Learning elliptic PDEs with randomized linear algebra

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Joint work with


Nicolas Boullé


Chris Earls

Introduction

Question: Can one "learn" an unknown linear PDE from input-output data?

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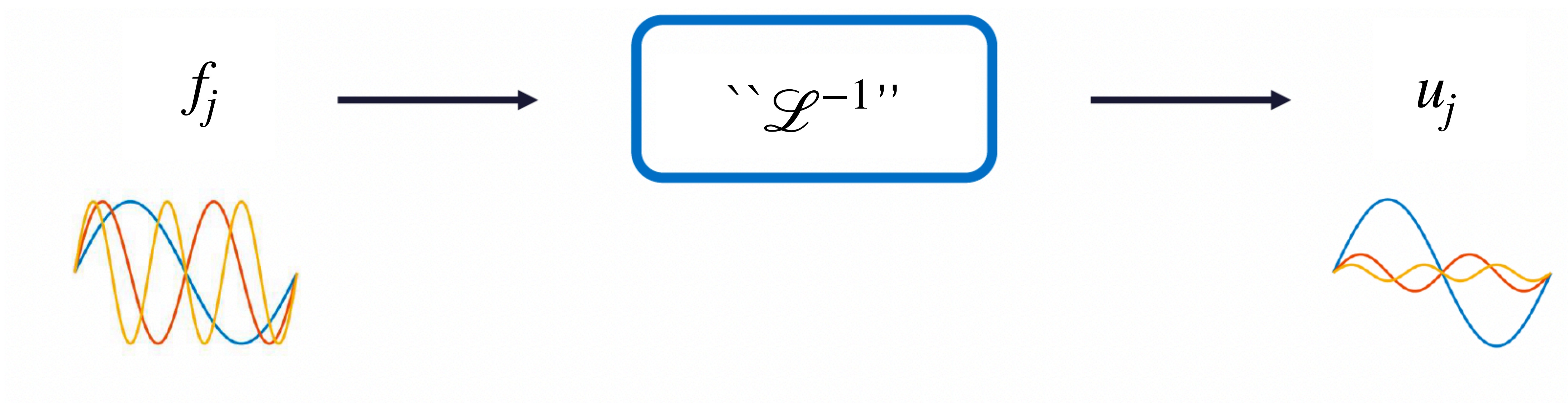

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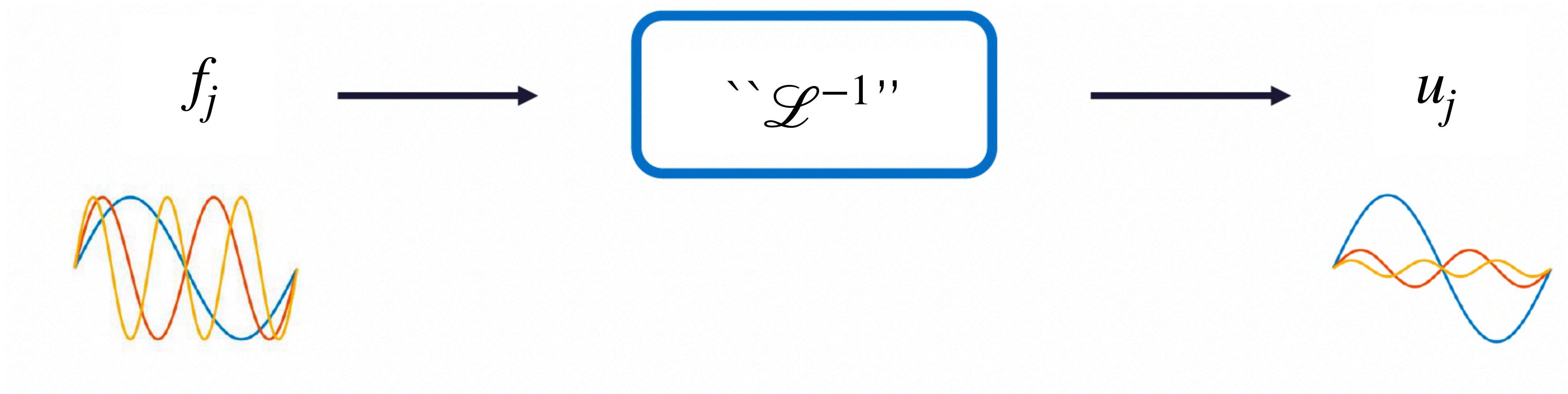

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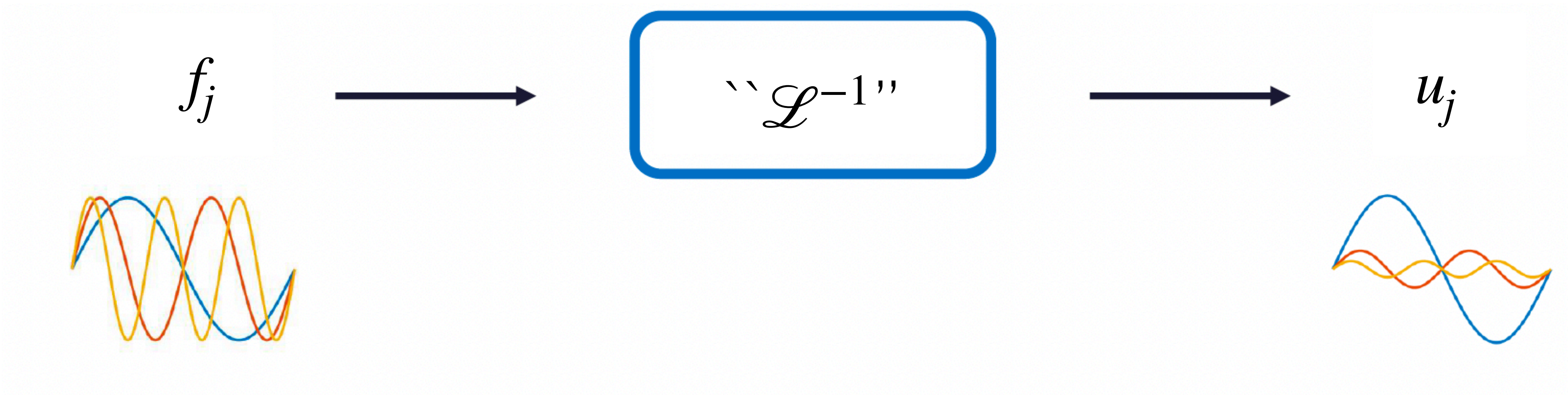

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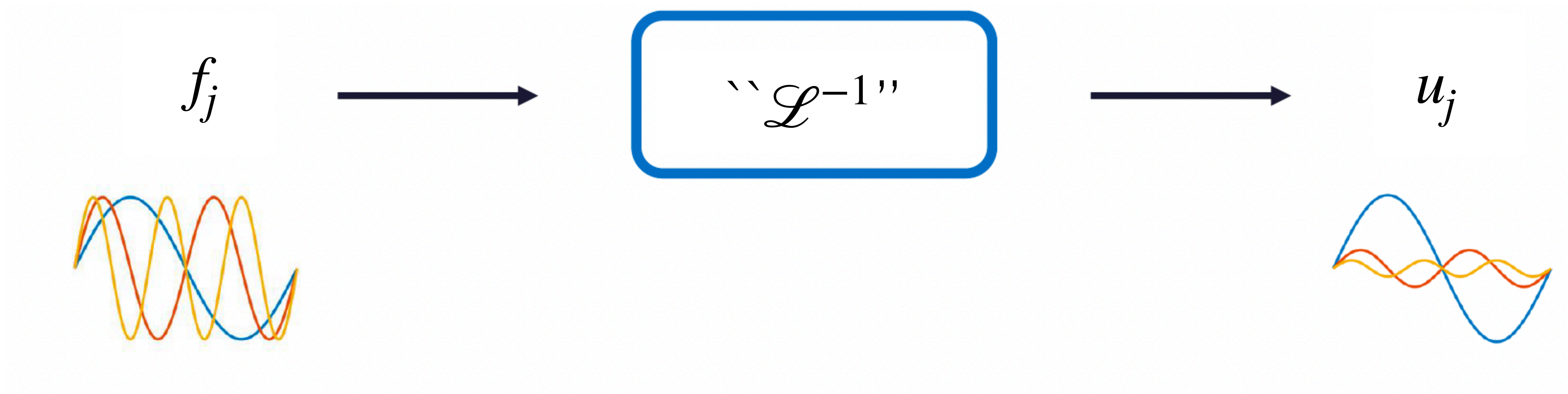

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Small selection of practical work:

[Brunton, Proctor, & Kutz, 16], [Rudy, Brunton, Proctor, & Kutz, 17], [Schaeffer, 17], [Raissi, Perdikaris, & Karniadakis, 17], [Raissi, 18], [Han, Jentzen, and E, 2018], [Khoo, Lu, & Ying, 2018], [Fan, Feliu-Faba, Lin, Ying, Zepeda-Nunez, 2018], [Raissi, Perdikaris, & Karniadakis, 19], [Gin, Shea, Brunton, & Kutz, 21]

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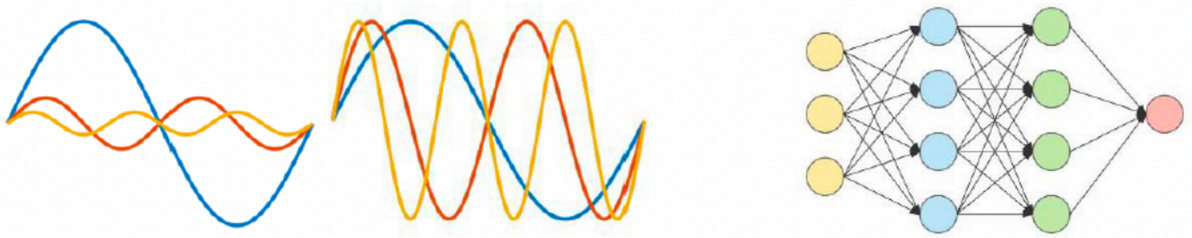
f_j

u_j $\longrightarrow$ $\boxed{\text{Train NN}}$



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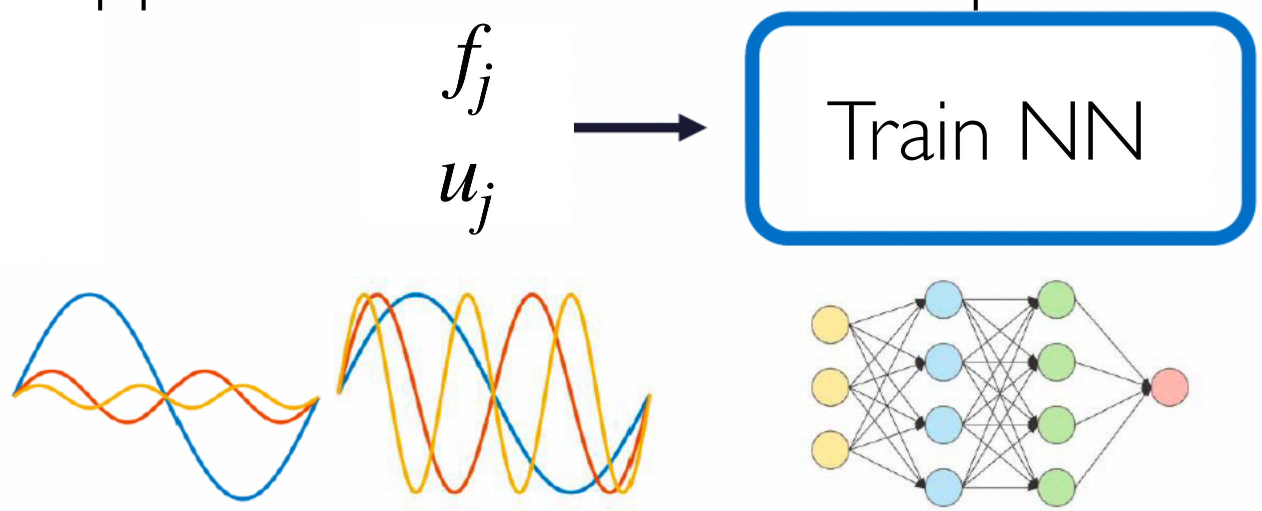
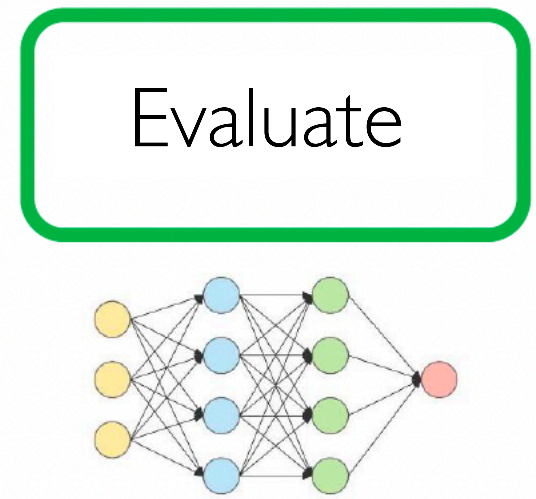


