Hierarchical structure

Level 2 Level 3 Level 4



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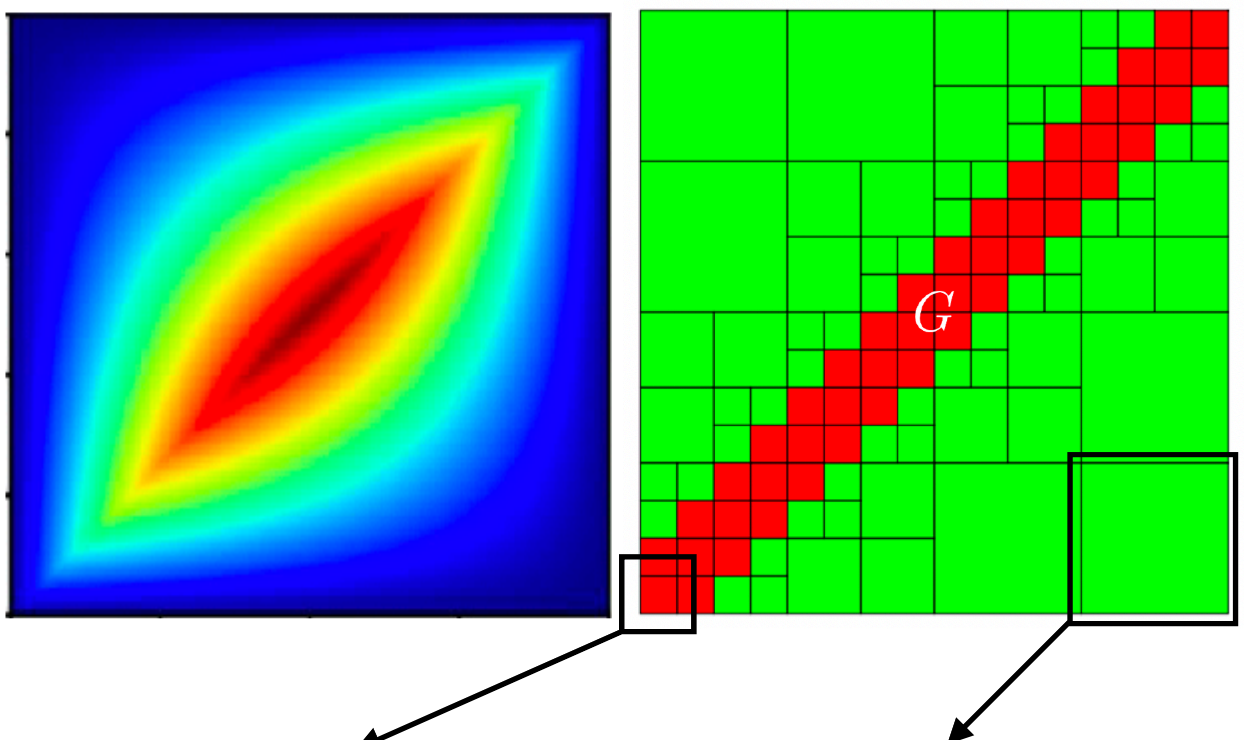

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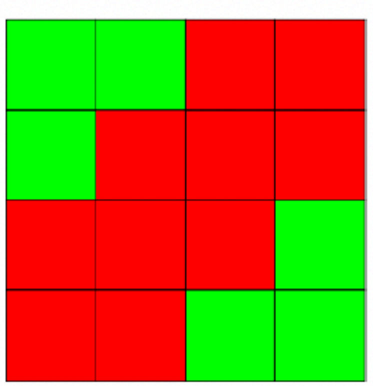
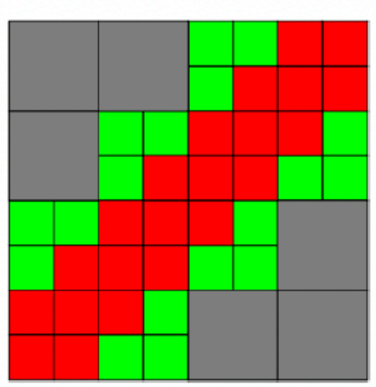
<u>Hierarchical structure</u>

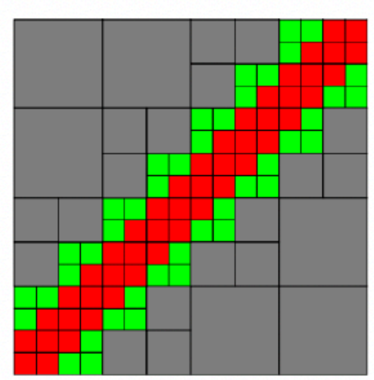
Level 2



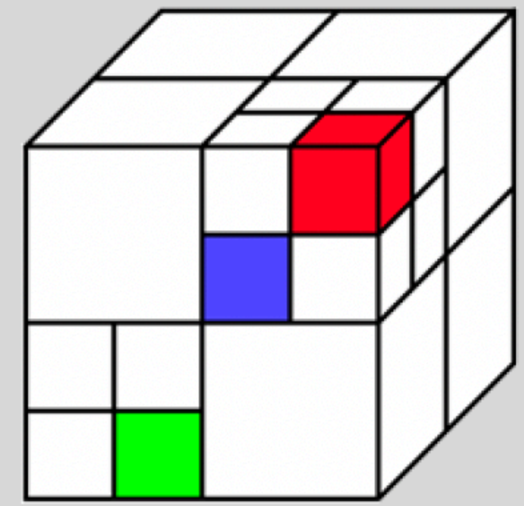
Level 3



Level 4



Three dimensions

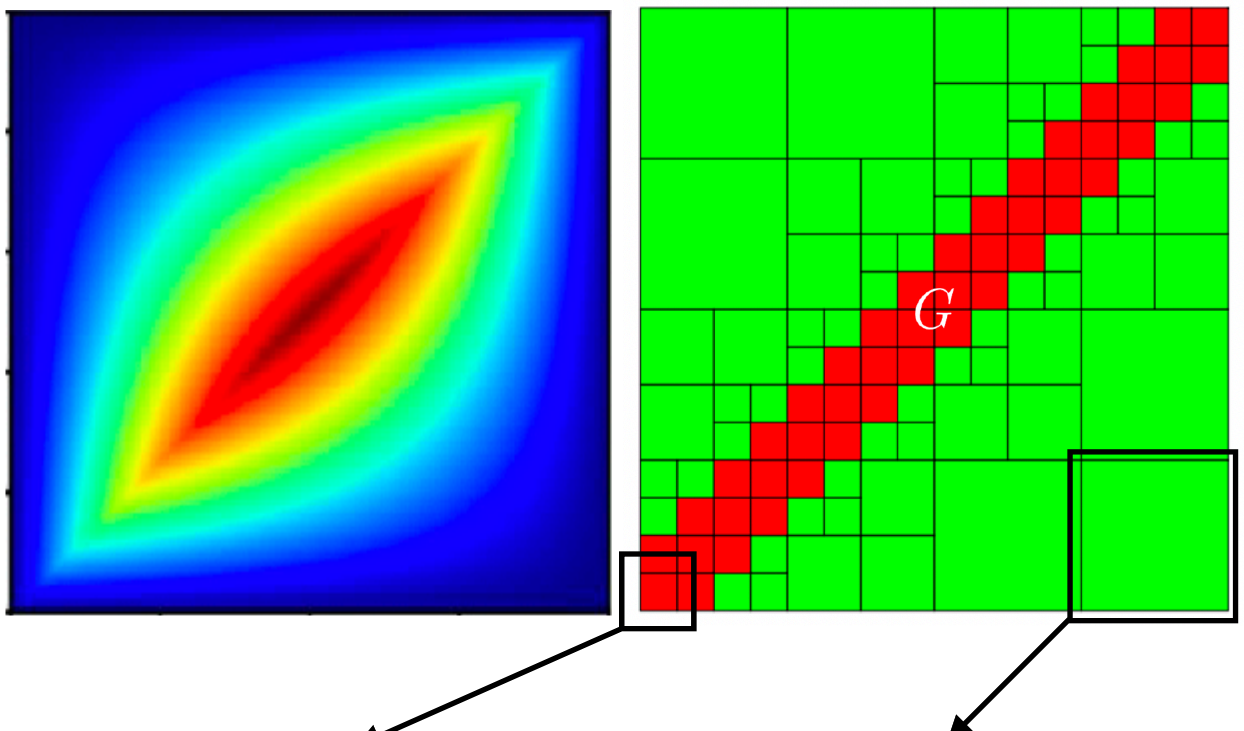


Low-rank structure on well separated domains.

