

Kernelization of Natural Gradient Methods for Physics Informed Neural Network (PINNs)

Thalès seminar

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February 19, 2026

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Inria

Scientific Machine-Learning (SciML) and Physics Informed Neural Networks (PINNs)

- **Data-driven modeling:** learn governing equations directly from observed trajectories (e.g., SINDy (Brunton et al., 2016), Neural ODEs (Chen et al., 2018)).
- **Operator learning:** approximate full solution operators for families of PDEs (e.g., DeepONet (Lu et al., 2021), FNO (Li et al., 2020)).
- **Physics-informed ML :** embed physical laws as constraints in the learning process (e.g., PINNs and extensions).

PIML aims to minimize:

$$\mathcal{L}(u) := \int_{\Omega} \|D[u] - f\|_{\mathbb{R}^n}^2 + \int_{\partial\Omega} \|B[u] - g\|_{\mathbb{R}^m}^2.$$

PINNs key idea

- model u with a neural network (Lagaris et al., 1998)
- use autodiff to compute D and B (Raissi et al., 2019)

Sampling yields the loss:

$$\begin{aligned} \hat{\ell}_{D,B}(\theta) := & \frac{1}{2S_D} \sum_{i=1}^{S_D} \left(D[u_{\theta}](x_i^D) - f(x_i^D) \right)^2 \\ & + \frac{1}{2S_B} \sum_{i=1}^{S_B} \left(B[u_{\theta}](x_i^B) - g(x_i^B) \right)^2. \end{aligned}$$

Problem: This leads to low accuracy when using usual optimizers.

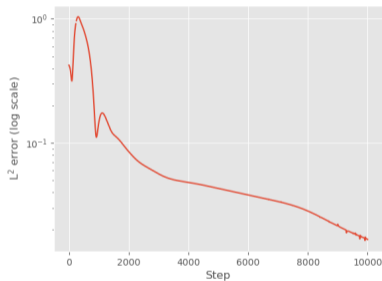


Figure: L^2 -error of a PINN optimized with Adam on the 2D Laplace equation.

PINNs main drawback : optimization error

- Highly nonconvex & ill-conditioned optimization
- Gradient imbalance between loss terms
- Spectral bias of neural nets : Low frequencies learned first; high-frequency or localized features missed.

Intuition from Fourier

$$S_N : (\alpha_k) \in \mathbb{C}^{\llbracket -N, N \rrbracket} \mapsto \sum_{k=-N}^N \alpha_k e^{2i\pi kx}.$$

S_N singular values are all 1. **BUT:**

$$\Delta[S_N] \text{ spectrum is } \{4\pi^2 k^2 : 1 \leq k \leq N\}$$

Δ strongly impact the spectral conditioning.

Natural Gradient

Classical quadratic regression problem, with batch (x_i) :

$$\hat{\ell}(\theta) := \frac{1}{2S} \sum_{i=1}^S (u_\theta(x_i) - f(x_i))^2.$$

In the population limit:

$$\hat{\ell}(\theta) \xrightarrow{S \rightarrow \infty} \mathcal{L}(u_\theta); \quad \mathcal{L}(u) := \frac{1}{2} \|u - f\|_{L^2(\Omega)}^2$$

This yields the Fréchet derivative:

$$d\mathcal{L}|_u(h) = \underbrace{\langle u - f, h \rangle}_{\nabla \mathcal{L}|_u} \Big|_{L^2(\Omega)},$$

and thus the gradient flow:

$$\begin{cases} u_0 \in L^2(\Omega) \\ \dot{u}_t = -\nabla \mathcal{L}|_{u_t} = f - u_t \end{cases}$$

Solution: $u_t = f - e^{-t}(f - u_0)$.

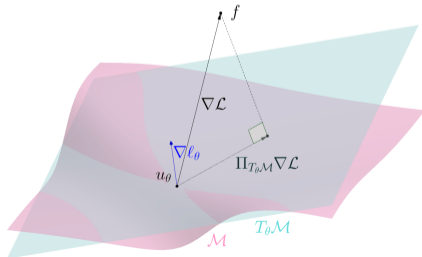
Natural gradient in functional space

The functional space is constrained to:

- $\mathcal{M} := \text{Im } u = \{u_\theta : \theta \in \mathbb{R}^P\}$
- $T_\theta \mathcal{M} := \text{Im } du_\theta = \text{Span}(\partial_p u_\theta)$

The Natural Gradient is then (Amari and Douglas, 1998):

$$\theta_{t+1} \leftarrow \theta_t - \eta du_{\theta_t}^\dagger \left(\Pi_{T_{\theta_t} \mathcal{M}}^\perp \nabla \mathcal{L}|_{u_{\theta_t}} \right),$$



Computational perspective on Natural Gradient

Definition-Proposition

The **Natural Neural Tangent Kernel (NNTK)** is the kernel of the projection $\Pi_{T_\theta \mathcal{M}} : L^2(\Omega) \rightarrow L^2(\Omega)$ onto $T_\theta \mathcal{M}$. It is given by the formula:

$$NNTK_\theta(x, y) := \sum_{1 \leq p, q \leq P} (\partial_p u_\theta(x)) G_{\theta pq}^\dagger (\partial_q u_\theta(y))^t; \quad G_{\theta p, q} := \langle \partial_p u_\theta, \partial_q u_\theta \rangle_{L^2(\Omega)}.$$

Corollary

The Natural Gradient update rewrites: $\theta_{t+1} \leftarrow \theta_t - \eta G_{\theta_t}^\dagger \nabla \ell(\theta_t)$; $\ell(\theta) := \mathcal{L}(u_\theta)$.