Solution operator



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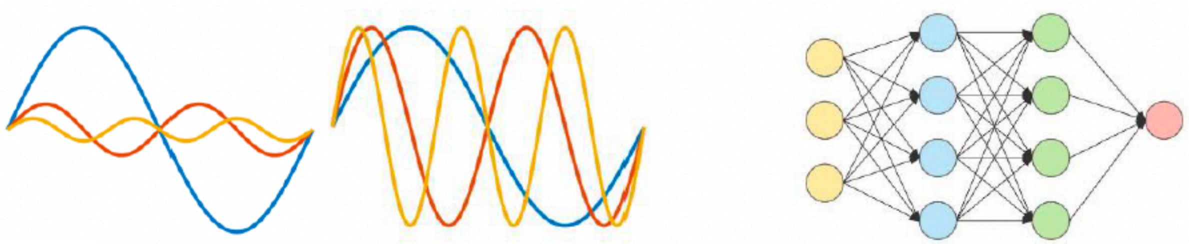
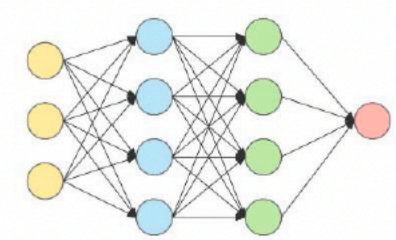
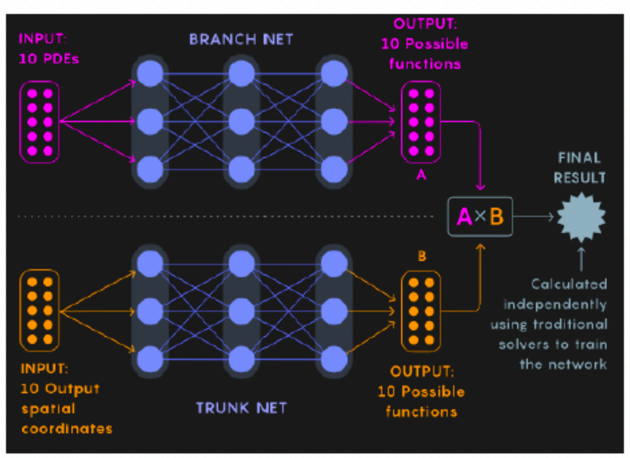


Solution operator

Evaluate

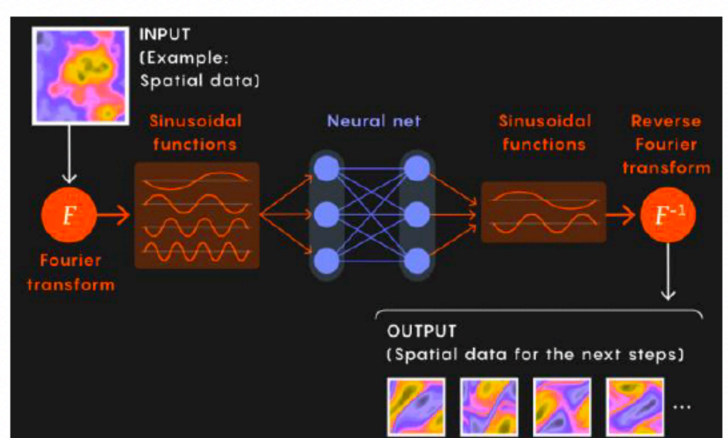


DeepONet



[Quanta Magazine; Lu et al, 2021]

Fourier Neural Operator



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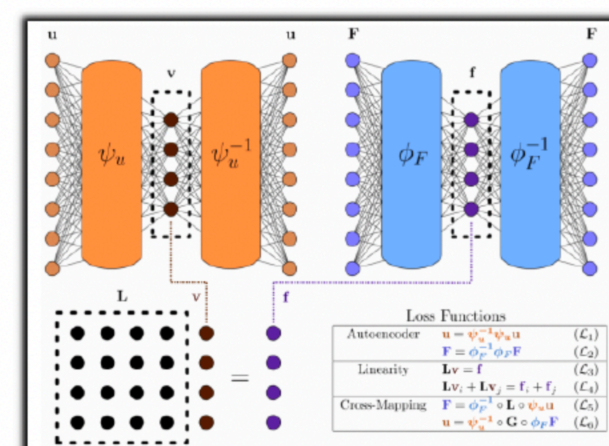
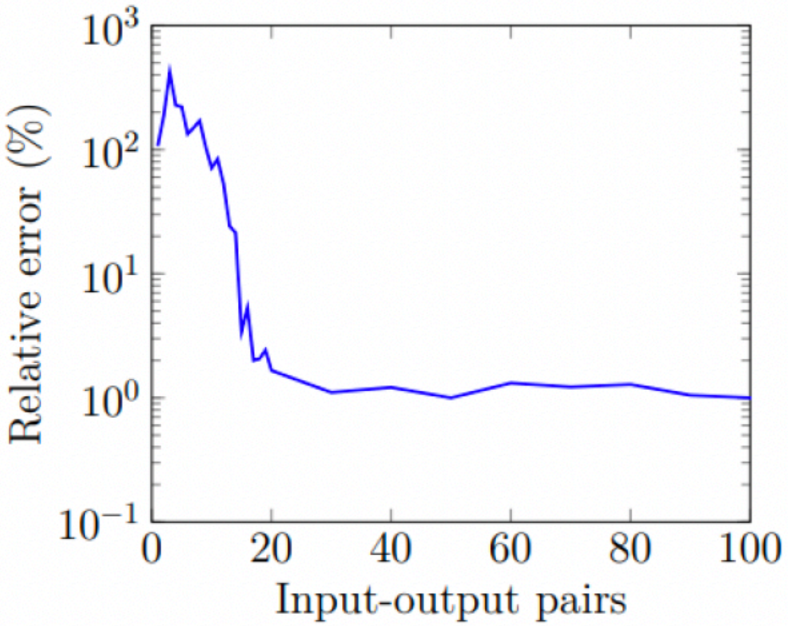
DeepGreen



[Gin et al., 2020]

Main challenges

1. Theoretical results



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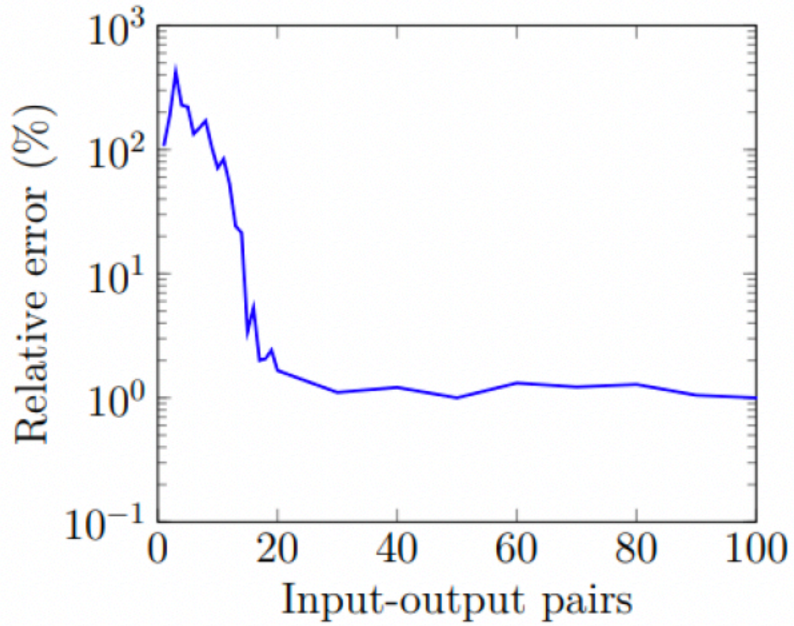

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- Performance guarantees
- Neural network architectures
- Noise robustness

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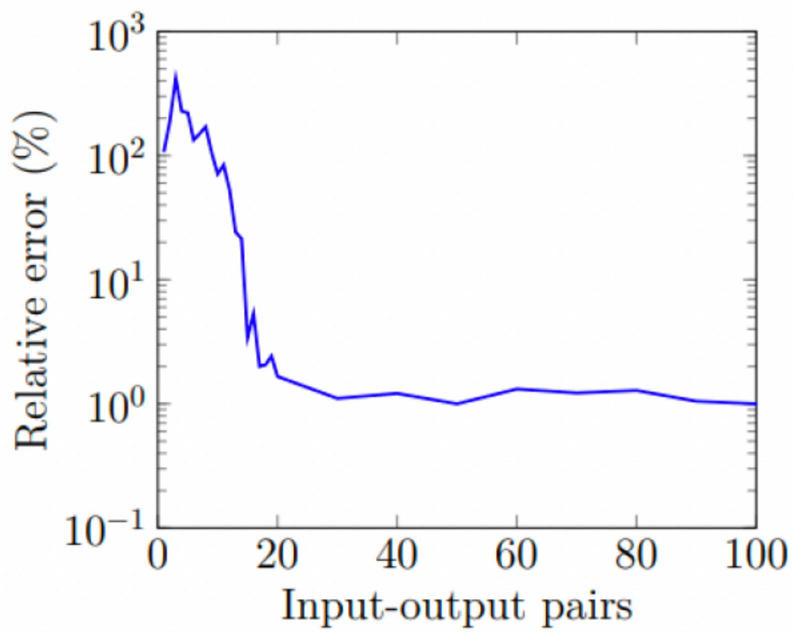

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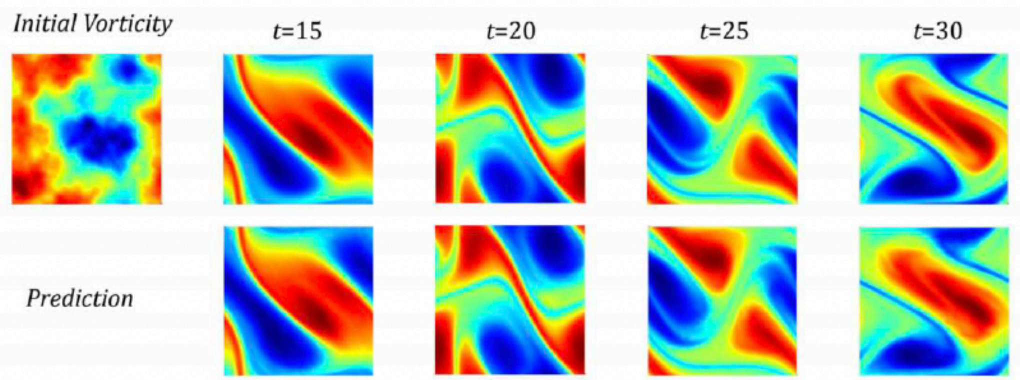

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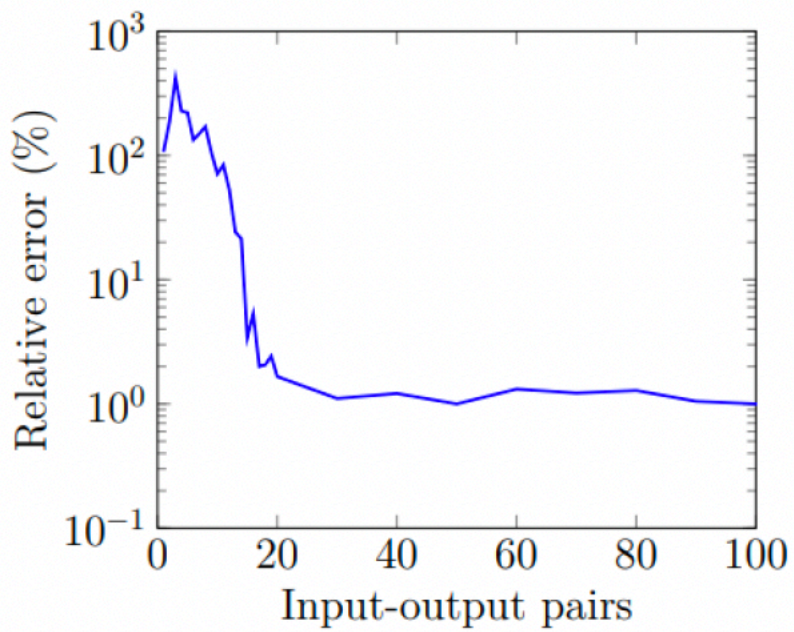

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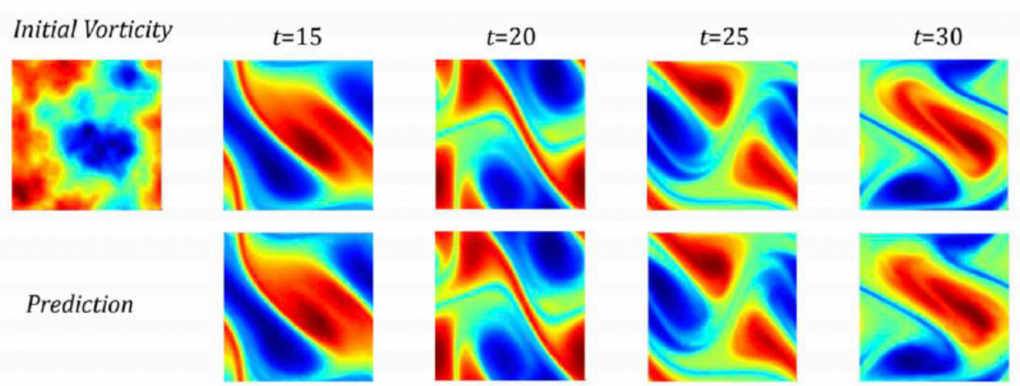

[Li et al, 2020]

- Dominant modes
- Symmetries
- Conservation laws
- Singularities

Green's function

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Equivalently, for a uniformly elliptic PDE, learn a Green's function such that

$$u_j(x) = \int_\Omega G(x,y) f_j(y) dy, \qquad x \in \Omega, \qquad 1 \leq j \leq k+5$$

This is a Hilbert-Schmidt (HS) integral operator.