[Bebendorf, Hackbush, 2003]

Green’s functions are low rank on separated blocks

One dimension



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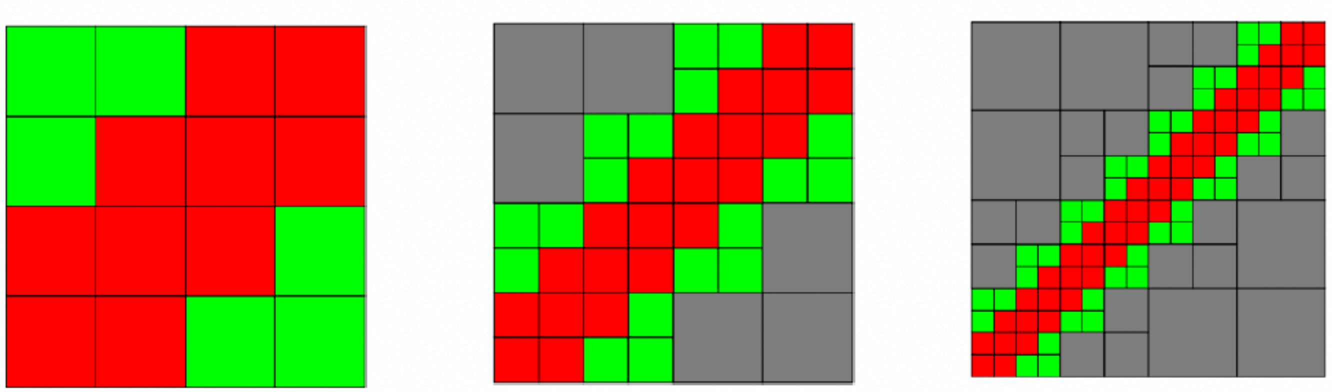

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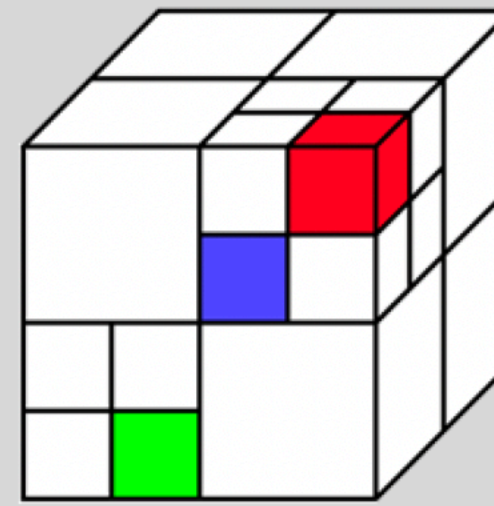

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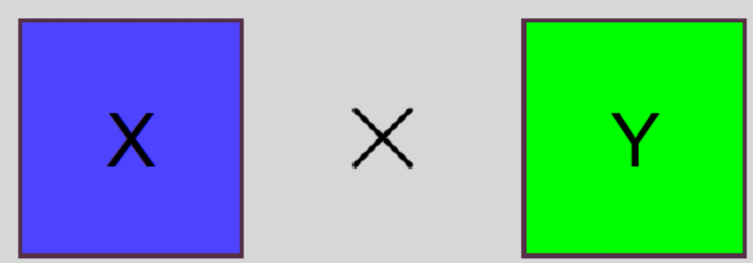
[Bebendorf, Hackbush, 2003]



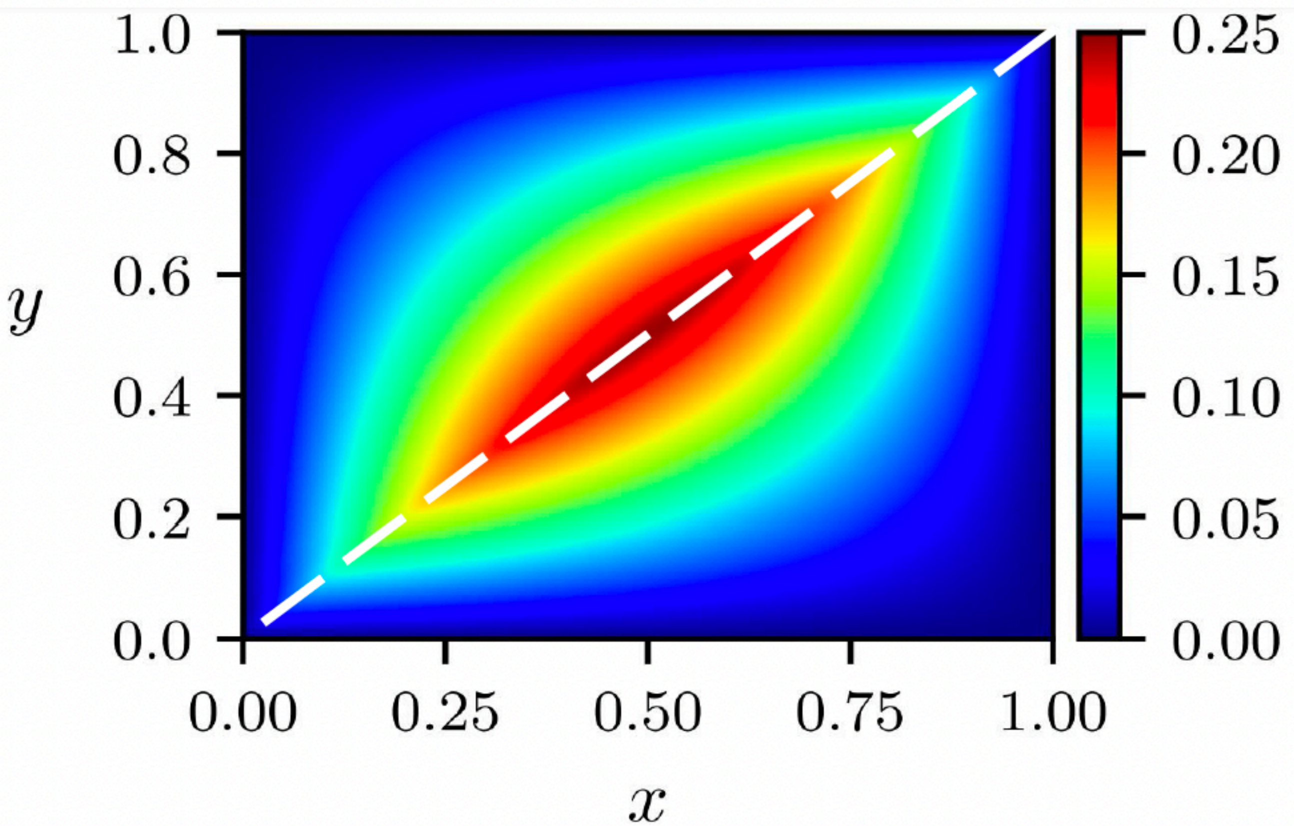
Related approaches for matrices:

[Martinsson, 2008], [Lin, Lu, & Ying, 2010], [Martinsson, 2016], [Levitt & Martinsson, 2022]