Shortcomings

- Computation of the Gram matrix G_{θ_t} is quadratic in the number of parameters.
- Inversion of G_{θ_t} is cubic

We introduce the empirical Natural Gradient that scales linearly with the number of parameters.

Reproducing Kernel Hilbert Spaces (RKHS) *détour*

Definition-Proposition

An Hilbert space \mathcal{H} of functions $\Omega \rightarrow \mathbb{R}$ is a RKHS if and only if the following equivalent conditions are met:

- 1 There exist a function $k : \Omega \times \Omega \rightarrow \mathbb{R}$ such that:
 - $\mathcal{H} = \overline{\text{Span}(k(x, \cdot) : x \in \Omega)}$
 - $\langle k(x, \cdot), k(y, \cdot) \rangle_{\mathcal{H}} = k(x, y)$
- 2 for all $x \in \Omega$, the evaluation form $e_x : f \in \mathcal{H} \mapsto f(x)$ is continuous.

Proposition

Any finite dimensional space \mathcal{H} is a RKHS

Proposition

If $\mathcal{H} := \overline{\text{Span}(u_i : i \in \mathbb{N})}$, is an RKHS, then its kernel is given by: for all $x, y \in \Omega$

$$k(x, y) = \sum_{i, j \in \mathbb{N}} u_i(x) G_{i, j}^{\dagger} u_j(y)$$

where $G_{ij} := \langle u_i, u_j \rangle_{\mathcal{H}}$.

Proposition

If $\mathcal{H} \supset \mathcal{H}_0$ is an RKHS with kernel k , then the orthogonal projection $\Pi_{\mathcal{H}_0}^{\perp}$ onto \mathcal{H}_0 is given by:

$$\Pi_{\mathcal{H}_0}^{\perp}(f)(x) = \langle k(x, \cdot), f \rangle_{\mathcal{H}}$$

Remark

Applying to $\mathcal{H}_0 = T_{\theta} \mathcal{M}$, we get natural gradient.

Intuition

$$\hat{\ell}(u) := \frac{1}{2S} \sum_{i=1}^S (u(x_i) - f(x_i))^2.$$

$$\frac{du_{\theta(t)}}{dt}(x) = -\frac{1}{S} \sum_{i=1}^S (u_{\theta}(x_i) - f(x_i)) \delta_{x_i}$$

Gradient descent (Jacot et al., 2018)

$$\frac{du_{\theta(t)}}{dt}(x) = -\frac{1}{S} \sum_{i=1}^S \text{NTK}_{\theta}(x, x_i) (u_{\theta}(x_i) - f(x_i))$$

$$\text{with: } \text{NTK}_{\theta}(x, y) := \sum_{p=1}^P \partial_p u_{\theta}(x) \partial_p u_{\theta}(y)^{\top}.$$

Natural Gradient (Rudner et al., 2019)

$$\frac{du_{\theta(t)}}{dt}(x) = -\frac{1}{S} \sum_{i=1}^S \text{NNTK}_{\theta}(x, x_i) (u_{\theta}(x_i) - f(x_i))$$

$$\text{with: } \text{NNTK}_{\theta}(x, y) := \sum_{1 \leq p, q \leq P} \partial_p u_{\theta}(x) G_{\theta, p, q}^{\dagger} \partial_q u_{\theta}(y)^{\top},$$

$$G_{\theta, p, q} = \langle \partial_p u_{\theta}, \partial_q u_{\theta} \rangle.$$

Neural Tangent Kernel (NTK)

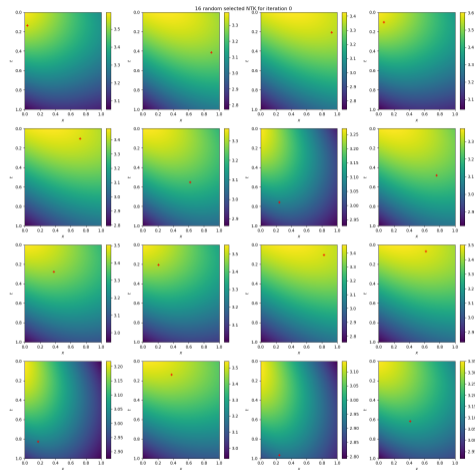


Figure: NTK for the Heat equation.

Reading: the plot represents the function

$\text{NTK}_{\theta_0}(\cdot, x_i)$; the red cross marks the point x_i .

empirical Natural Gradient

Recall the the functional dynamics of (N)GD on the empirical loss $\hat{\ell}$:

$$\frac{d\mathbf{u}_{\theta_t}}{dt}(\mathbf{x}) = - \sum_{i=1}^S (N)NTK_{\theta_t}(\mathbf{x}, \mathbf{x}_i)(\mathbf{u}_{\theta_t}(\mathbf{x}_i) - y_i),$$

Key Observation

The empirical dynamics takes place in:

$$\hat{T}_{\theta_t}\mathcal{M} := \text{Span}((N)NTK_{\theta_t}(\mathbf{x}_i, \cdot) : (\mathbf{x}_i)_{1 \leq i \leq N}).$$

We can define the empirical Natural Gradient:

$$\theta_{t+1} = \theta_t - \eta d\mathbf{u}_{\theta_t}^\dagger \left(\Pi_{\hat{T}_{\theta_t}\mathcal{M}}^\perp \nabla \mathcal{L}|_{\mathbf{u}_{\theta_t}} \right).$$

Theorem (ANaGRAM)

Under mild assumptions:

$$d\mathbf{u}_{\theta_t}^\dagger \left(\Pi_{\hat{T}_{\theta_t}\mathcal{M}}^\perp \nabla \mathcal{L}|_{\mathbf{u}_{\theta_t}} \right) \simeq \hat{\phi}_{\theta_t}^\dagger \widehat{\nabla \mathcal{L}}_{\theta_t},$$

with: for all $1 \leq p \leq P, 1 \leq i \leq S$

- $\hat{\phi}_{\theta_{t i}, p} := \partial_p \mathbf{u}_{\theta_t}(\mathbf{x}_i)$
- $\widehat{\nabla \mathcal{L}}_{\theta_{t i}} := \nabla \mathcal{L}|_{\mathbf{u}_{\theta_t}}(\mathbf{x}_i)$

Key fact

$\hat{\phi}_{\theta_t}^\dagger$ can be computed with a SVD, with complexity $O(\min(P^2S, P^2S))$.