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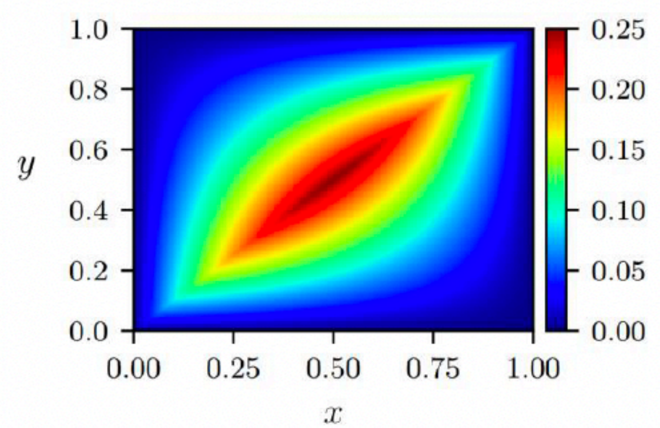
Poisson equation

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

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



Helmholtz equation

$$\nabla^2 u + k^2 u = f$$

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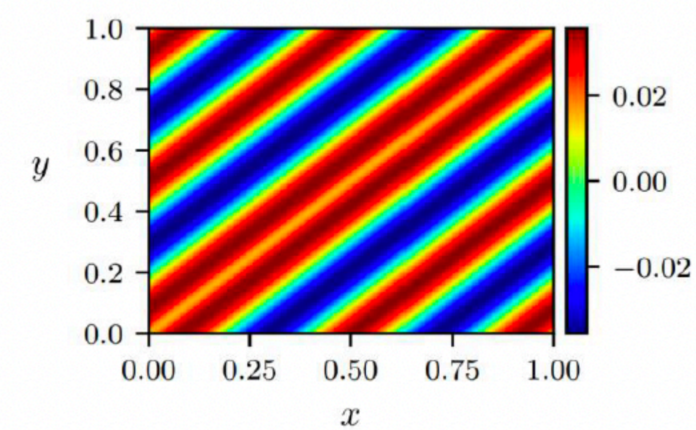

Final theoretical result

Symmetric pos. def. matrix with bounded coefficients

Self-adjoint elliptic PDEs in 1D, 2D, or 3D of the form:

$$\mathcal{L}u := -\nabla \cdot (A(x)\nabla u) = f \longrightarrow u(x) = \int_{\Omega} G(x,y) f(y)\,\mathrm{d}y$$

Theorem [Boullé & T., 2021]

There is a randomized algorithm that, for any $\epsilon > 0$, can construct an approximation $\tilde{G}$ of G with $O(\epsilon^{-6}\log^4(1/\epsilon)/\Gamma_\epsilon)$ input-output pairs (f, u) such that

$$||G - \tilde{G}||_{L^2(D\times D)} = O(\Gamma_\epsilon^{-3/4}\log^3(1/\epsilon)\,\epsilon)\,,$$

with high probability.

Proof

1. Randomized numerical linear algebra
2. Regularity of the Green's function

Randomized numerical linear algebra

Randomized SVD

We can learn symmetric low-rank matrices via matrix-vector products $v \mapsto Xv$:

Randomized SVD:

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

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Randomized SVD:

1 $n \times (k+5)$

$Y =$ 

Tall-skinny Gaussian matrix
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$A_k = QQ^*X$

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Theorem (Halko, Martinsson, Tropp, 2011).

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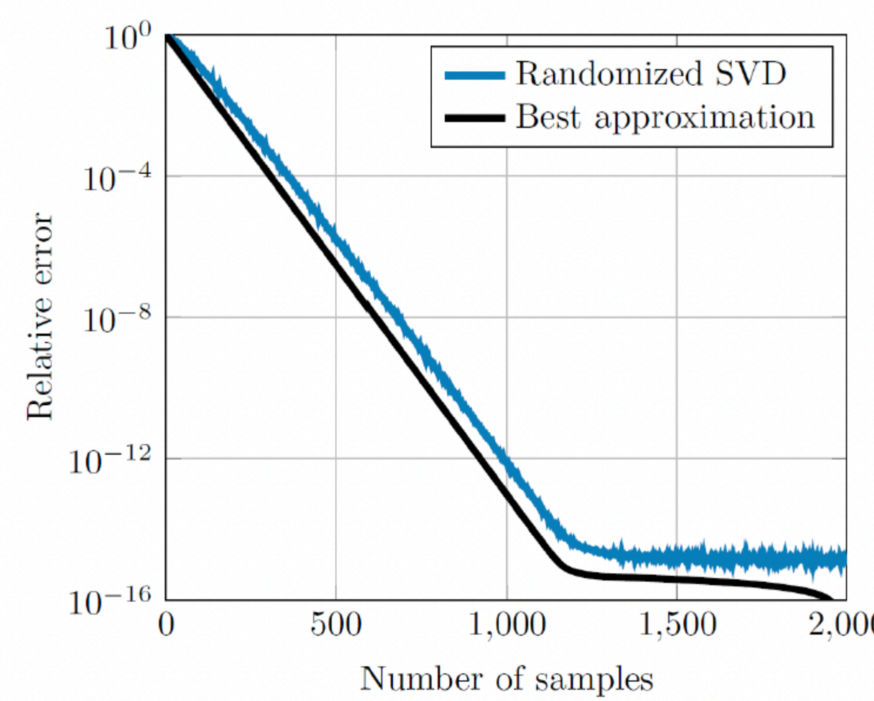

Generalization of the randomized SVD

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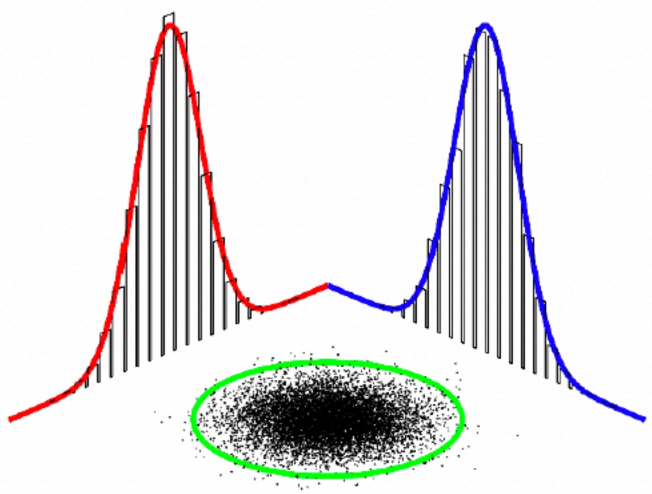
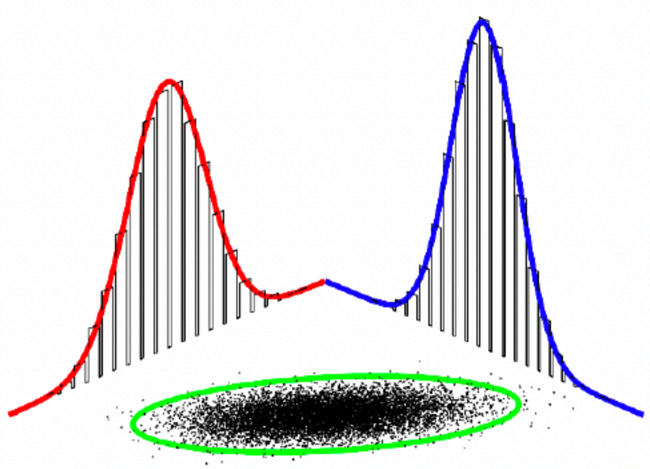
Standard Gaussian vectors



Correlated Gaussian vectors



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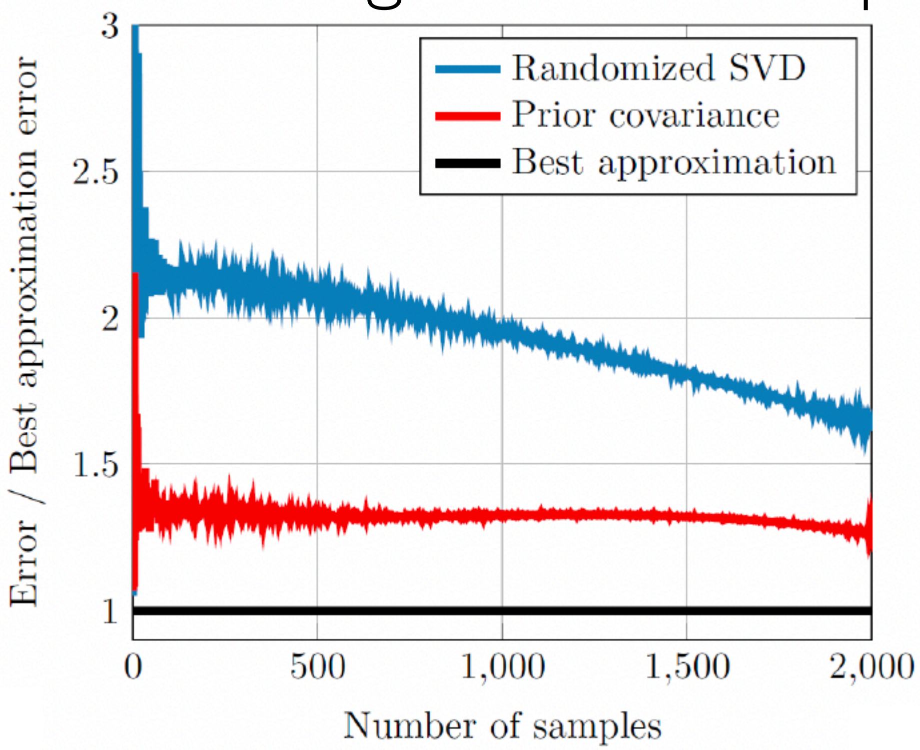
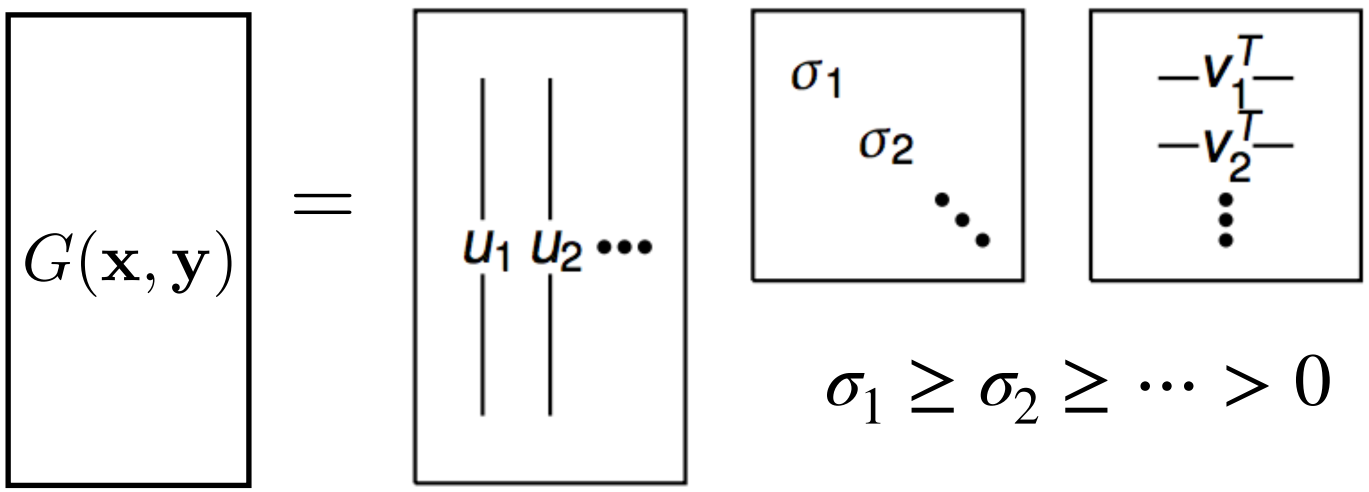
Prior knowledge about A helps:



Singular values of a function

Singular value expansion of a square-integrable function $G : \Omega_1 \times \Omega_2 \to \mathbb{R}$:

Σ = diagonal, U, V = orthonormal columns



At least formally

$$\sigma_1 \geq \sigma_2 \geq \cdots > 0$$

[Schmidt 1907], [Weyl 1912], [Hammerstein 1923], [Smithies 1937]

$$k = \text{rank}_\epsilon(G)$$

means

$$\sqrt{\sum_{j=k+1}^{\infty} \sigma_j^2} \leq \epsilon \|G\|_{L^2(\Omega_1 \times \Omega_2)}$$

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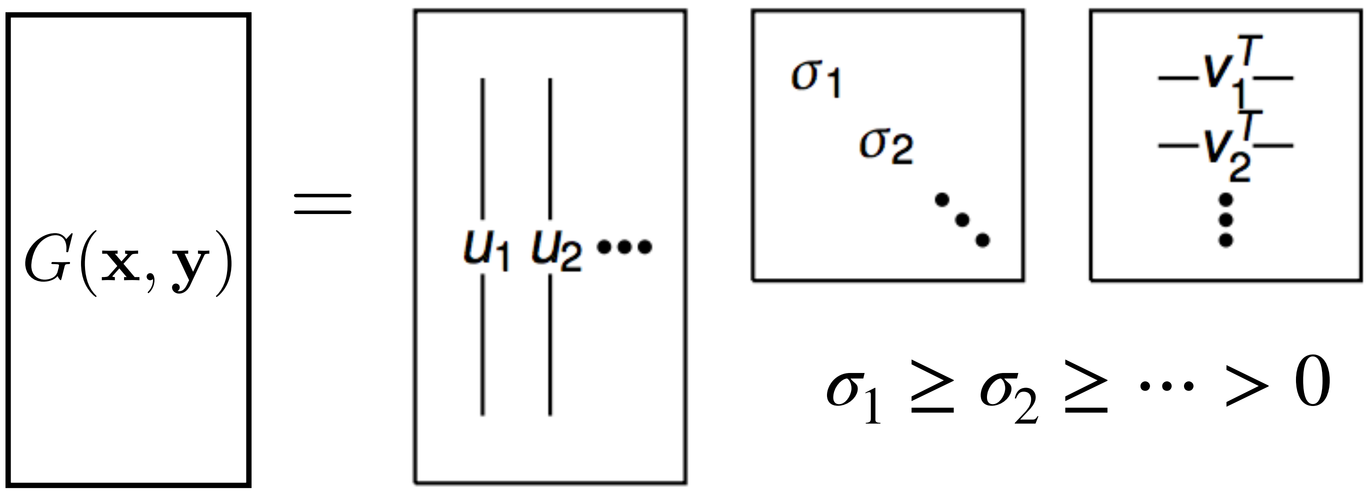