Off-diagonal decay

Green's function of the Laplace operator:

$$-\nabla^2 u = f$$

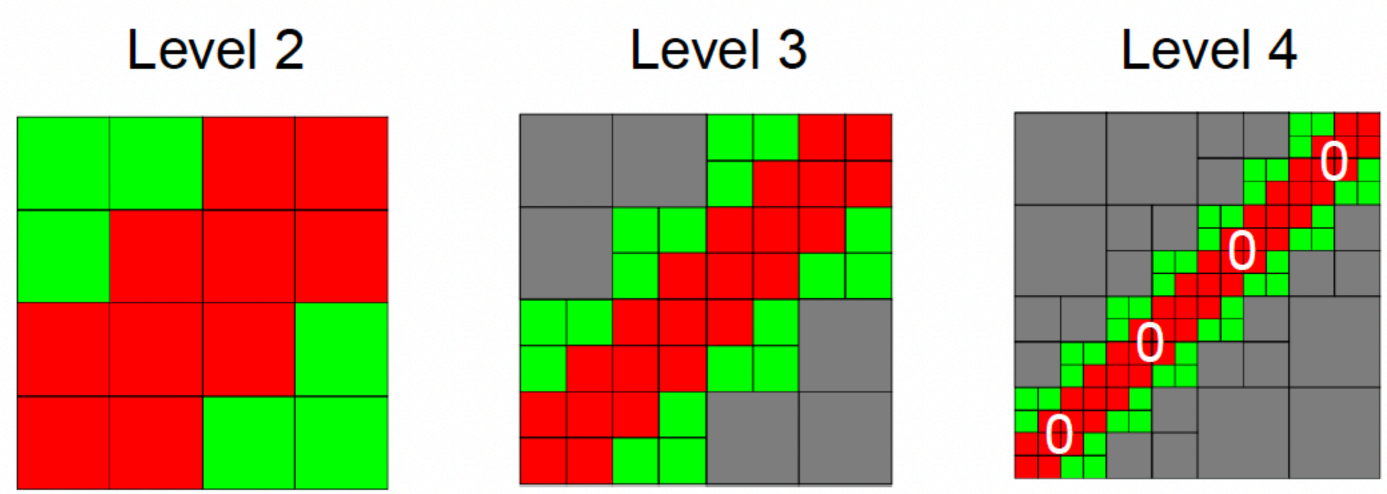


Green's functions are smooth and decay off the diagonal. [Grüter, Widman, 1982]

$$G(x,y) \leq \frac{1}{\|x-y\|}$$

(for 3D elliptic PDEs)

<u>Hierarchical structure</u>

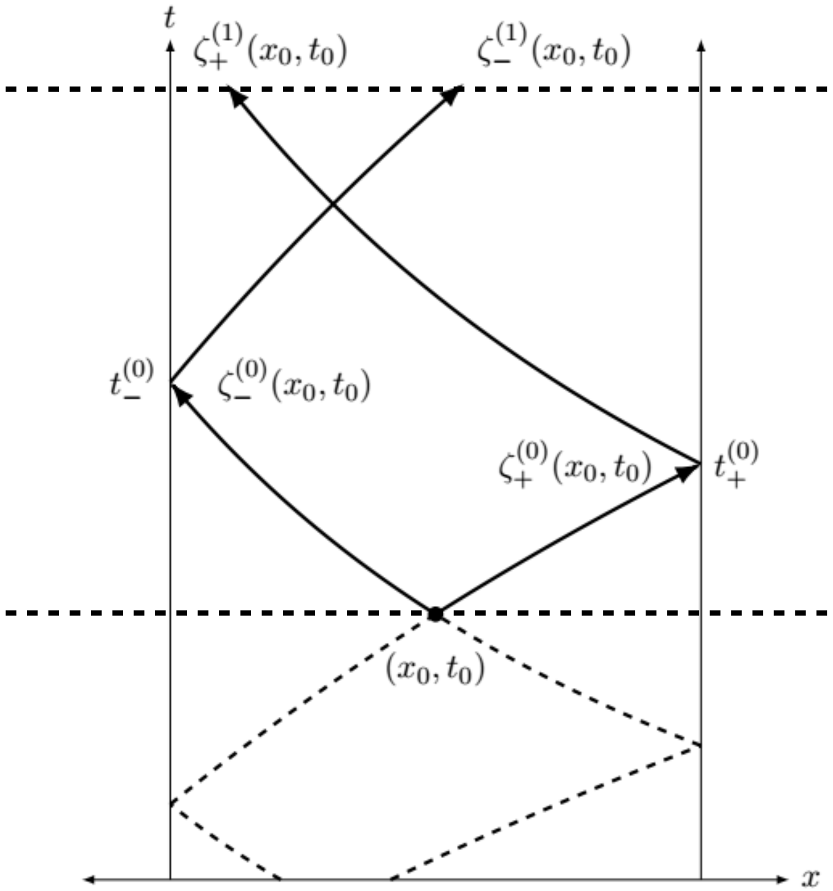


(Pictures are in 1D for illustration purposes.)

Green's functions associated with 1D hyperbolic PDEs

[Wang & T., 2024]

Solution operators for 1D hyperbolic PDEs have Green's functions with jumps along characteristics.



2D slice through the 4D Green's function

Chris Wang

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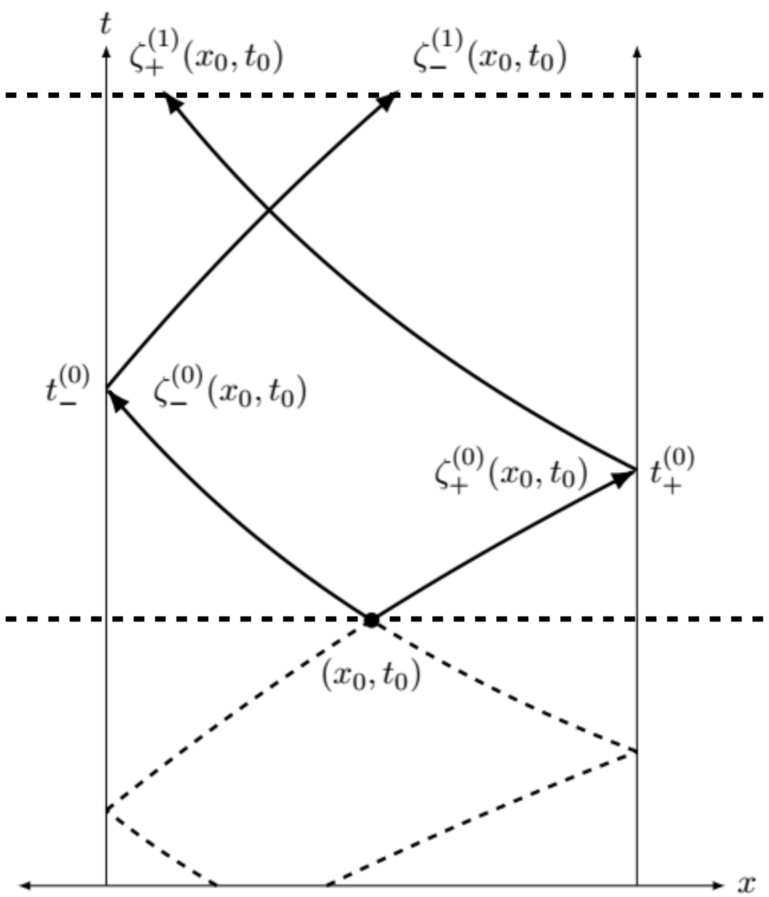

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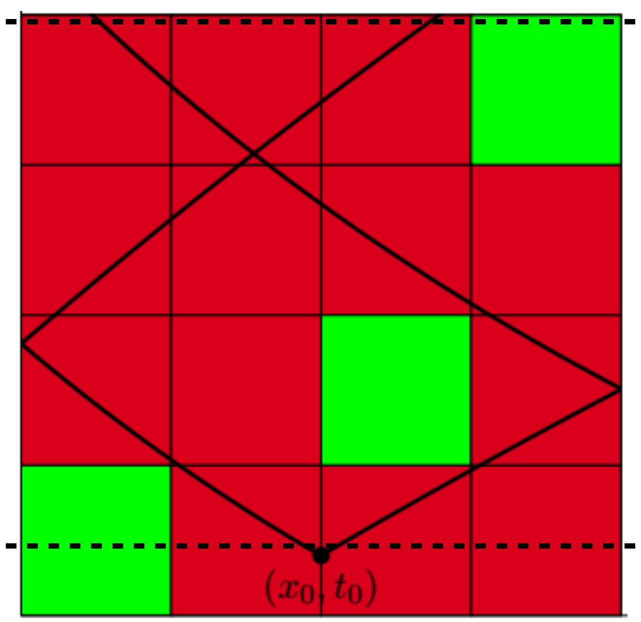