Corollary

There exists P points $(\hat{\mathbf{x}}_i)$ such that:

$$\Pi_{\hat{T}_{\theta_t}\mathcal{M}}^\perp \nabla \mathcal{L}|_{\mathbf{u}_{\theta_t}} = \Pi_{T_{\theta_t}\mathcal{M}}^\perp \nabla \mathcal{L}|_{\mathbf{u}_{\theta_t}}.$$

Recall the the functional dynamics of (N)GD on the empirical loss $\hat{\ell}$:

$$\frac{du_{\theta_t}}{dt}(x) = - \sum_{i=1}^S (N)NTK_{\theta_t}(x, x_i)(u_{\theta_t}(x_i) - y_i),$$

Key Observation

The empirical dynamics takes place in:

$$\hat{T}_{\theta} \mathcal{M} := \text{Span} \left((N)NTK_{\theta}(x_i, \cdot) : (x_i)_{1 \leq i \leq N} \right).$$

We can define the empirical Natural Gradient:

$$\theta_{t+1} = \theta_t - \eta du_{\theta_t}^{\dagger} \left(\Pi_{\hat{T}_{\theta_t} \mathcal{M}}^{\perp} \nabla \mathcal{L}|_{u_{\theta_t}} \right).$$

Byproduct

Yields an optimal criterion for (x_i) choice:

$$(x_i)^{\star} = \underset{(x_i) \in \Omega^S}{\text{argmin}} \left\| \Pi_{\hat{T}_{\theta, K}^{(x_i)} \mathcal{M}}^{\perp} \nabla \mathcal{L}|_{u_{\theta_t}} - \nabla \mathcal{L}|_{u_{\theta_t}} \right\|_{L^2(\Omega)}$$

Theorem (ANaGRAM)

Under mild assumptions:

$$du_{\theta_t}^{\dagger} \left(\Pi_{\hat{T}_{\theta_t} \mathcal{M}}^{\perp} \nabla \mathcal{L}|_{u_{\theta_t}} \right) \simeq \hat{\phi}_{\theta_t}^{\dagger} \widehat{\nabla \mathcal{L}}_{\theta_t},$$

with: for all $1 \leq p \leq P, 1 \leq i \leq S$

- $\hat{\phi}_{\theta_t i, p} := \partial_p u_{\theta_t}(x_i)$
- $\widehat{\nabla \mathcal{L}}_{\theta_t i} := \nabla \mathcal{L}|_{u_{\theta_t}}(x_i)$

Key fact

$\hat{\phi}_{\theta_t}^{\dagger}$ can be computed with a SVD, with complexity $O(\min(P^2 S, S^2 P))$.

Corollary

There exists P points (\hat{x}_i) such that:

$$\Pi_{\hat{T}_{\theta} \mathcal{M}}^{\perp} \nabla \mathcal{L}|_{u_{\theta}} = \Pi_{T_{\theta} \mathcal{M}}^{\perp} \nabla \mathcal{L}|_{u_{\theta}}.$$

Application to PINNs

Key remark

The only difference between the losses:

$$\hat{\ell}_{D,B}(\theta) := \frac{1}{2S_D} \sum_{i=1}^{S_D} \left(D[u_\theta](x_i^D) - f(x_i^D) \right)^2 + \frac{1}{2S_B} \sum_{i=1}^{S_B} \left(B[u_\theta](x_i^B) - g(x_i^B) \right)^2,$$

and $\hat{\ell}(u) := \frac{1}{2S} \sum_{i=1}^S (u(x_i) - f(x_i))^2$ is the use of the operators D and B .

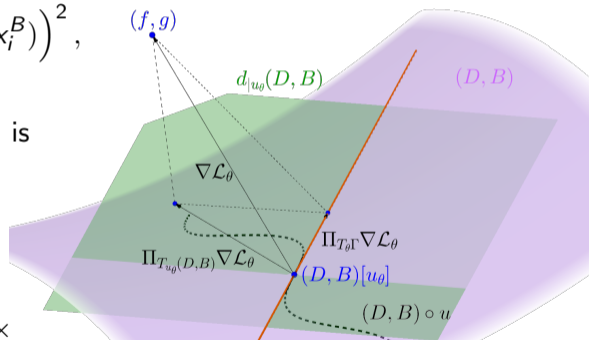
Proposition

PINNs are a quadratic regression problem with model: $(D, B) \circ u$:

$$\begin{cases} \mathbb{R}^P & \rightarrow \mathcal{H} & \rightarrow L^2(\Omega \rightarrow \mathbb{R}, \mu) \times \\ & & L^2(\partial\Omega \rightarrow \mathbb{R}, \sigma) \\ \theta & \mapsto u_\theta & \mapsto (D[u_\theta], B[u_\theta]) \end{cases}$$

Natural Gradient of PINNs

Figure: Illustration of PINNs Natural Gradient



Empirical Evidence for the Natural Gradient Relative to Adapted Model (*ANaGRAM*) Algorithm