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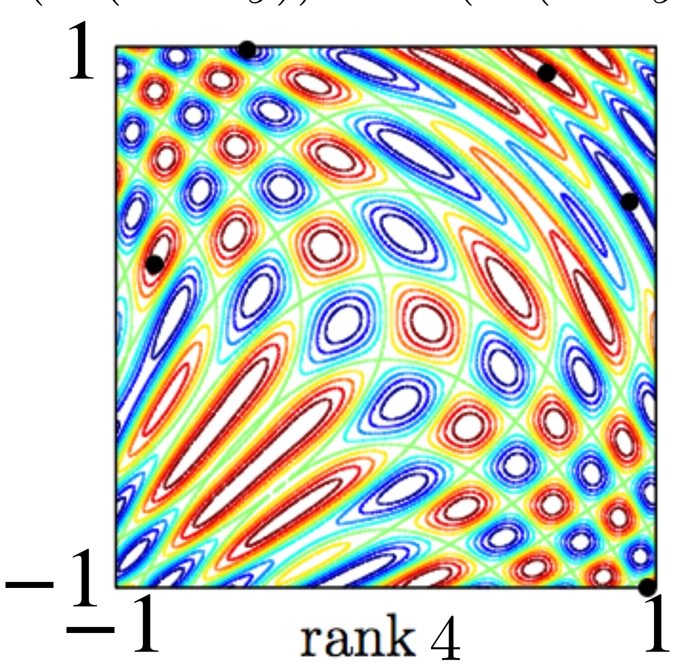
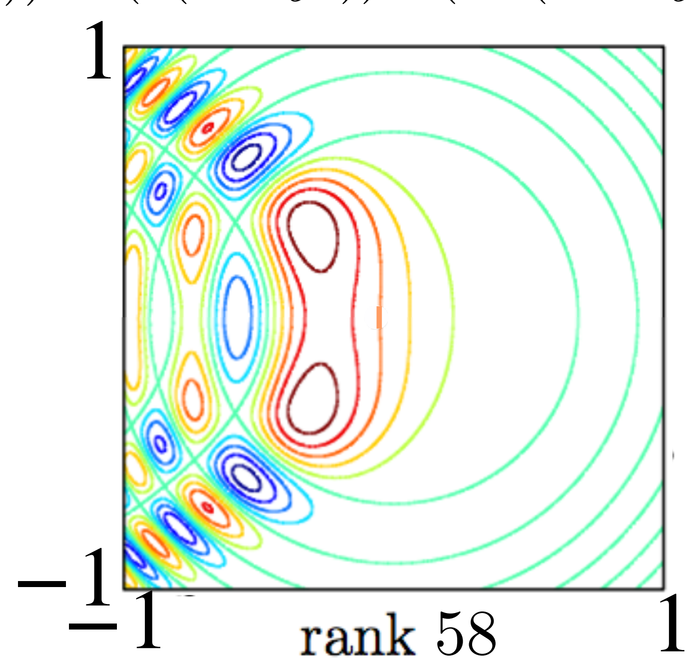
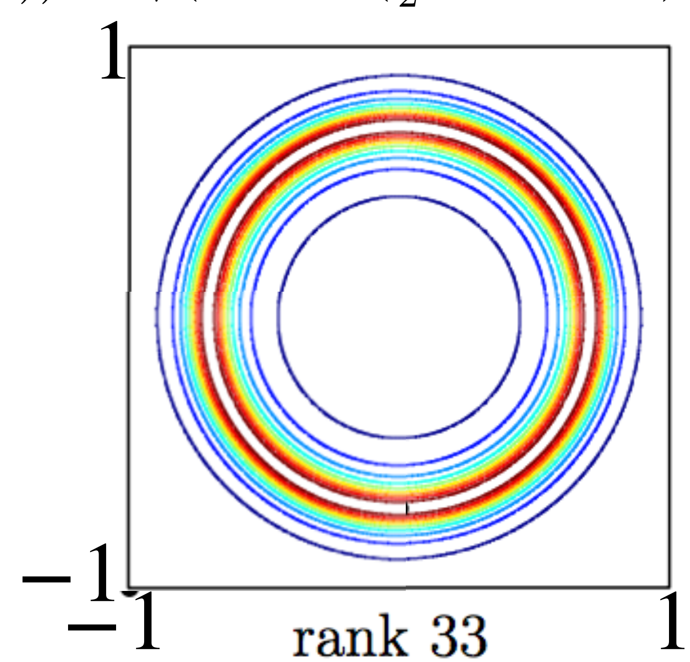
$\cos(10(x^2 + y)) + \sin(10(x + y^2))$



$\mathrm{Ai}(5(x + y^2))\mathrm{Ai}(-5(x^2 + y^2))$



$1/(1 + 100(\frac{1}{2} - x^2 - y^2)^2)$



$$\epsilon = 10^{-15}$$

Also, see: [T. & Trefethen, 14], [Hashemi & Trefethen, 17], [Gorodetsky, Karaman, & Marzouk, 18]

Randomized SVD for Green's functions

[Boulle & T., 21]

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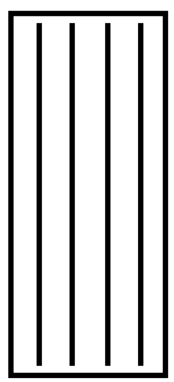
$Y =$ 

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

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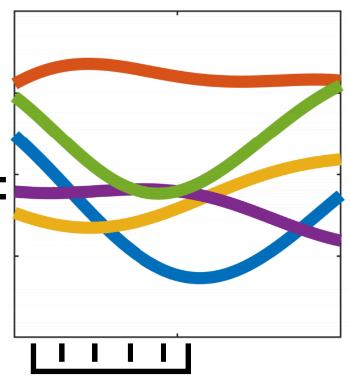
$Y =$ 

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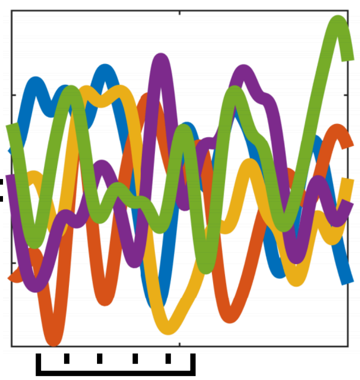
$Y =$ 

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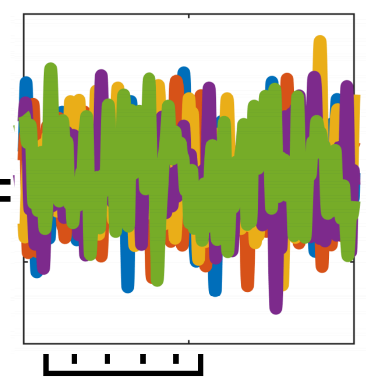
$Y =$ 

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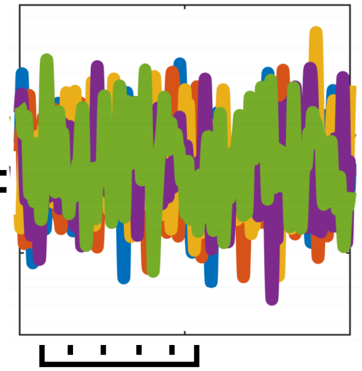
$Y =$ 

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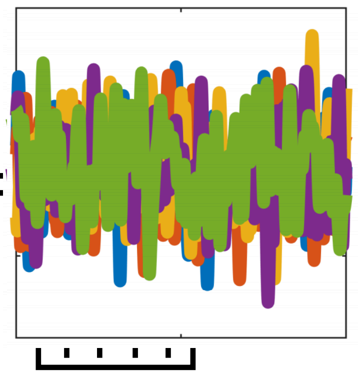
$Y =$ 

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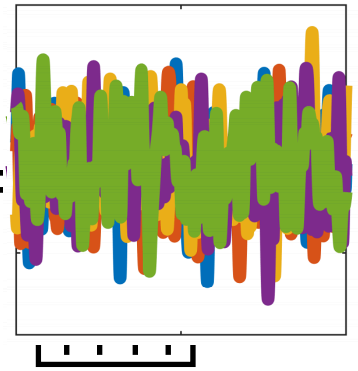
$Y =$ 

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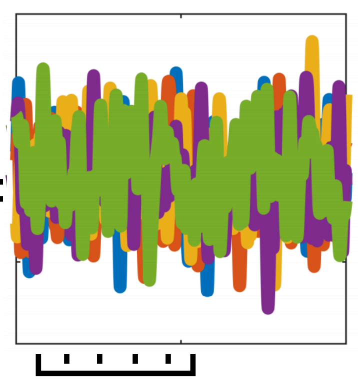
$Y =$ 

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2 $Z_i(x) = \int_\Omega G(x,y)Y_i(y)dy$

Input-output data

3 $Q = \mathrm{orth}(Z)$

orthonormal basis for $\mathrm{col}(Z)$

``$G_k = QQ^*G$''

Theorem [Boullé & T., 2021]

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

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

Problem:

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

ϵ_k **decays very slowly with k**

Smoothness implies low-rank

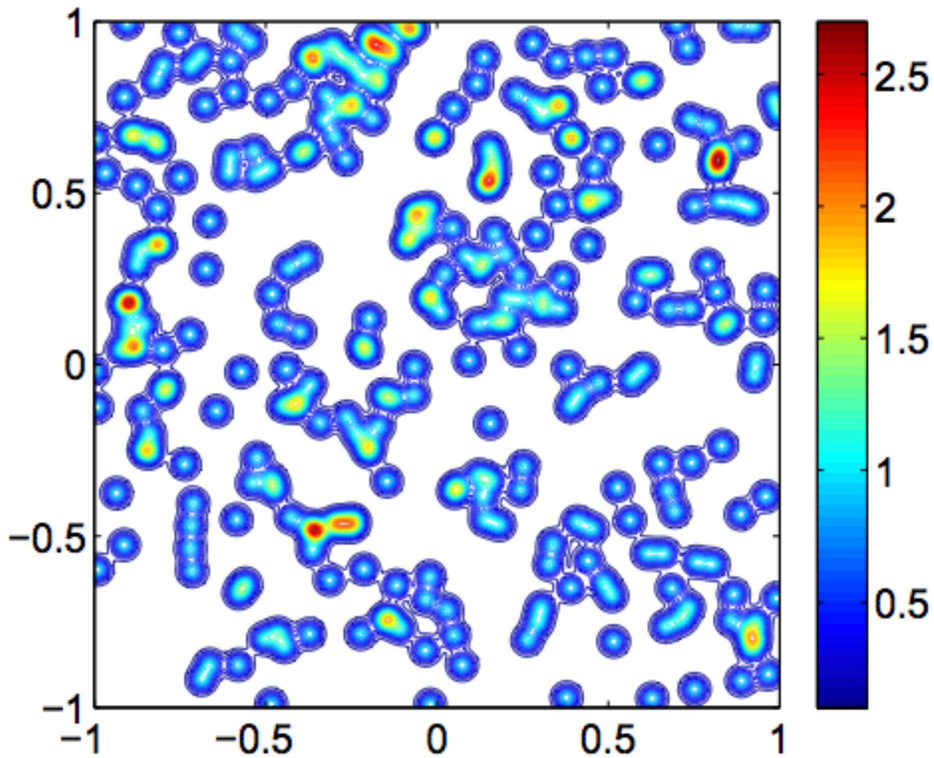
Suppose $X_{ij} = G(x_i, y_j)$, where $G : [-1,1]^2 \to \mathbb{R}$ is a continuous function.

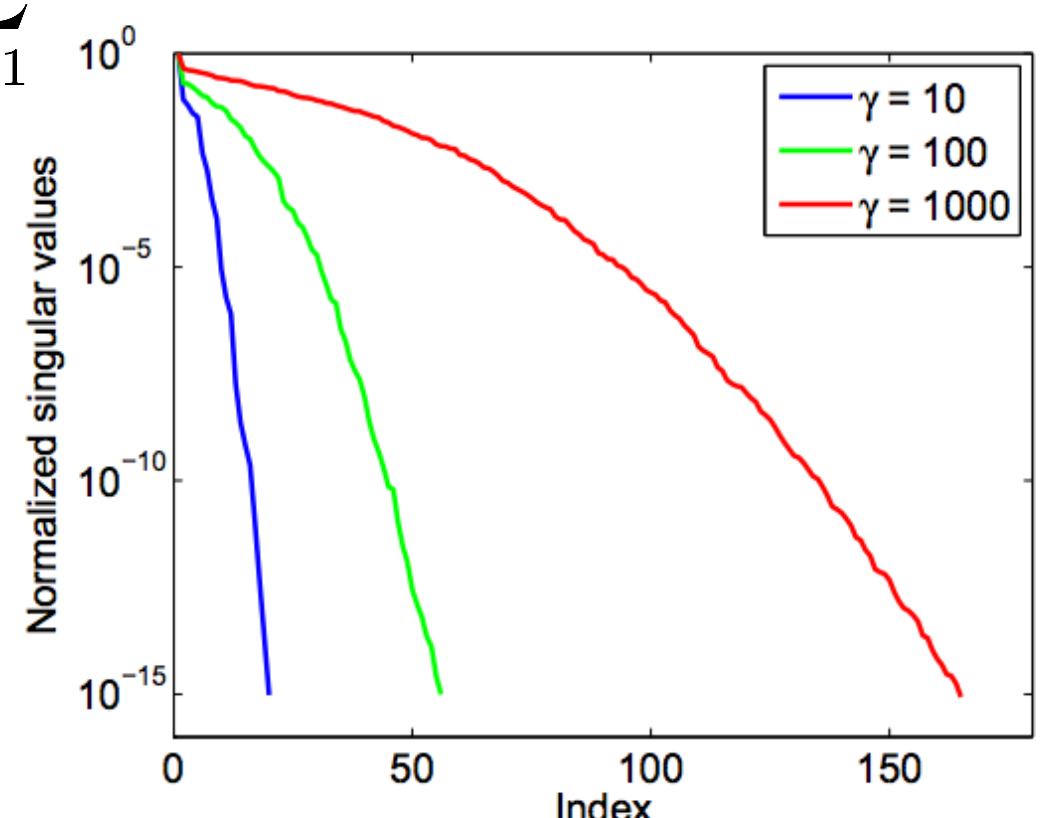
$G(\cdot, y)$ is ν-times diff. with bounded variation: $\sigma_k(G) = \mathcal{O}(k^{-\nu})$

$G(\cdot, y)$ is bounded analytic in neighborhood of $[-1,1]$: $\sigma_k(G) = \mathcal{O}(\rho^{-k})$

[Reade, 83], [Little & Reade, 84], [Ibragimov & Rjasanow, 09], [Khoromskij, 10], [Trefethen, 13]

$$G(x,y) = \sum_{j=1}^{300} e^{-\gamma\left((x-x_j)^2+(y-y_j)^2\right)}$$





Extensions to multivariate functions and tensors [Khoromskij, 10].