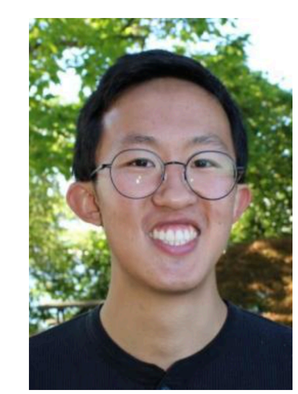

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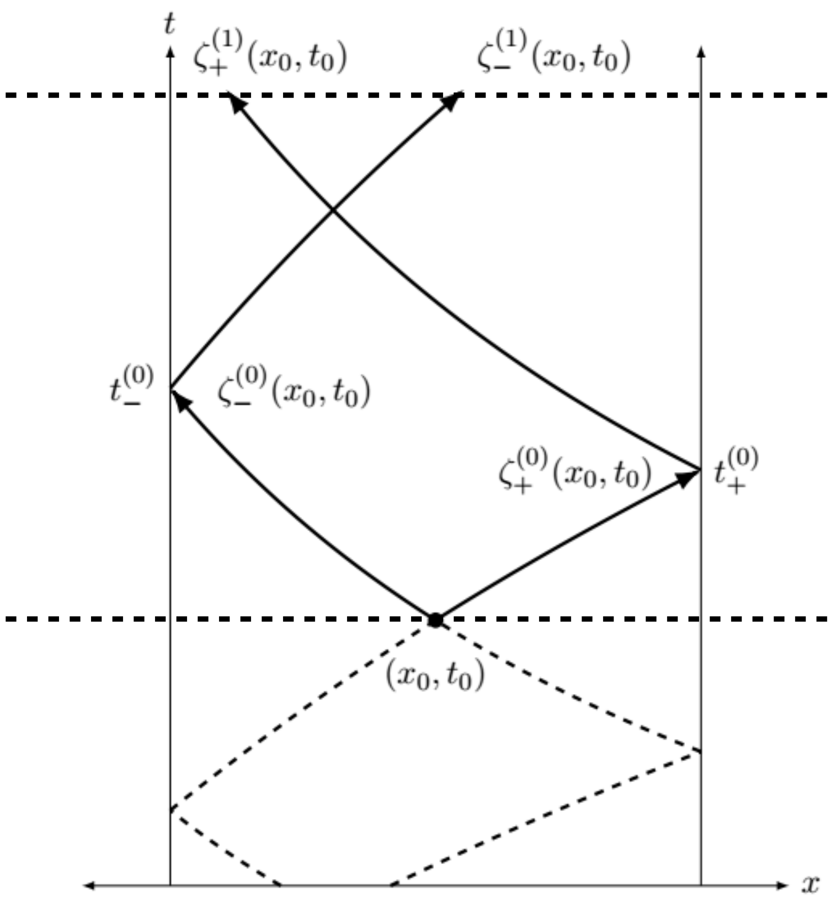

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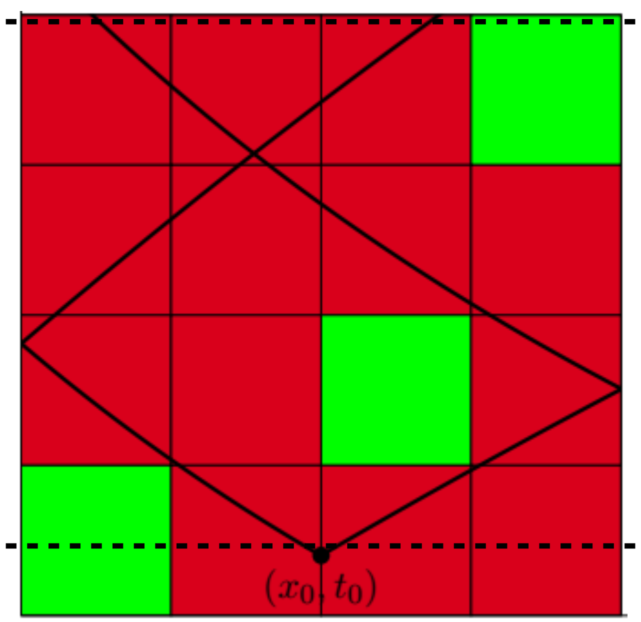