2D Laplace equation

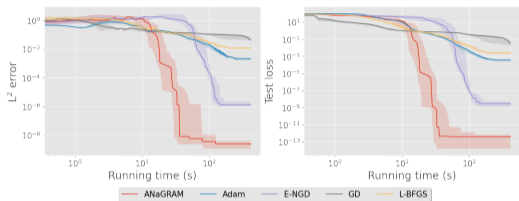


Figure: Performance comparison w.r.t running time for Laplace equation in 2 D:

$$\begin{cases} \Delta u = -2\pi^2 \sin(\pi x_1) \sin(\pi x_2) & \text{in } [0, 1]^2 \\ u = 0 & \text{on } \partial[0, 1]^2 \end{cases}$$

1+1 D Heat equation

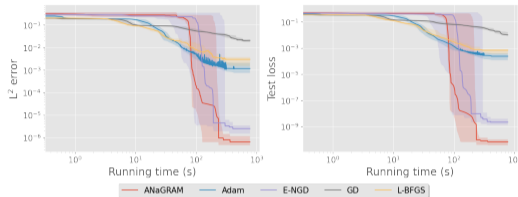


Figure: Performance comparison w.r.t running time for Heat equation in 1+1 D:

$$\begin{cases} \partial_t u - \frac{1}{4} \partial_{xx} u = 0 & \text{in } [0, 1]^2 \\ u = 0 & \text{on } [0, 1] \times \{0, 1\} \\ u = \sin(\pi x) & \text{on } \{0\} \times [0, 1] \end{cases}$$

5 D Laplace equation

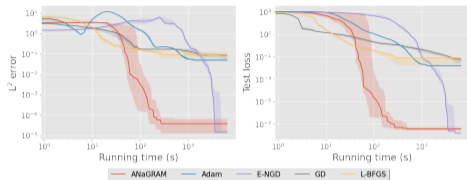


Figure: Performance comparison w.r.t running time for Laplace equation in 5 D:

$$\begin{cases} \Delta u = \pi^2 \sum_{k=1}^5 \sin(\pi x_k) & \text{in } \Omega = [0, 1]^5 \\ u = \sum_{k=1}^5 \sin(\pi x_k) & \text{on } \partial\Omega \end{cases} \quad \begin{cases} \partial_t u - 10^{-3} \partial_{xx} u = 5(u - u^3) & \text{in } \Omega = [0, 1] \times [-1, 1] \\ u = -1 & \text{on } \partial\Omega_b = [0, 1] \times \{-1, 1\} \\ u(0, x) = x^2 \cos(\pi x) & \text{on } \partial\Omega_0 = \{0\} \times [-1, 1] \end{cases}$$

1+1 D Allen-Cahn equation

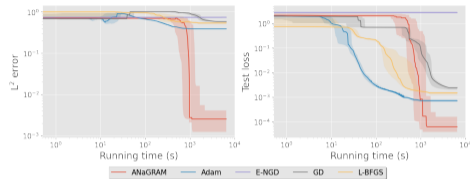
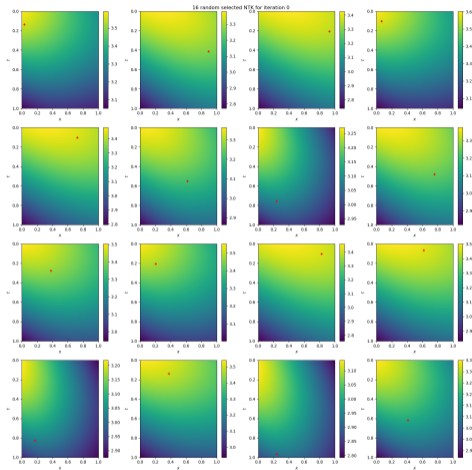
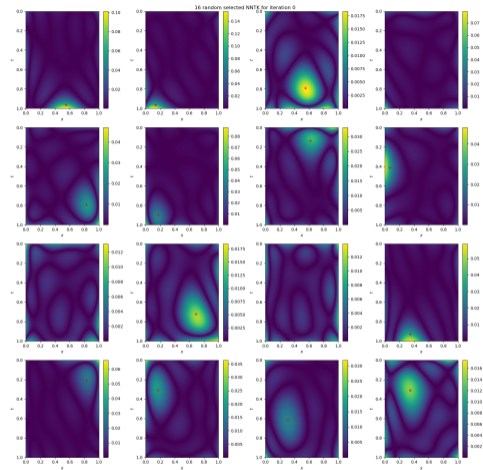


Figure: Performance comparison w.r.t running time for Allen-Cahn equation in 1+1 D:

NTK vs NNTK of PINNs



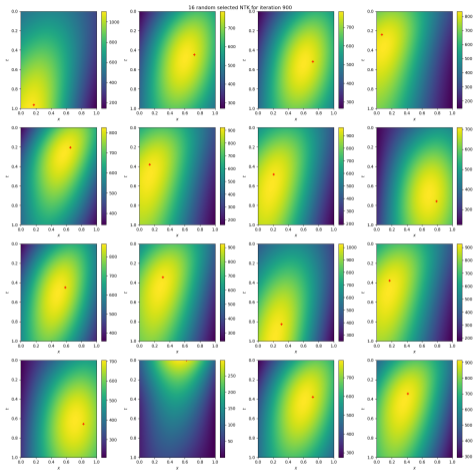
(a) NTK



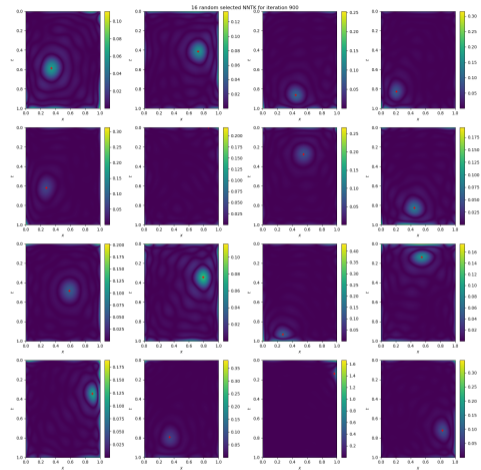
(b) NNTK

Figure: Comparison of NTK and NNTK at **initialization** for Heat equation in 1+1 D