Aside: Covariance quality factor

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

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

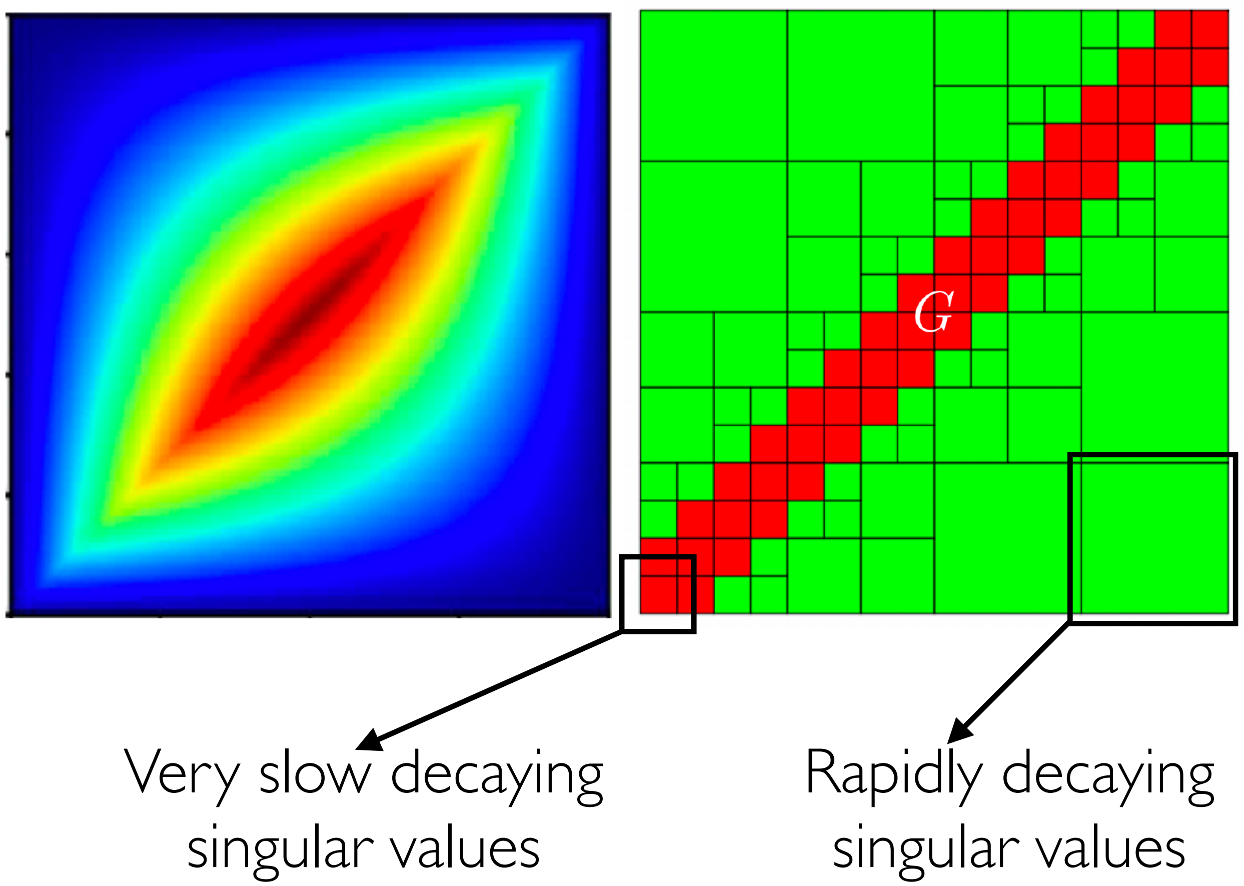
where v_i is the ith right singular vectors of G.

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

Regularity of Green's functions

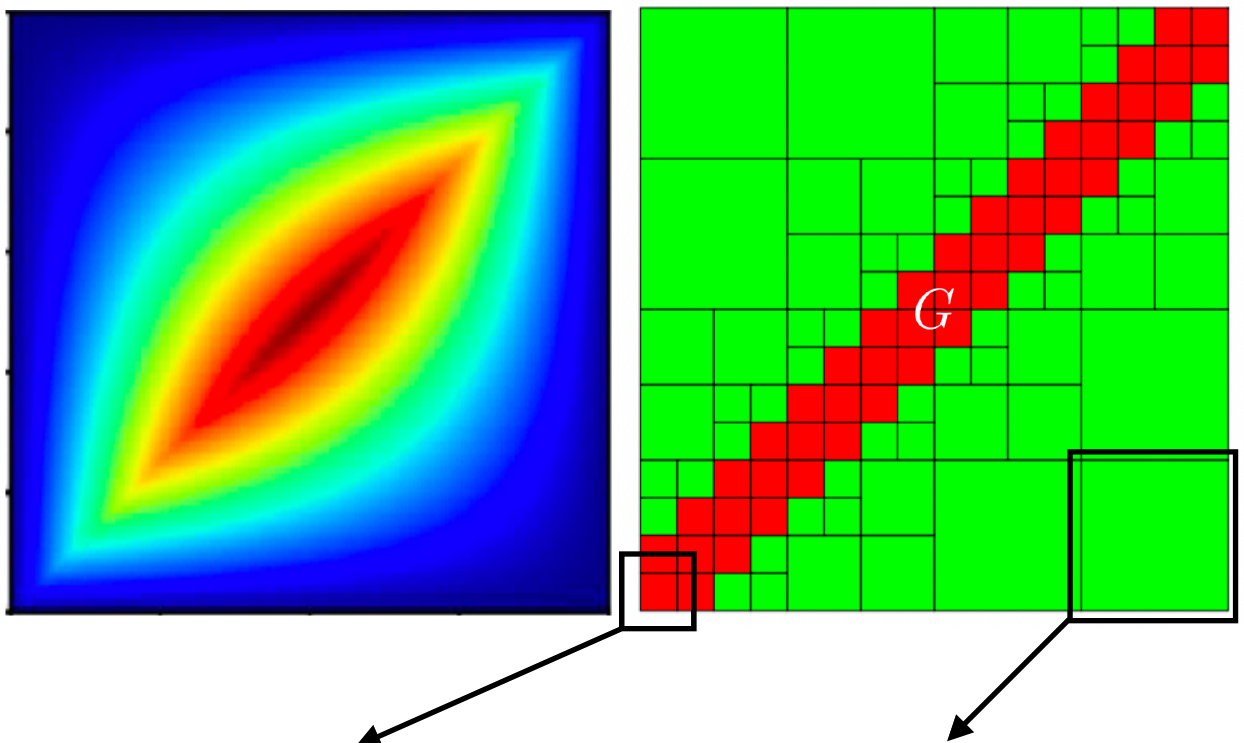
Green's functions are low rank on separated blocks

One dimension



Green's functions are low rank on separated blocks

One dimension

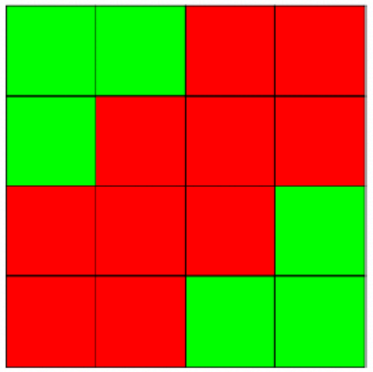


Very slow decaying singular values

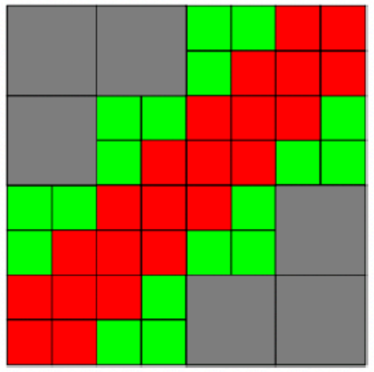
Rapidly decaying singular values

Hierarchical structure

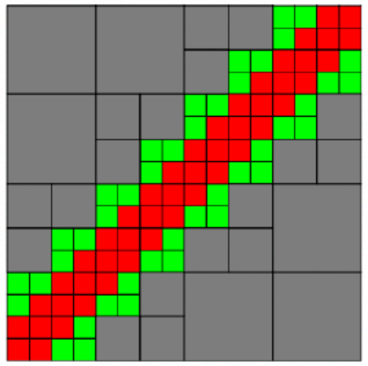
Level 2



Level 3

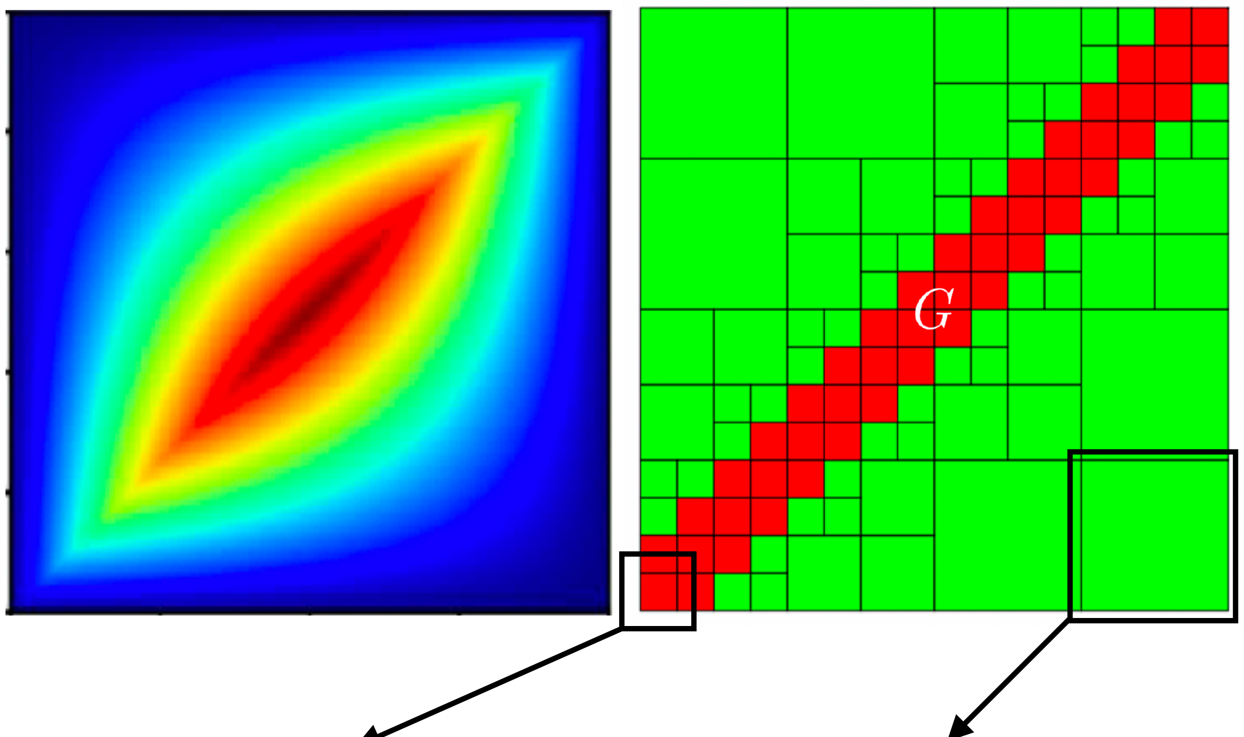


Level 4



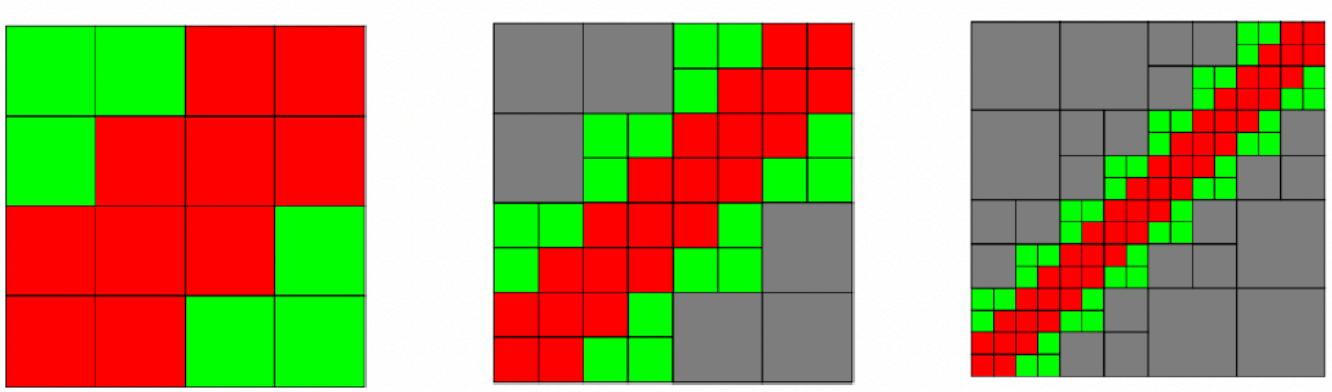
Green’s functions are low rank on separated blocks