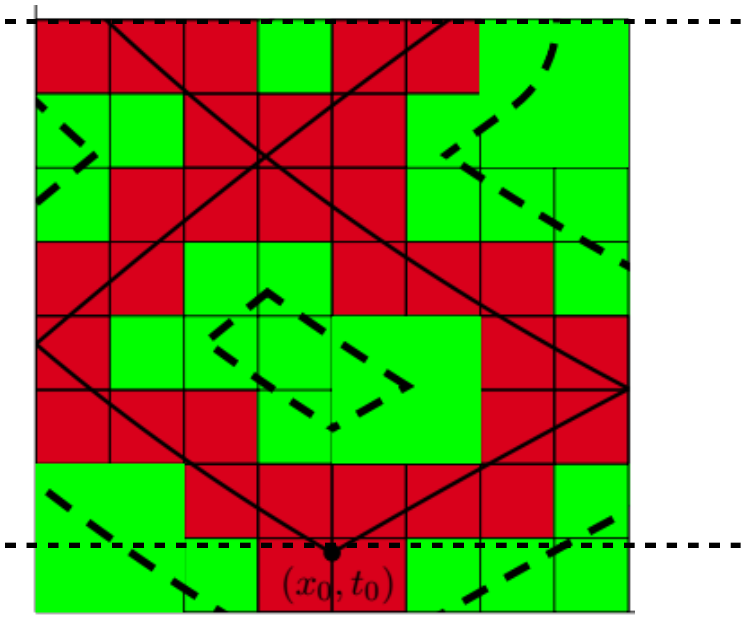

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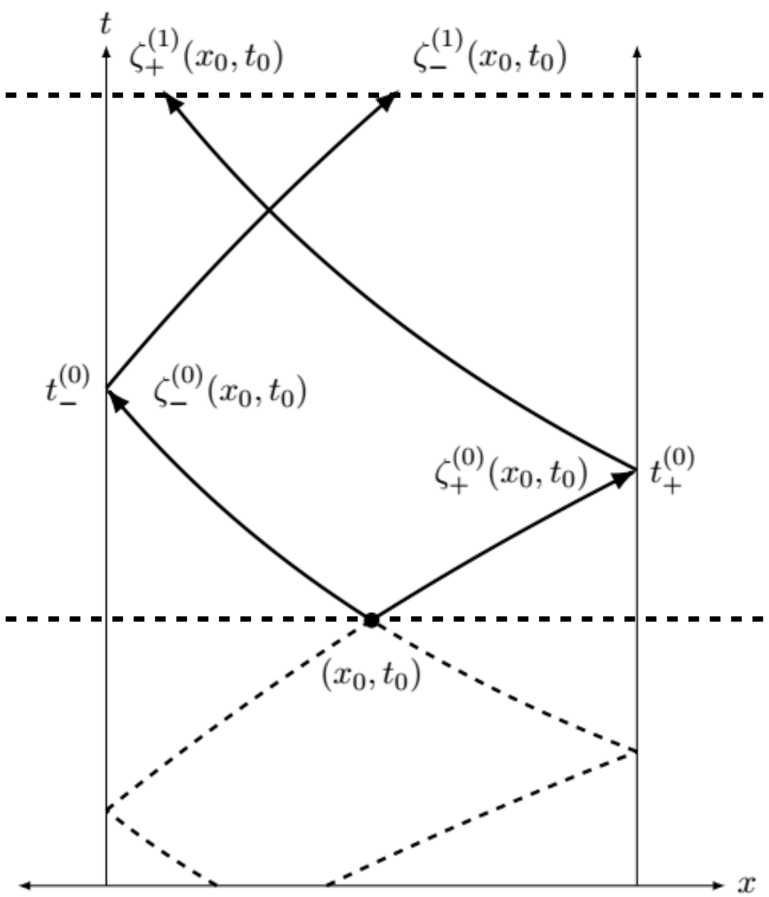
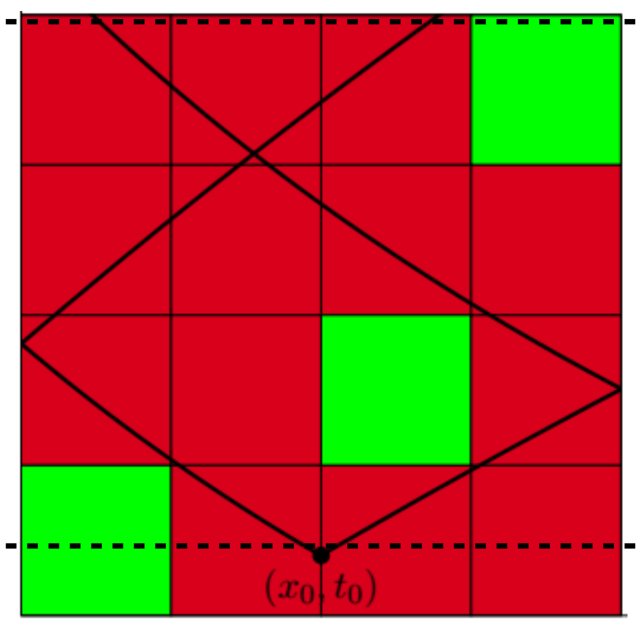
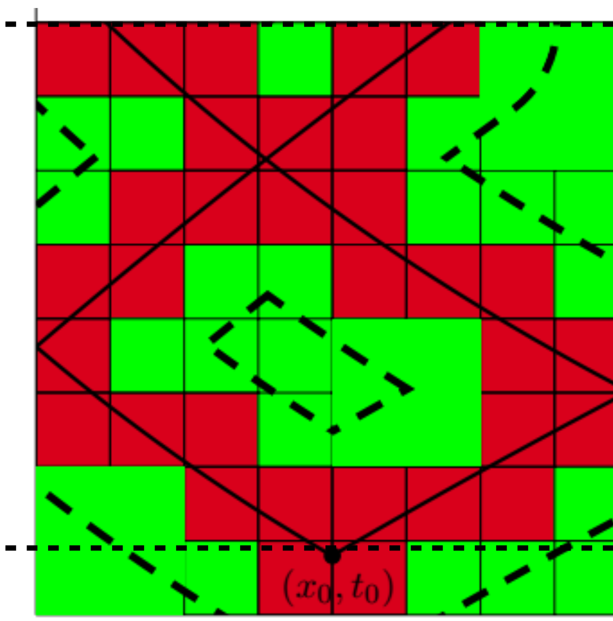


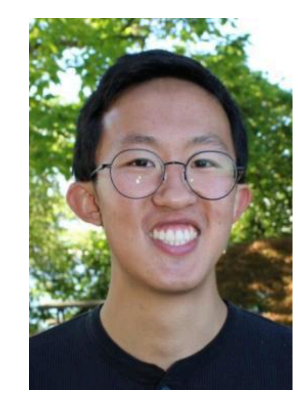




2D slice through the 4D Green's function

Using input-output data to:

1. Adaptively partition domain to isolate characteristics in tiny regions
2. Recover Green's function off the characteristics



Chris Wang

Green's function recovery

Theorem: [Boullé & T., 2021], [Boullé, Kim, Tianyi & T., 2022], [Boullé, Hailikas & T., 2023] [Wang & T., 2024]
There is a randomized algorithm that, for any $\epsilon > 0$, can construct an approx. G of $\hat{G}$ for PDE class with $\boxed{??}$ input-output pairs (f_j, u_j) such that

$$\|G - \hat{G}\|_{L^p} \leq \epsilon \|G\|_{L^p}$$

with high probability.

PDE class	$\boxed{??}$	p
uniformly self-adjoint elliptic in $d = 1,2,3$	$\mathcal{O}(\log^{d+2}(1/\epsilon)/\Gamma_\epsilon)$	2
uniformly parabolic in $d \geq 1$ (and uni. self-adjoint elliptic in $d \geq 4$.)	$\mathcal{O}(\log^{d+4}(1/\epsilon)/\Gamma_\epsilon)$	1
uniformly self-adjoint hyperbolic in $d = 1$	$\mathcal{O}(\epsilon^{-(6+1/r)}\log^3(1/\epsilon)/\Gamma_\epsilon)$	2

Quality of training data

In our theoretical results, Γ_ϵ is a measure of the quality of the training data.

Theorem

We can construct an approximation G_k of G from k+5 random input functions f such that

$$\mathbb{P}\left[\|G - G_k\|_{L^2} \leq \mathcal{O}\left(\sqrt{k^2/\gamma_k}\right)\epsilon_k\right] \geq 0.999$$

$$f \sim \mathcal{GP}(0, K)$$

where $K(x, y)$ is the covariance kernel

Definition: $\gamma_k = k/(\lambda_1 \mathrm{Tr}(\mathbf{C}^{-1}))$

$$\mathbf{C}_{ij} = \int_{\Omega\times\Omega} v_i(x)K(x,y)v_j(y)\,\mathrm{d}x\,\mathrm{d}y$$

where v_i is the ith right singular vectors of G.

- $0 < \gamma_k \leq 1$
- We can impose prior knowledge on the covariance kernel
- Explicit bounds for the covariance quality factor are available

Operator learning without the adjoint

Question:

Can operator learning be data-efficient with only input-output $\{f_i, \mathcal{G}(f_i)\}_{i=1}^N$ data?

Operator learning with and without the adjoint

Consider

$$(\mathcal{G}f) = \int_0^1 G(x, y)f(y)dy, \text{ where } G \text{ is a 1-Lipschitz smooth function}$$

$$\ldots\text{and } G(x, y) = g(x)h(y)$$

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Then, $$(\mathcal{G}f)(x) = \left(\int_0^1 h(y)f(y)dy\right)g(x)$$

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The adjoint is $(\mathscr{G}^*f)(x) = \left(\int_0^1 g(y)f(y)dy\right)h(x)$

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Training dataset size to achieve ϵ accuracy

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	With the adjoint	Without the adjoint
Training dataset size to achieve ϵ accuracy		

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	With the adjoint	Without the adjoint
Training dataset size to achieve ϵ accuracy	$\mathscr{O}(1)$ Input-output pairs	

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$$\text{The adjoint is } (\mathscr{G}^*f)(x) = \left(\int_0^1 g(y)f(y)dy\right)h(x)$$

	With the adjoint	Without the adjoint
Training dataset size to achieve ϵ accuracy	$\mathcal{O}(1)$ Input-output pairs	$\mathcal{O}(1/\epsilon)$ Input-output pairs