NTK vs NNTK of PINNs



(a) NTK



(b) NNTK

Figure: Comparison of NTK and NNTK at the **end of optimization** for Heat equation in 1+1D

In-Depth Empirical Analysis of *Cutoff* Regularization in *ANaGRAM*

In-Depth Empirical Analysis of *Cutoff* Regularization in ANaGRAM

Intuition on RCE

SVD pseudoinverse details

$$\hat{\phi}_\theta = \hat{V} \hat{\Delta} \hat{U}^\top; \quad \hat{\phi}_{\theta_t}^\dagger = \hat{U} \hat{\Delta}^\dagger \hat{V}^\top.$$

Singular values

In practice, we apply a *cutoff*:

$$\hat{\Delta}^{\dagger\alpha} := \begin{cases} \hat{\Delta}_i^{-1} & \text{if } \hat{\Delta}_i \geq \alpha \\ 0 & \text{otherwise} \end{cases},$$

with $\alpha > 0$ the cutoff level. Thus:

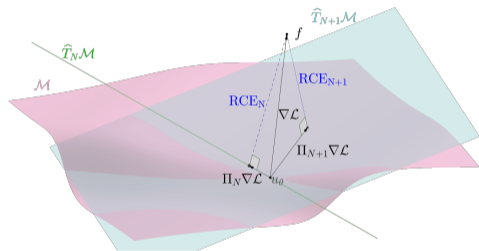
$$\hat{\phi}_\theta^{\dagger\alpha} \widehat{\nabla \mathcal{L}_\theta} = \sum_{i=1}^{r_\alpha} \hat{U}_i \hat{\Delta}_i^{-1} \hat{V}_i^\top \widehat{\nabla \mathcal{L}_\theta},$$

with $r_\alpha := \#\{i : \hat{\Delta}_i \geq \alpha\} \leq \min(P, S)$.

Reconstruction Error (RCE)

$$\text{RCE}_n = \frac{1}{\sqrt{S}} \left\| \widehat{\nabla \mathcal{L}_\theta} - \sum_{i=1}^n \hat{V}_i \hat{V}_i^\top \widehat{\nabla \mathcal{L}_\theta} \right\|_{\mathbb{R}^S}$$

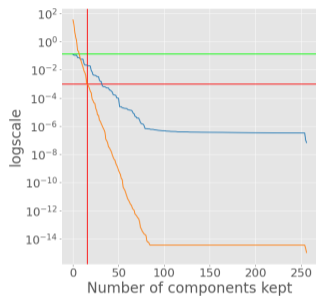
RCE_n accounts for the part of $\nabla \mathcal{L}_\theta$ orthogonal to the n most important components of $\hat{T}_\theta \mathcal{M}$.



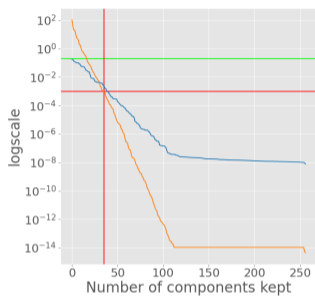
Remark

- $\lim_{S \rightarrow \infty} \hat{T}_\theta \mathcal{M} = T_\theta \mathcal{M}$
- $\text{RCE}_0^2 = \frac{1}{S} \left\| \widehat{\nabla \mathcal{L}_\theta} \right\|_{\mathbb{R}^S}^2 = \hat{\ell}(\theta)$

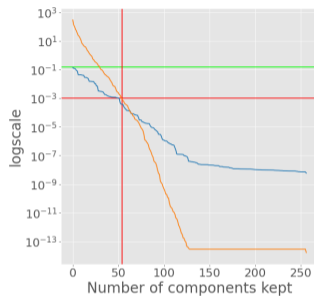
Empirical insights on the *cutoff* impact in ANaGRAM



(a) Iteration 0: intersection point between singular values and RCE lies before cutoff.



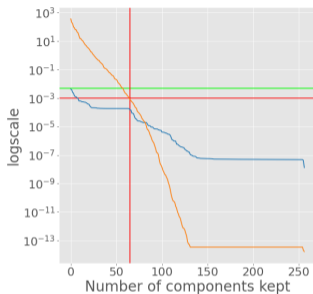
(b) Iteration 40: intersection point shifts rightward toward cutoff.



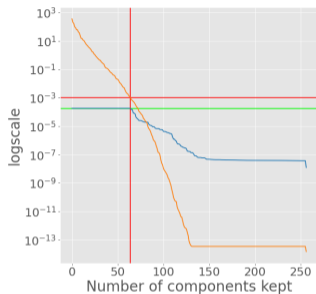
(c) Iteration 90: intersection point passes the cutoff threshold.



Empirical insights on the *cutoff* impact in ANaGRAM



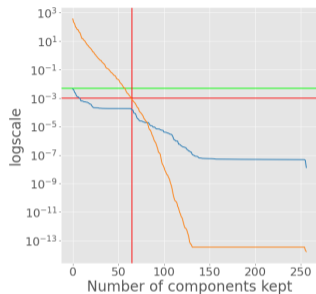
(d) Iteration 120. Beginning of *flattening*: RCE stabilizes at constant level before cutoff.