One dimension

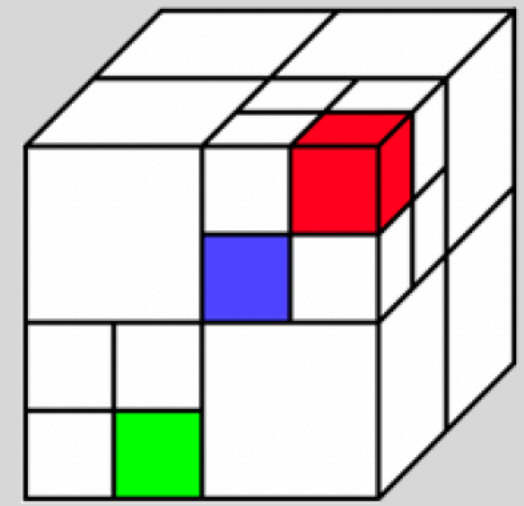


<u>Hierarchical structure</u>

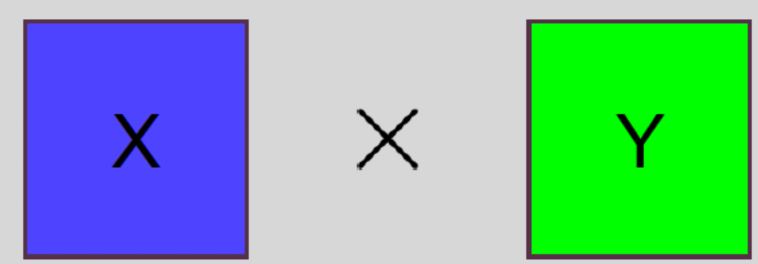
Level 2 | Level 3 | Level 4



Three dimensions

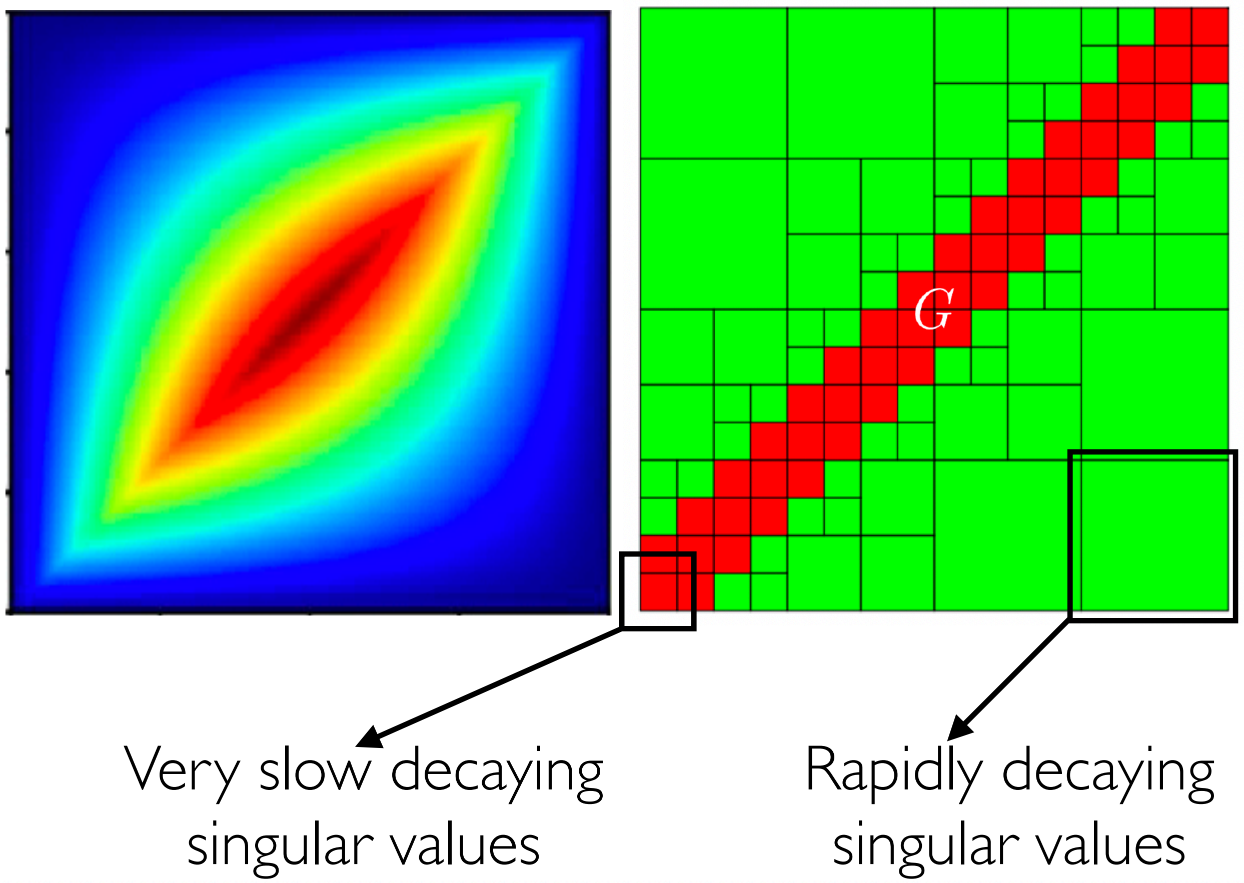


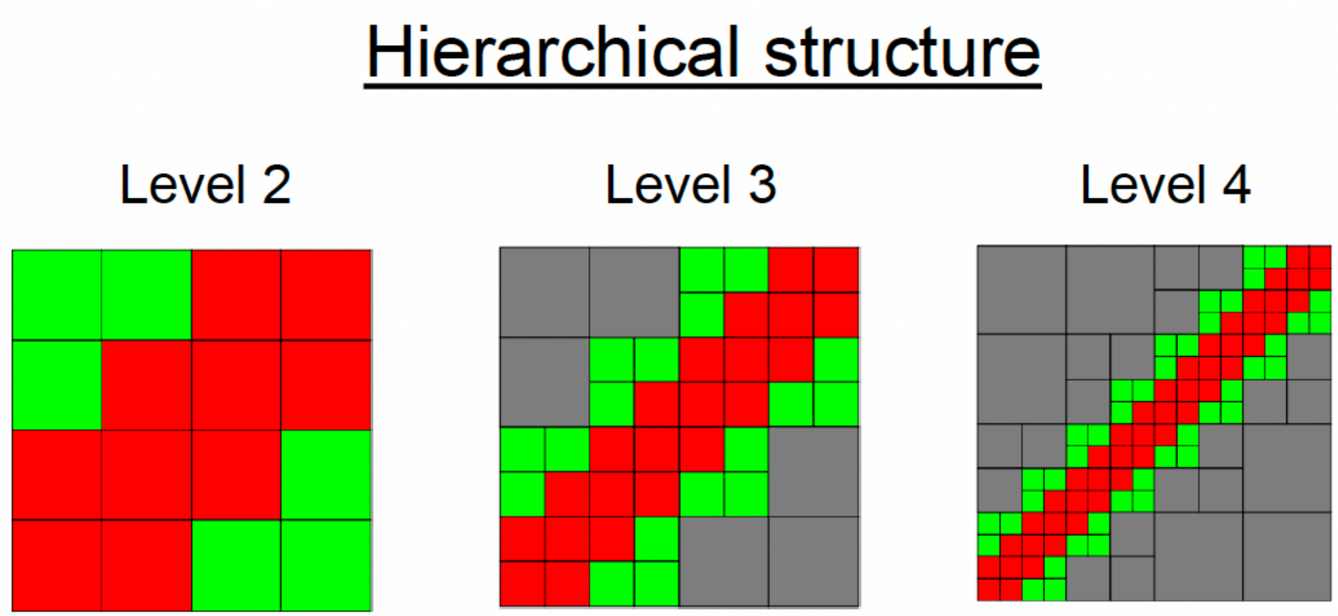
Low-rank structure on well separated domains.
[Bebendorf, Hackbush, 2003]



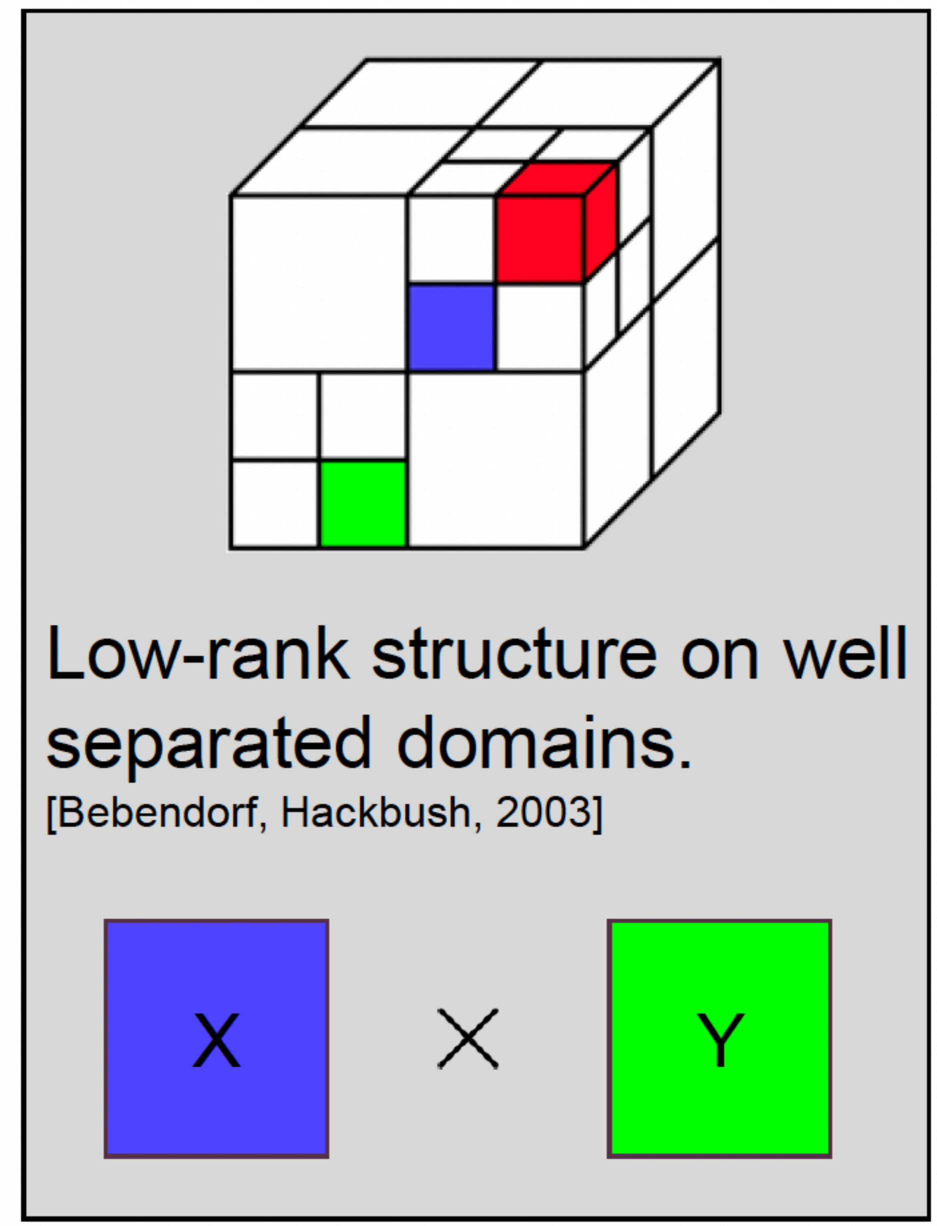
Green's functions are low rank on separated blocks

One dimension





Three dimensions

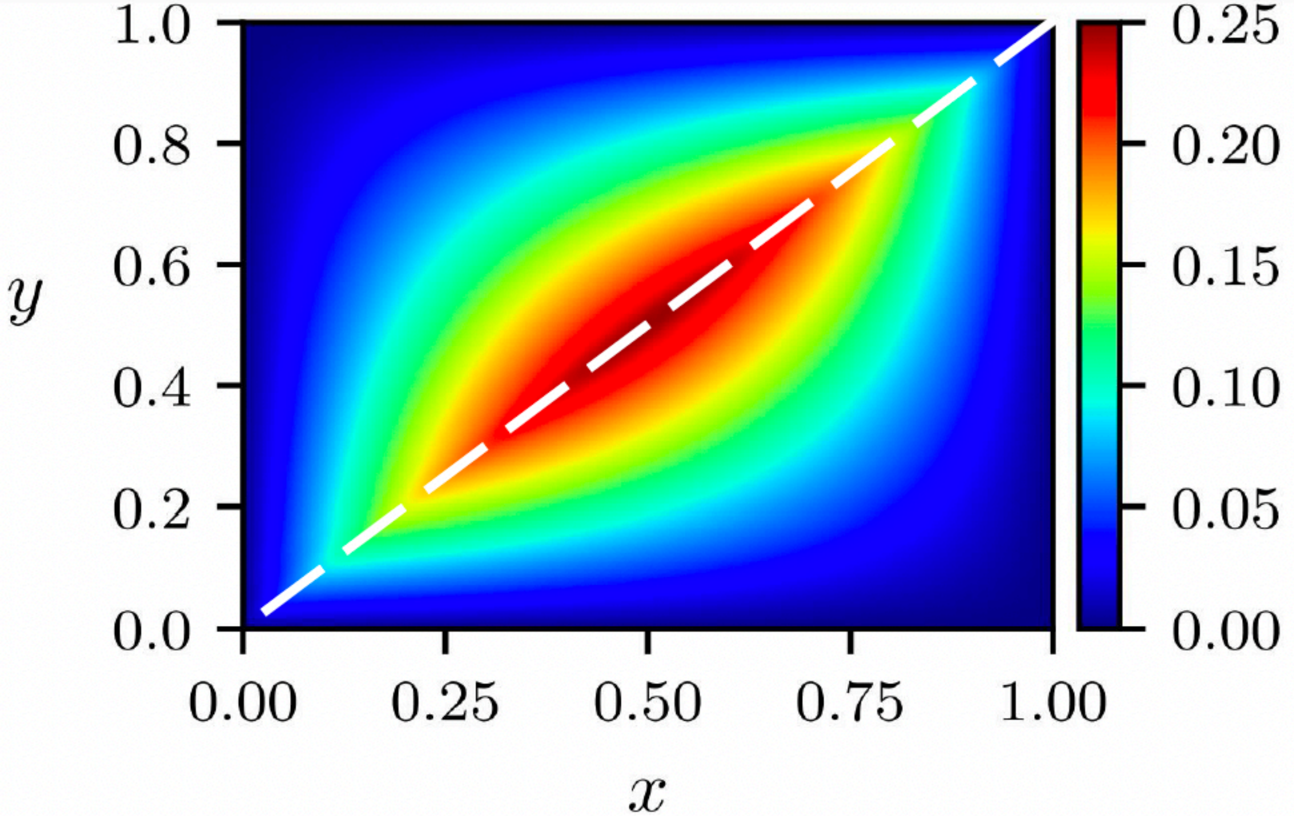


Related approaches for matrices:
[Martinsson, 2008], [Lin, Lu, Ying, 2010], [Martinsson, 2016]