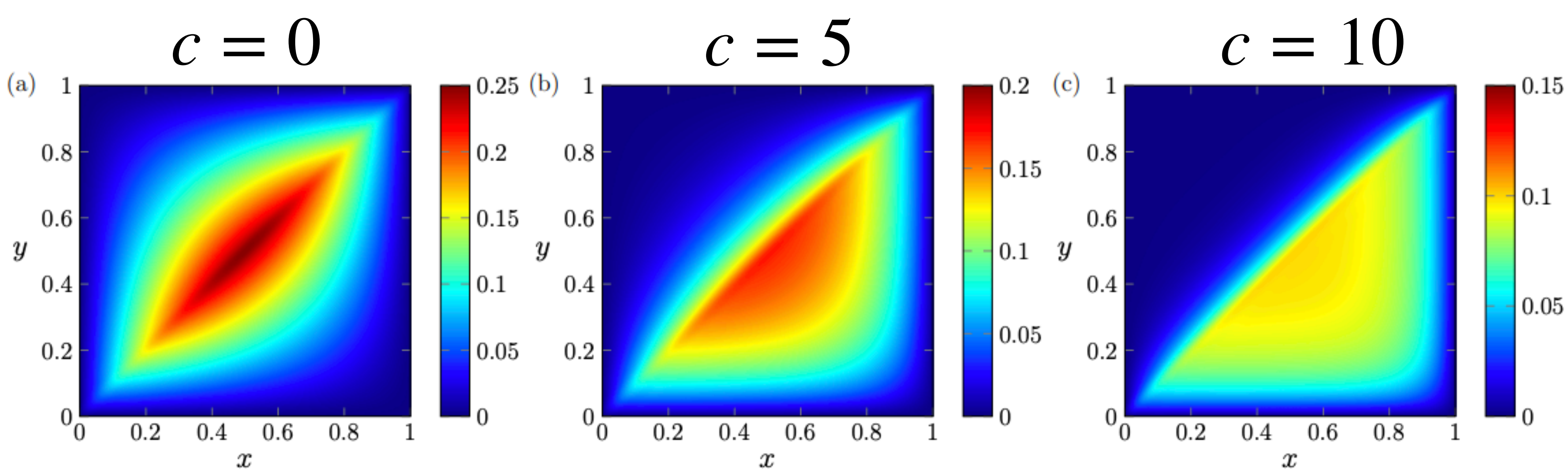
[Halikias & T., 22]

The adjoint mystery

[Boullé, Halikias, Otto & T., 2024], [Levitt & Martinsson, 2024]

Forcing terms: N input-output functions drawn from a Gaussian process.

$$-\frac{d^2u}{dx^2} + c\frac{du}{dx} = f, \quad u(0) = u(1) = 0, \quad x \in [0,1].$$



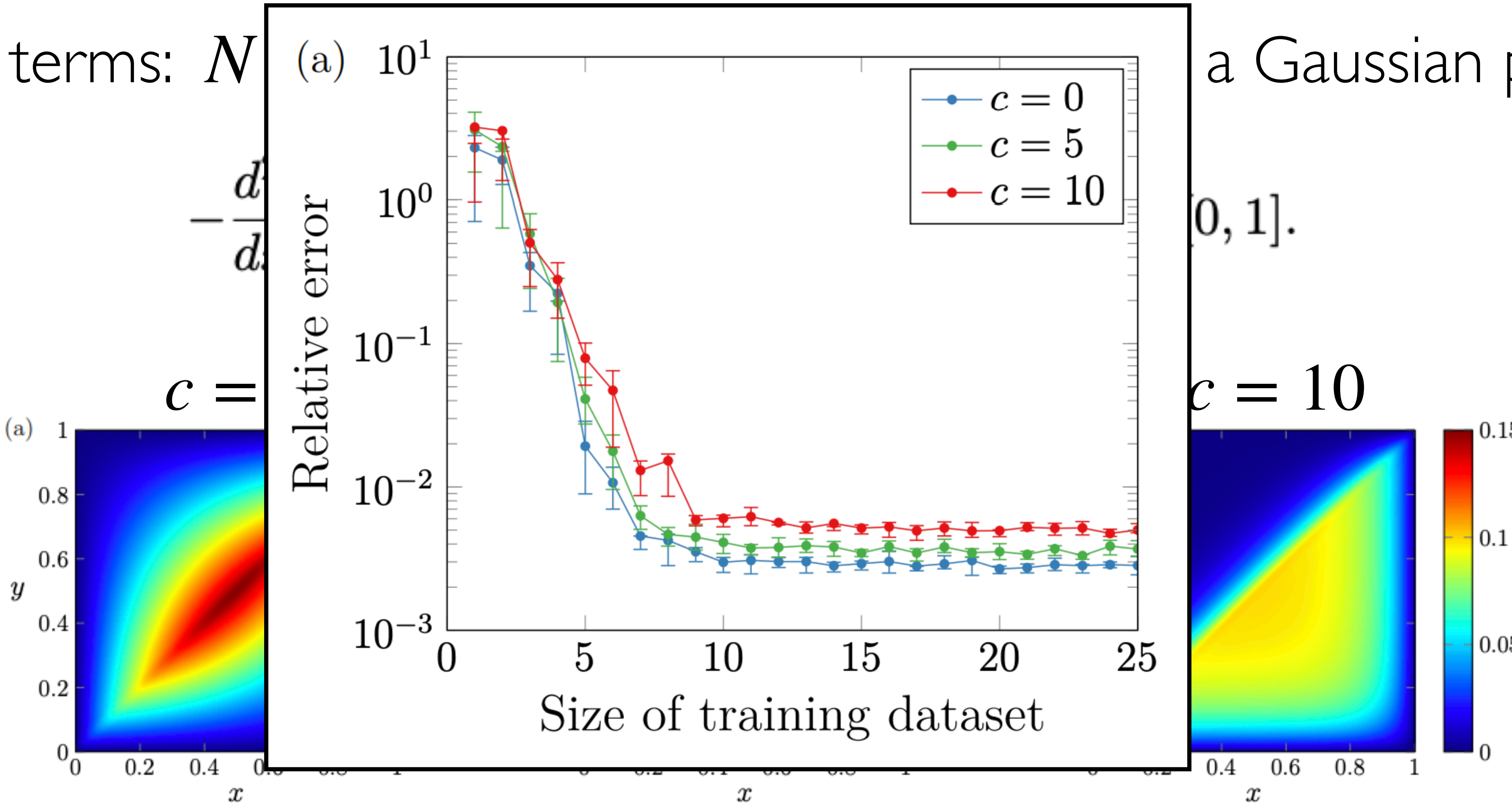
The adjoint mystery

[Boullé, Halikias, Otto & T., 2024], [Levitt & Martinsson, 2024]

Forcing terms: N … a Gaussian process.

$$-\frac{d}{d} \quad \ldots \quad [0,1].$$

$c =$ … $c = 10$



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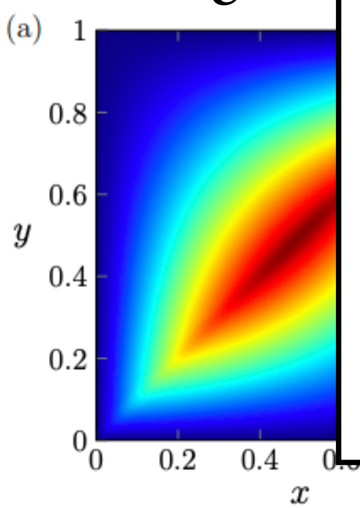