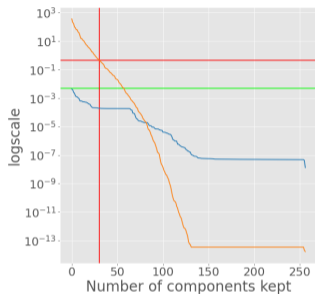
(e) Iteration 150: End of the *flattening phenomenon*. The train loss reaches the flattened part of the RCE.



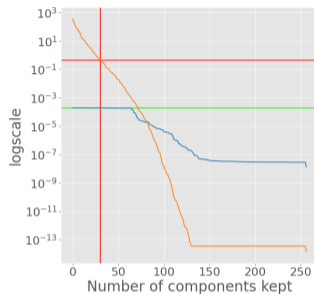
Incomplete and instant *flattening*



(f) Incomplete flattening of the RCE with a fixed cutoff at 10^{-3} .



(g) New cutoff located roughly at the location of the "elbow" in the RCE curve.



(h) Complete flattening after one natural gradient step with the new cutoff.



Adaptive Multi-cutoff Strategy Modification for ANaGRAM
(*AMStramGRAM*) algorithm

Algorithm 1: *AMStramGRAM* (sketch)

Input:

Initial parameters: $\theta_0 \in \mathbb{R}^P$

Precision target: $\epsilon > 0$

1 repeat

2 $\hat{U}_t, \hat{\Delta}_t, \hat{V}_t \leftarrow \text{SVD}(\hat{\phi}_t)$

3 Compute RCE_t

4 $r_\cap \leftarrow \#\{n : \text{RCE}_{t_n} \geq \hat{\Delta}_{t_n}\}$

5 $r_\epsilon \leftarrow \#\{n : \text{RCE}_{t_n} \geq \epsilon\}$

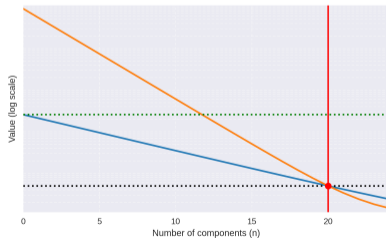
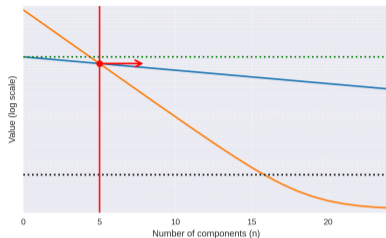
6 Apply ANaGRAM with cutoff rank

$r_\alpha \leftarrow \min(r_\cap, r_\epsilon)$

7 $t \leftarrow t + 1$

8 until $r_\epsilon = 0$ or $t \geq T_{\max}$

Output: θ_t



Algorithm 1: *AMStramGRAM* (sketch)

Input:

Initial parameters: $\theta_0 \in \mathbb{R}^P$

Precision target: $\epsilon > 0$

1 repeat

2 $\hat{U}_t, \hat{\Delta}_t, \hat{V}_t \leftarrow \text{SVD}(\hat{\phi}_t)$

3 Compute RCE_t

4 $r_\cap \leftarrow \#\{n : \text{RCE}_{t_n} \geq \hat{\Delta}_{t_n}\}$

5 $r_\epsilon \leftarrow \#\{n : \text{RCE}_{t_n} \geq \epsilon\}$

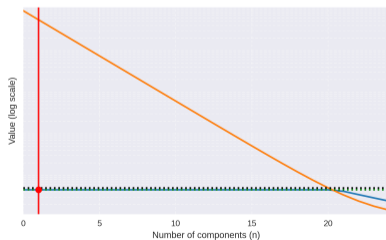
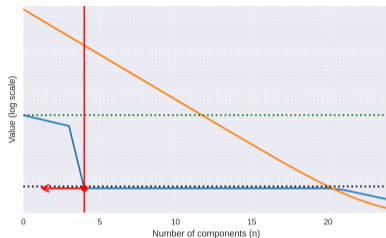
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$r_\alpha \leftarrow \min(r_\cap, r_\epsilon)$

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8 until $r_\epsilon = 0$ or $t \geq T_{\max}$

Output: θ_t



Experiment	Train Loss		L_2 Error	
	AMStramGRAM	ANaGRAM	AMStramGRAM	ANaGRAM
Heat Equation	6.29e-29 \pm 6.78e-30	8.56e-11 \pm 7.05e-11	2.32e-14 \pm 1.14e-14	1.28e-06 \pm 1.75e-06
Laplace 2D	1.46e-28 \pm 1.87e-29	4.27e-13 \pm 4.66e-13	2.24e-15 \pm 2.52e-16	3.49e-09 \pm 3.58e-09
Laplace 5D	2.04e-08 \pm 1.16e-08	6.37e-08 \pm 7.01e-08	2.12e-05 \pm 8.15e-06	4.00e-05 \pm 2.93e-05
Allen–Cahn	3.19e-11 \pm 2.37e-11	2.19e-04 \pm 4.16e-04	5.87e-05 \pm 6.25e-06	4.32e-03 \pm 5.93e-03

Experiment	Train Loss		L_2 Error	
	AMStramGRAM	SSBroyden	AMStramGRAM	SSBroyden
Burgers (1+1 D)	2.99e-12 \pm 9.26e-13	2.92e-10 \pm 1.45e-10	1.5e-06 \pm 9.43e-7	1.59e-06 \pm 1.02e-6
Non-Linear Poisson	8.51e-24 \pm 2.24e-24	3.03e-16 \pm 3.82e-16	6.81e-10 \pm 1.41e-09	9.29e-12 \pm 5.85e-12
Allen–Cahn	3.19e-11 \pm 2.37e-11	6.42e-12 \pm 5.52e-12	5.87e-05 \pm 6.25e-06	3.94e-06 \pm 1.72e-06