Off-diagonal decay

Green's function of the Laplace operator:

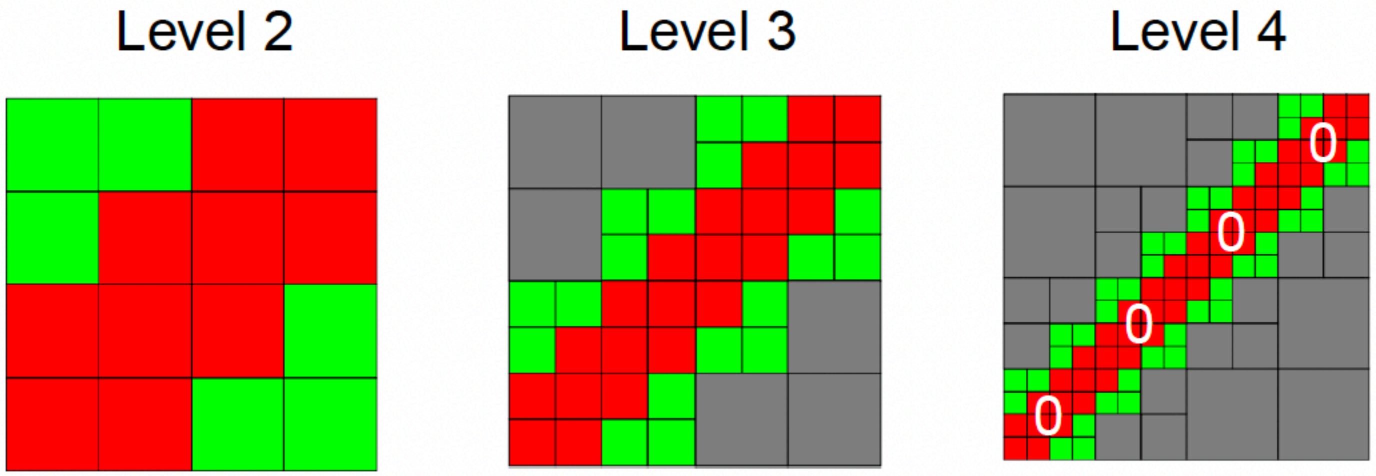
$$-\nabla^2 u = f$$



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

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

Hierarchical structure



PDE learning with a rigorous "learning rate"

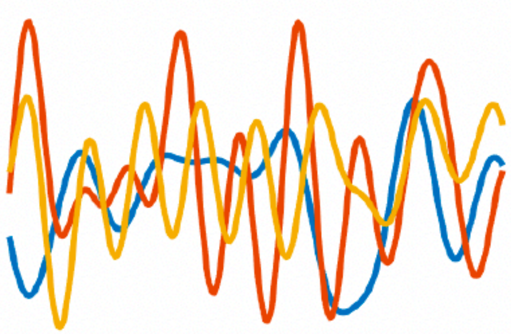
Theorem [Boullé & T., 2021]

There is a randomized algorithm that, for any $\epsilon > 0$, can construct an approximation $\tilde{G}$ of G with $O(\epsilon^{-6}\, log^4(1/\epsilon)/\Gamma_\epsilon)$ input-output pairs (f, u) such that

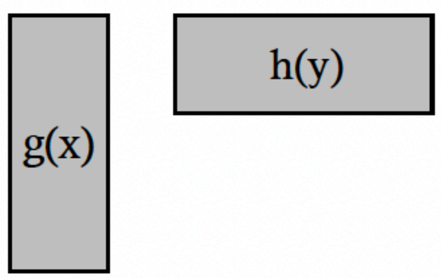
$$\|G - \tilde{G}\|_{L^2(D\times D)} = O(\Gamma_\epsilon^{-3/4} \log^3(1/\epsilon)\,\epsilon)\ ,$$

with high probability.

Randomized linear algebra



Low-rank structure



Off-diagonal decay

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

PDE learning with a rigorous "learning rate"

Coming soon…

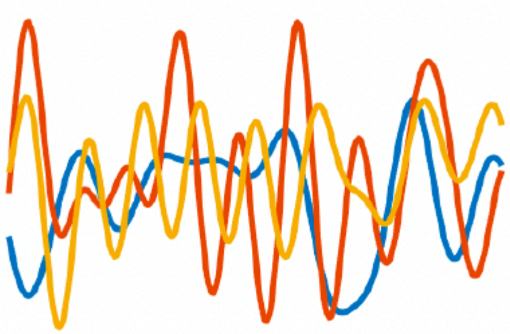
Theorem [Boullé & T., 2021]

There is a randomized algorithm that, for any $\epsilon > 0$, can construct an approximation $\tilde{G}$ of G with $\boxed{O(\quad log^4(1/\epsilon)/\Gamma_\epsilon)}$ *input-output pairs (f, u) such that*

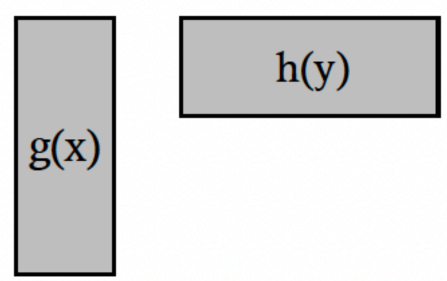
$$||G - \tilde{G}||_{L^2(D\times D)} = O(\Gamma_\epsilon^{-3/4} \log^3(1/\epsilon)\, \epsilon)\ ,$$

with high probability.

Randomized linear algebra



Low-rank structure



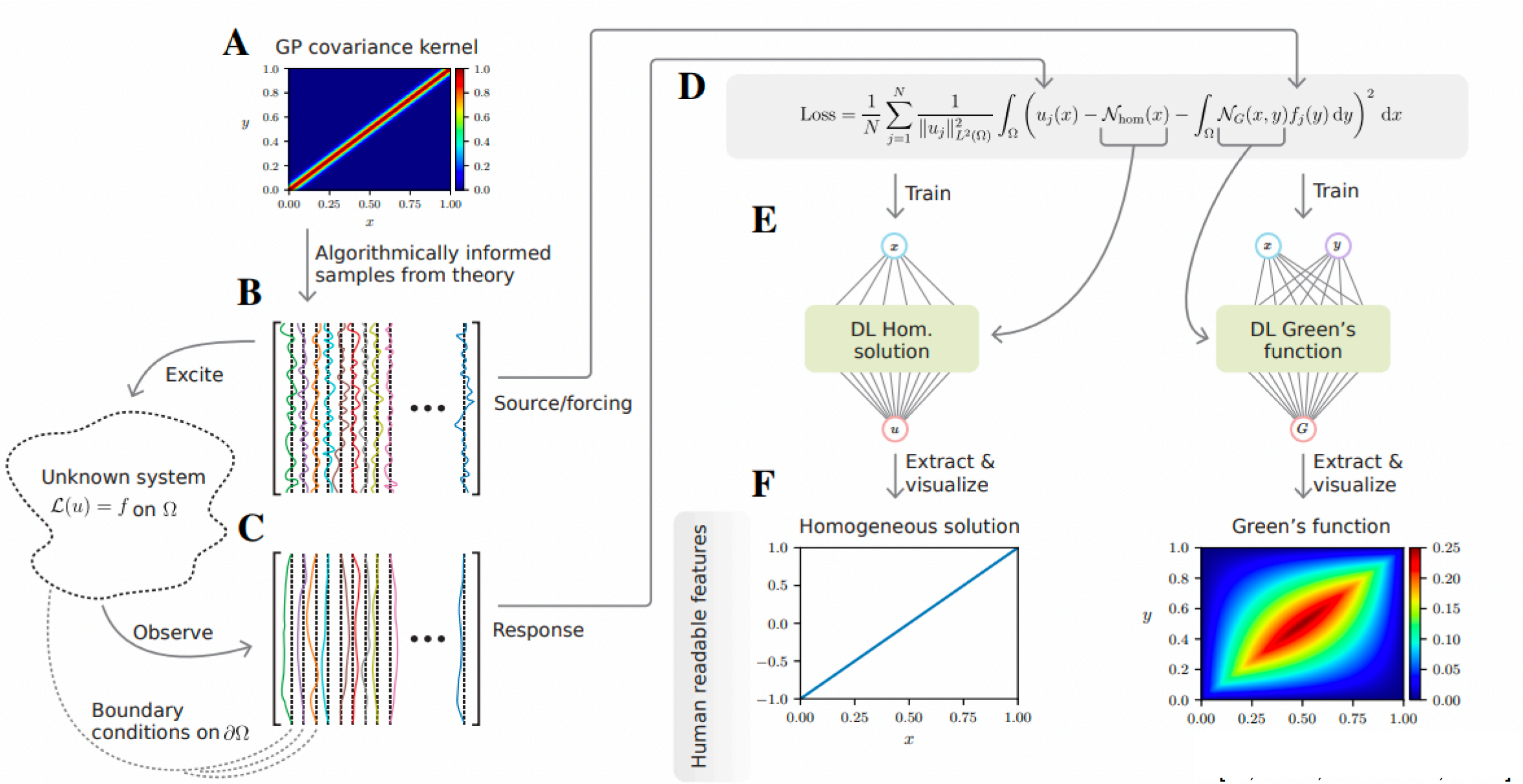
Off-diagonal decay

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

Learning Green's functions in practice

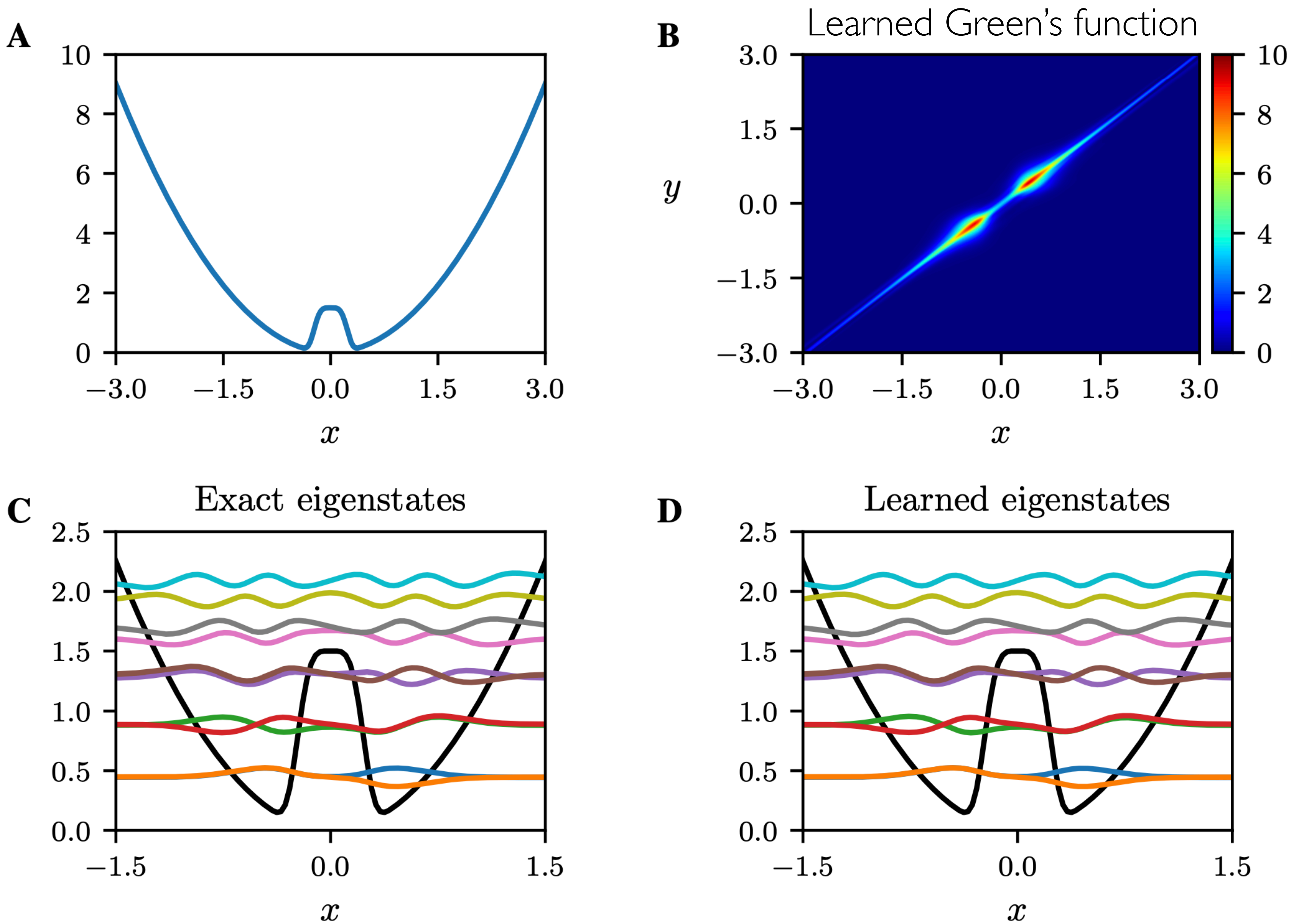
Deep learning method

[Boullé, Earls, T., 2021]