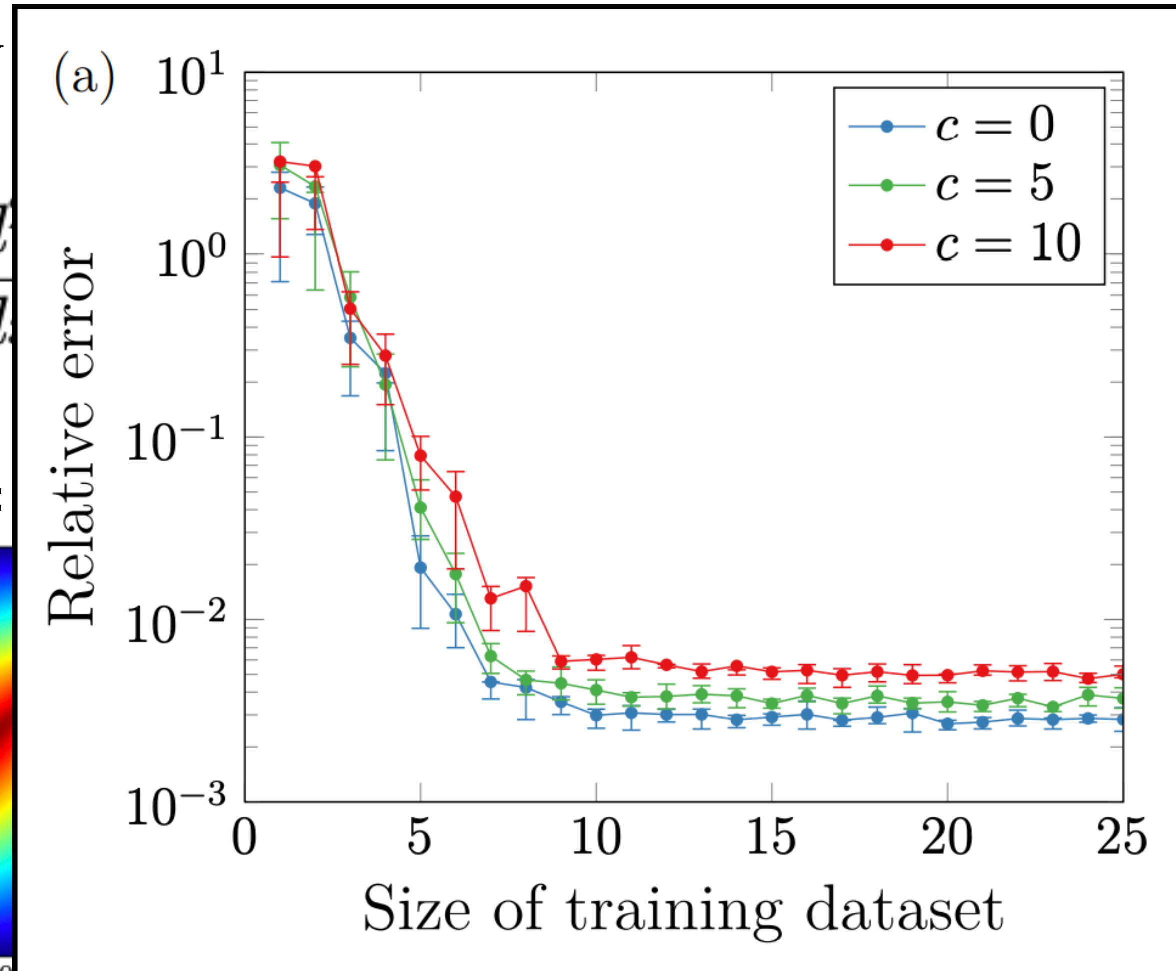

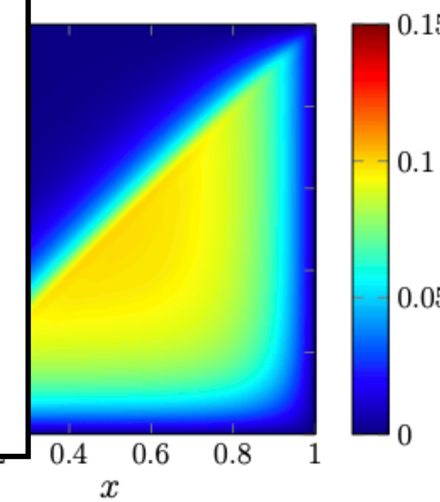

PDE class	With adjoint	Without adjoint

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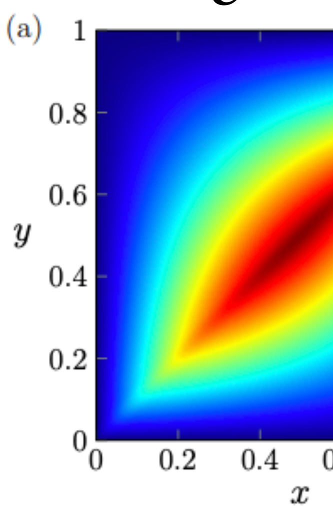

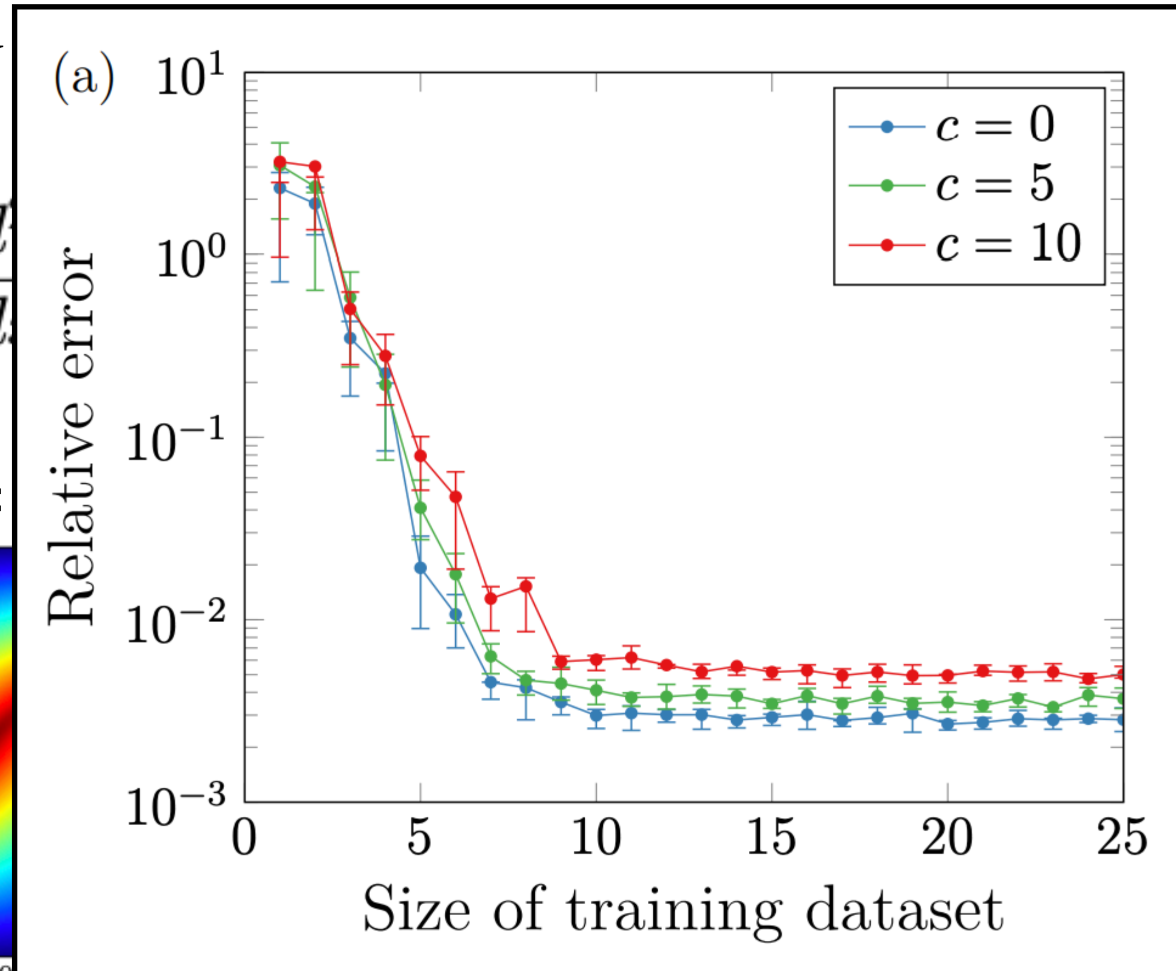

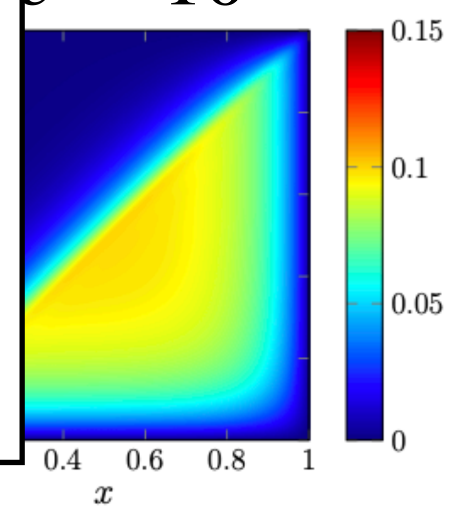

PDE class	With adjoint	Without adjoint
Constant coeff., elliptic $d = 1,2,3$	$\mathcal{O}(1)$	$\mathcal{O}(1)$