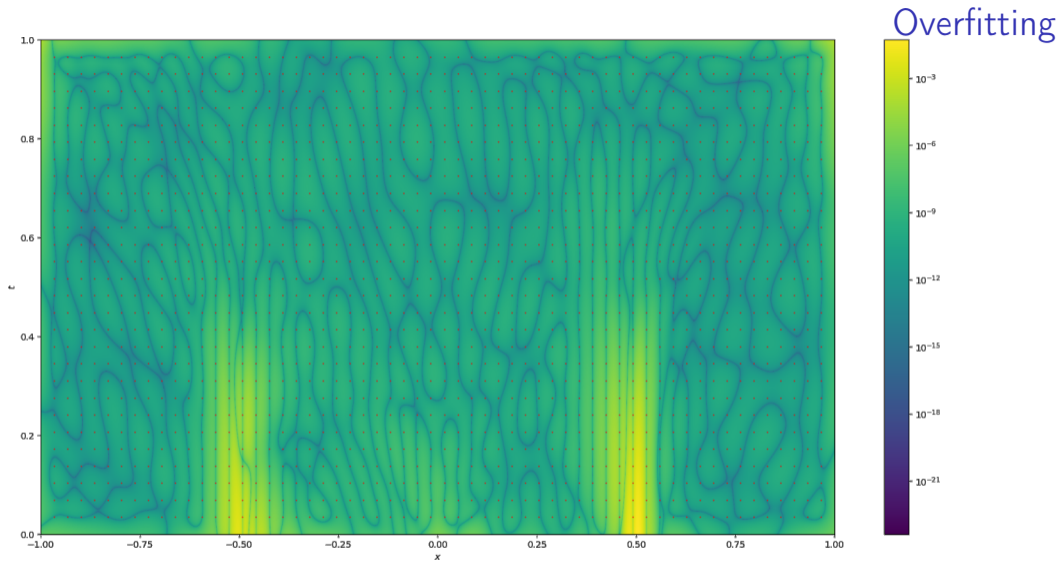


Figure: Overfitting on Allen–Cahn: residual lines align with sampling lines.

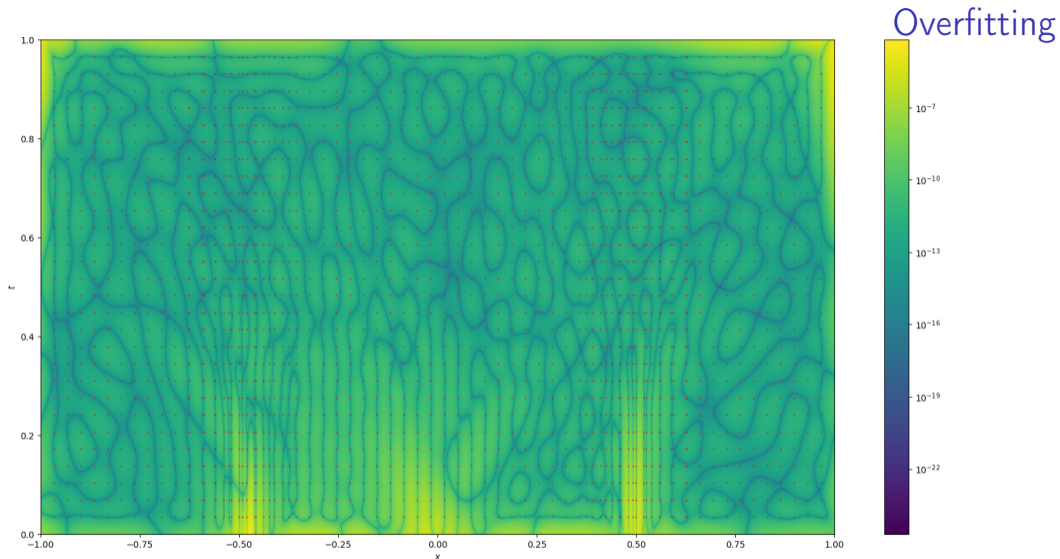


Figure: Overfitting on Allen–Cahn: densifying the sampling in overfitted regions mitigates overfitting.

Natural Gradient and Green's function

Definition (Green's function of D)

A Green's function is any kernel function $g : \Omega \times \Omega \rightarrow \mathbb{R}$ such that the operator:

$$R : f \in D[\mathcal{H}] \mapsto \left(x \in \Omega \mapsto \int_{\Omega} g(x, s) f(s) \mu(ds) \right) \in \mathcal{H}$$

verifies the equation: $D \circ R = I_{D[\mathcal{H}]}$

Definition (generalized Green's function of D on $\mathcal{H}_0 \subset \mathcal{H}$)

A generalized Green's function is any kernel function $g : \Omega \times \Omega \rightarrow \mathbb{R}$ such that the operator:

$$R : f \in L^2(\Omega \rightarrow \mathbb{R}, \mu) \mapsto \left(x \in \Omega \mapsto \int_{\Omega} g(x, s) f(s) \mu(ds) \right) \in \mathcal{H}$$

verifies the equation: $D \circ R = \Pi_{D[\mathcal{H}_0]}^{\perp}$

Natural gradient of PINNs is a Greens's function

Theorem

Let $D : \mathcal{H} \rightarrow L^2(\Omega \rightarrow \mathbb{R}, \mu)$ be a linear differential operator and $u : \mathbb{R}^P \rightarrow \mathcal{H}$ a parametric model. Then for all $\theta \in \mathbb{R}^P$, the generalized Green's function of D on $T_\theta \mathcal{M} = \text{Im } du_\theta$ is given by: for all $x, y \in \Omega$

$$g_{T_\theta \mathcal{M}}(x, y) := \sum_{1 \leq p, q \leq P} \partial_p u_\theta(x) G_{p,q}^\dagger \partial_q D[u_\theta](y),$$

with: for all $1 \leq p, q \leq P$

$$G_{pq} := \langle \partial_p D[u_\theta], \partial_q D[u_\theta] \rangle_{L^2(\Omega \rightarrow \mathbb{R}, \mu)}.$$