Schrödinger equation, double well potential

$$\mathscr{L}u = -(0.1)^2\frac{d^2u}{dx^2} + V(x)u, \quad u(\pm 3) = 0$$

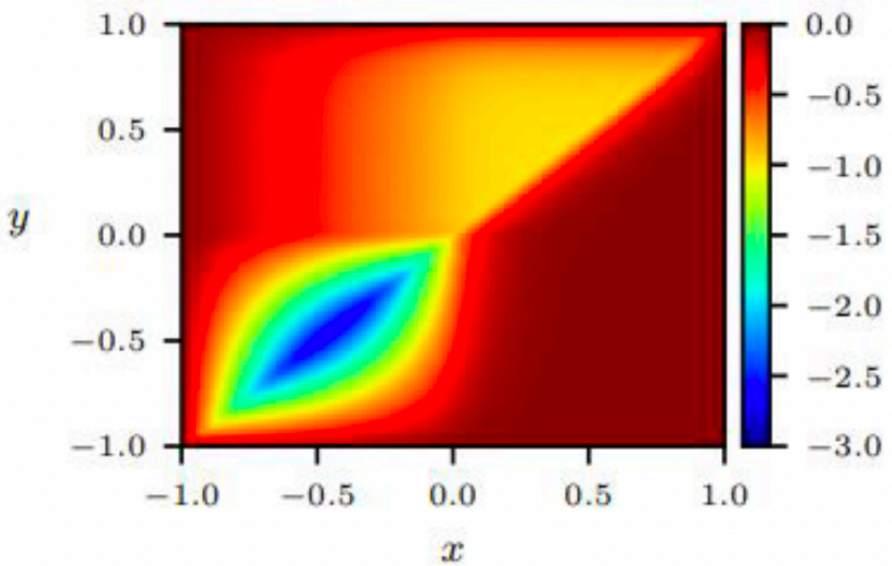


Advection-diffusion equation

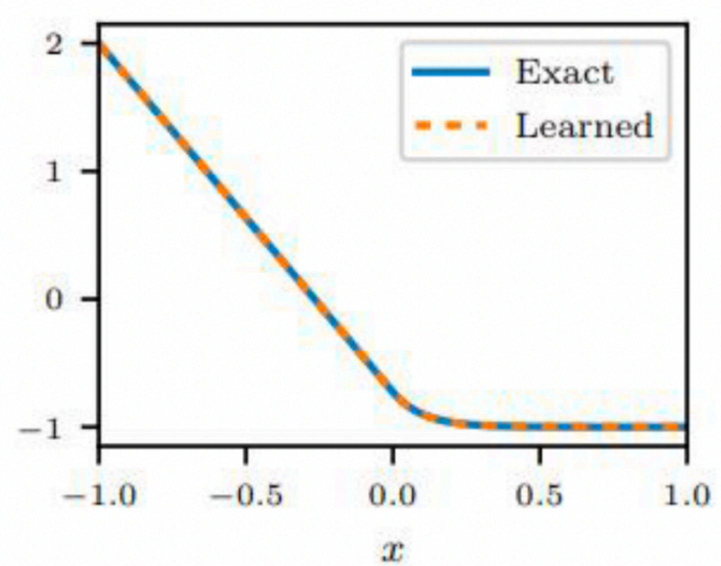
Equation:

$$\mathcal{L}u = 0.1\frac{d^2u}{dx^2} + (x \geq 0)\frac{du}{dx}, \qquad u(-1) = 2, \quad u(1) = -1$$

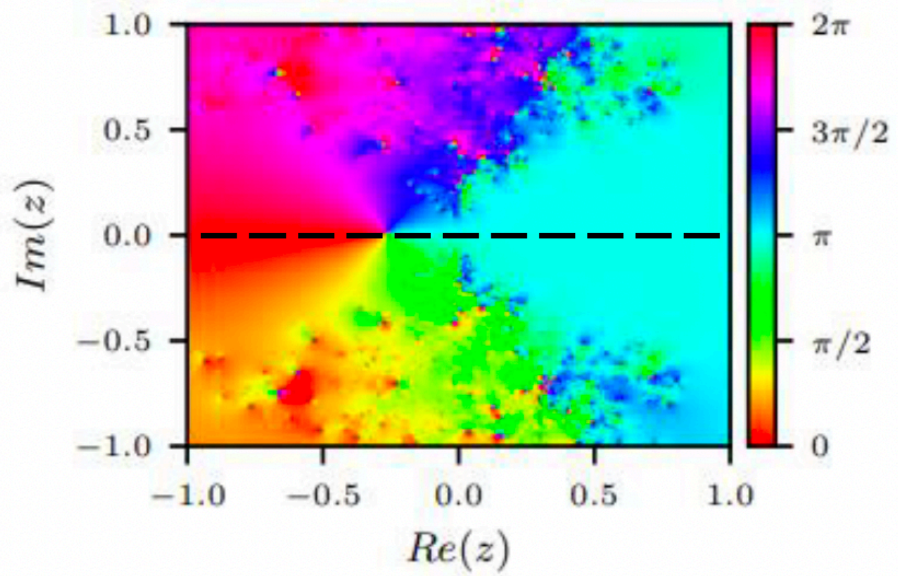
Green's function



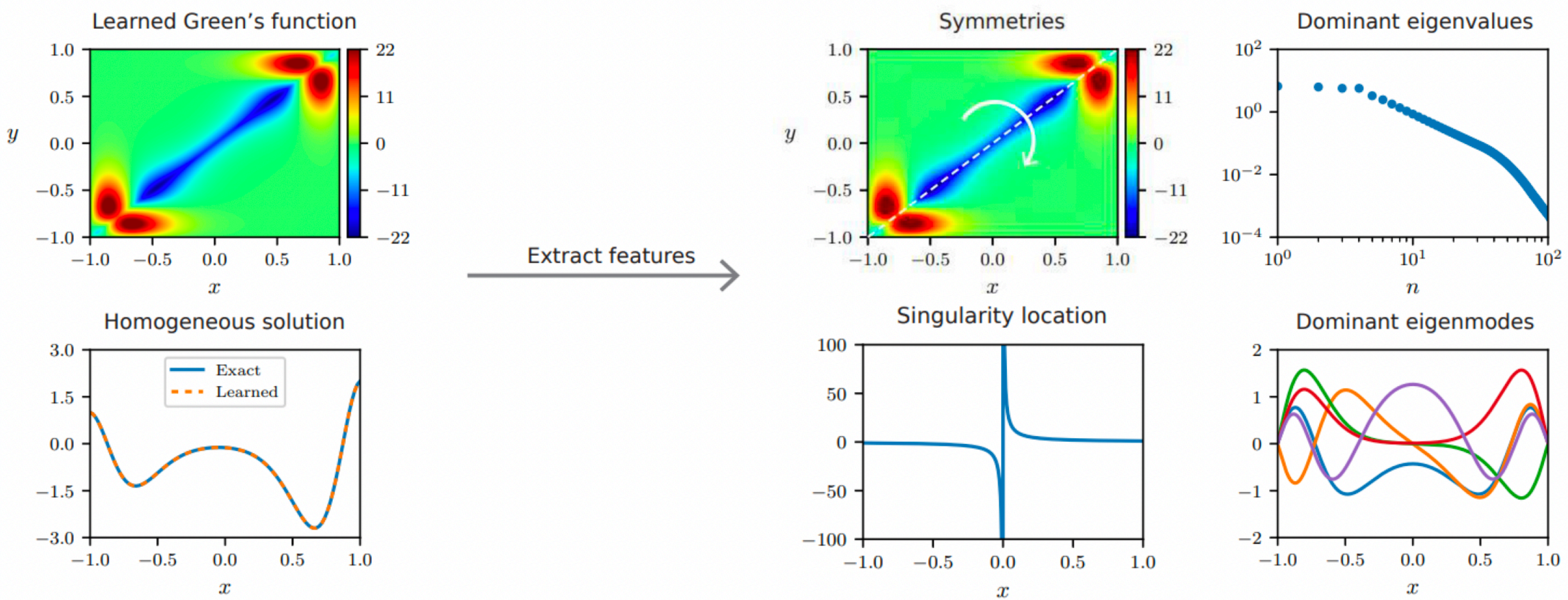
Homogeneous solution



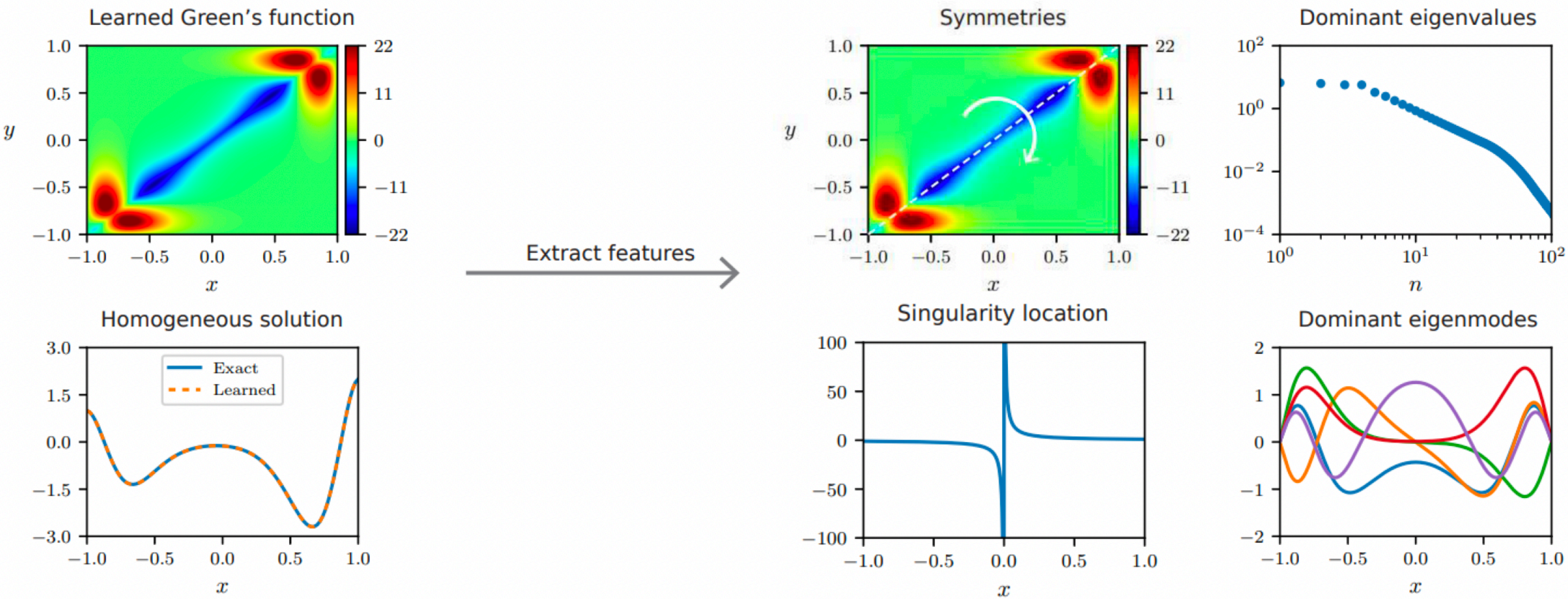
Phase portrait



Recovering PDE properties from its Green's function



Recovering PDE properties from its Green's function



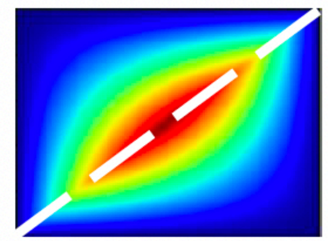
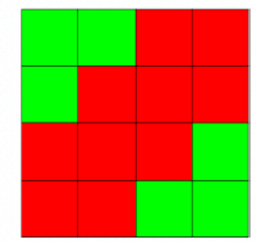
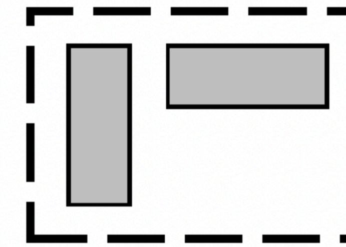
Question for the audience:

What PDE properties can we recover from a noisy /inaccurate Green's function?

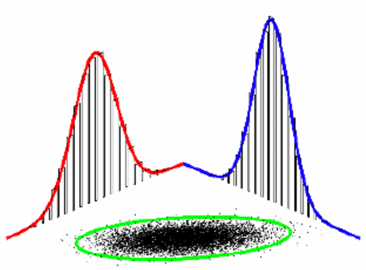
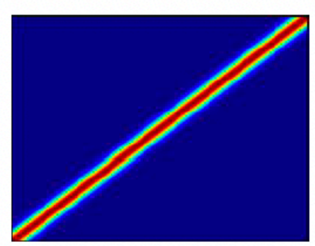
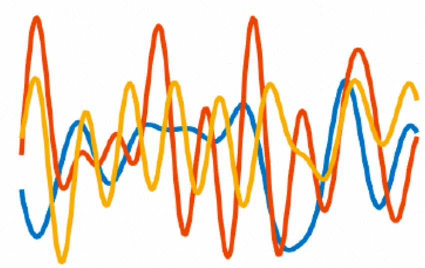
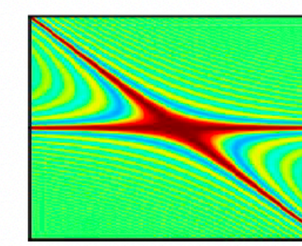
Summary

1. Theory for learning Green's functions

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

2. Generalization of the randomized SVD

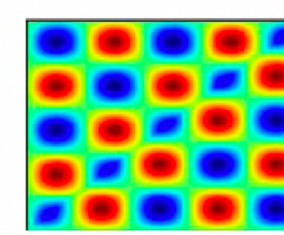





3. Deep learning approach

TensorFlow

Python package

`pip install greenlearning`



https://github.com/NBoulle/greenlearning