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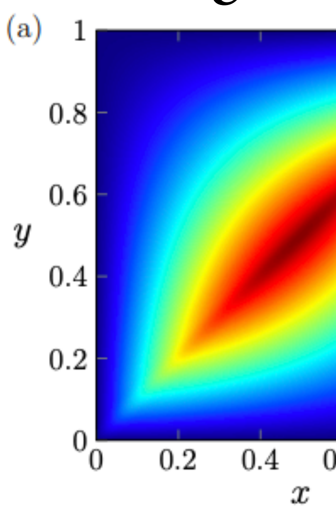
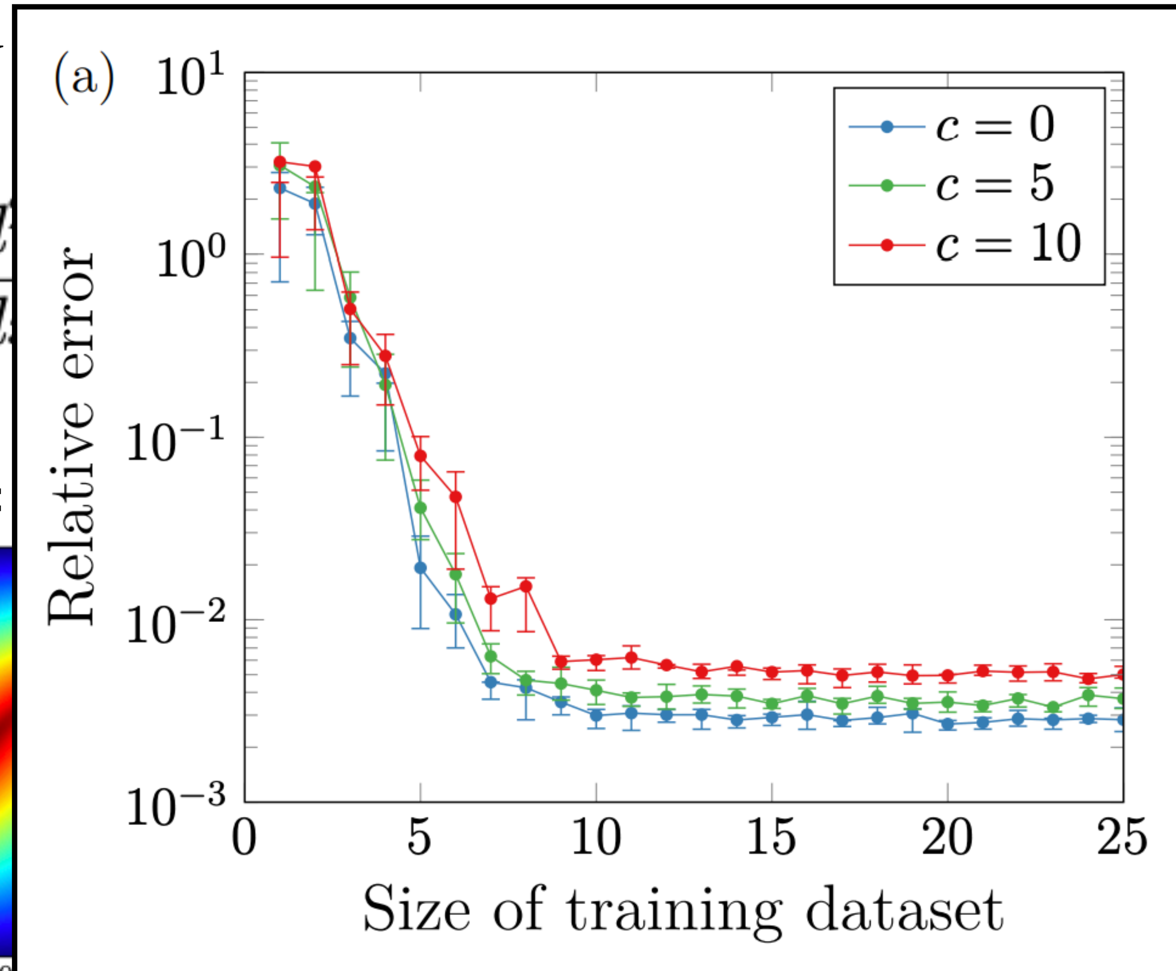
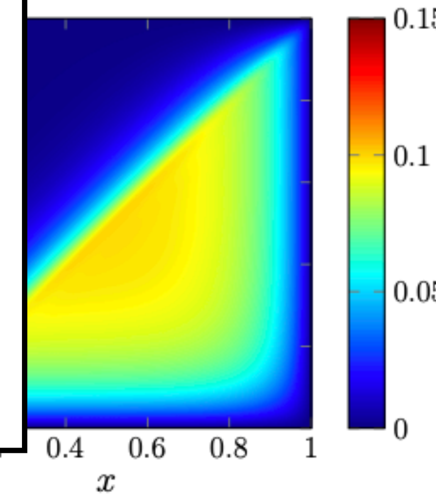




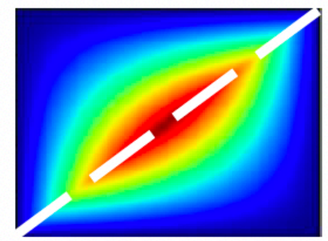


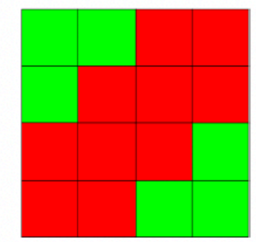
PDE class	With adjoint	Without adjoint
Constant coeff., elliptic $d = 1,2,3$	$\mathcal{O}(1)$	$\mathcal{O}(1)$
General 2nd order uniform elliptic $d = 1,2,3$	$\mathcal{O}(\log^{d+2}(1/\epsilon))$	$\mathcal{O}(\epsilon^{-d/2})$

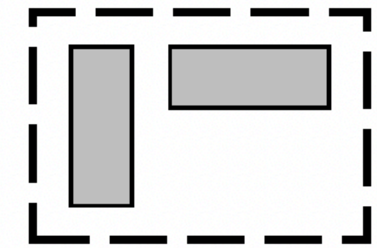
Summary

1. Theory for learning Green's functions

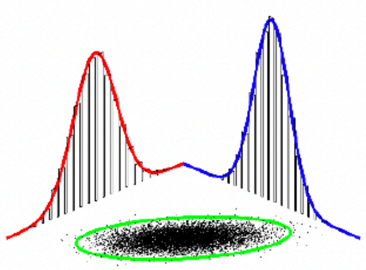
$$\mathcal{L}u = -\nabla \cdot (A(x)\nabla u)$$

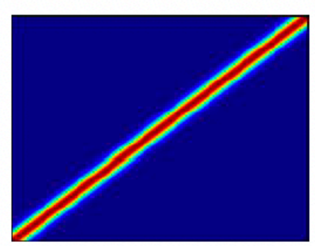


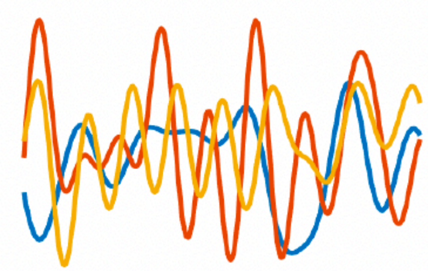


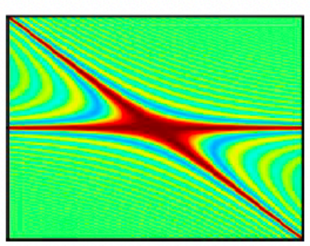


2. Generalization of the randomized SVD









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Can operator learning be data-efficient with only input-output $\{f_i, \mathcal{G}(f_i)\}_{i=1}^{N}$ data?