In particular, the natural gradient of PINNs can be rewritten:

$$\theta_{t+1} \leftarrow \theta_t - \eta du_{\theta_t}^\dagger \left(x \in \Omega \mapsto \int_{\Omega} g_{T_{\theta_t} \mathcal{M}}(x, y) \nabla \mathcal{L}_{\theta_t}(y) \mu(dy) \right).$$

Theorem

Let $D : \mathcal{H} \rightarrow L^2(\Omega \rightarrow \mathbb{R}, \mu)$ be a linear differential operator and $\mathcal{H}_0 \subset \mathcal{H}$ an RKHS with kernel k_0 . Given the spectral decomposition:

$$\Pi_{\mathcal{H}_0} D^* D \Pi_{\mathcal{H}_0} = \int_0^{+\infty} \lambda \pi_{D, \mathcal{H}_0}(d\lambda) \quad I_{\mathcal{H}_0} = \int_0^{+\infty} \pi_{D, \mathcal{H}_0}(d\lambda)$$

Then the generalized Green's function at regularization level $\alpha > 0$ is given by:
for all $x, y \in \Omega$

$$g_{\mathcal{H}_0, \alpha}(x, y) := D \left[\int_{\alpha^2}^{+\infty} \lambda^{-1} \pi_{D, \mathcal{H}_0}(d\lambda) [k(x, \cdot)] \right] (y)$$

Conclusion and Perspectives

Conclusions

- Anagram: lowers natural-gradient cost from $O(P^3)$ to $O(\min(PN^2, P^2N))$ (overfactor $\min(P, N)$ w.r.t SGD).
- AMStramGRAM gives a principled way to adapt cutoff reaching machine-level error.
- We prove that PINNs natural gradient corresponds to an optimal linear update following the Green's function.
- Empirical results are competitive with state-of-the-art PINNs optimizers.

Perspectives

- Design of an optimal collocation points procedure, coupled with AMStramGRAM's cutoff adaptation strategy.
- Include data assimilation in this theoretical setting, and understand its regularizing effect.
- Include common optimization techniques (e.g. Momentum)
- Extend it to Operator learning

Thank you for your attention !

Publications

- Schwencke, N. and C. Furtlehner (2025): “ANaGRAM: A Natural Gradient Relative to Adapted Model for Efficient PINNs Learning,” in The Thirteenth International Conference on Learning Representations.
- Marie-Anne, J., C. Rousselot, N. Schwencke, and A. Shilova (2025): “Implicit Function Theorem in Physics-Informed Neural Networks to Solve Parameterized Differential Equations,” in EurIPS 2025 Workshop: Differentiable Systems and Scientific Machine Learning.

Preprint

- Schwencke, N., C. Rousselot, A. Shilova, and C. Furtlehner (2025): “AMStramGRAM: Adaptive Multi-Cutoff Strategy Modification for ANaGRAM,” arXiv Preprint.

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- URBÁN, J. F., P. STEFANOPOULOS, AND J. A. PONS (2025): “Unveiling the Optimization Process of Physics Informed Neural Networks: How Accurate and Competitive Can PINNs Be?” *Journal of Computational Physics*, 523, 113656.

Ongoing work : Implicit Curriculum Learning

- Marie-Anne, J., C. Rousselot, N. Schwencke, and A. Shilova (2025): “Implicit Function Theorem in Physics-Informed Neural Networks to Solve Parameterized Differential Equations,” in EurIPS 2025 Workshop: Differentiable Systems and Scientific Machine Learning.

Implicit Curriculum Learning

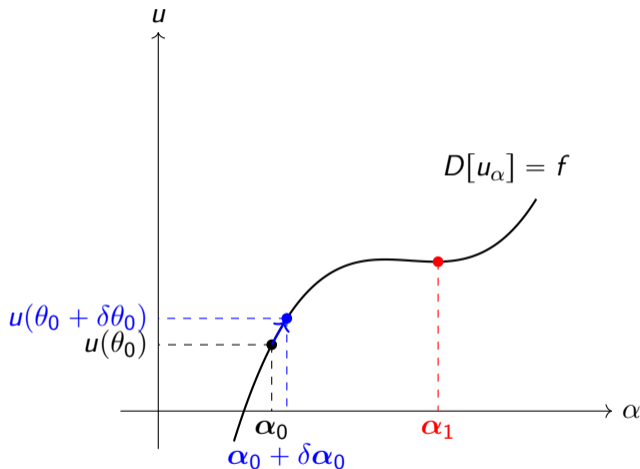


Figure: Illustration of implicit function theorem.

Credits : Julien Marie-Anne

Parameterized PDE

Let $\alpha \in \mathcal{A} \subset \mathbb{R}$ and consider

$$D[\alpha, u] = f \quad \text{in } \Omega.$$

Implicit function theorem

If $dD_{\alpha, u} \neq 0$, there is $[a, b] \ni \alpha$ and v such that for all $\beta \in [a, b]$

$$D[\beta, v(\beta)] = f.$$

with v solution to the ODE:

$$\frac{d}{d\beta} v = \partial_u D_{\beta, v(\beta)}^{-1} \left[\frac{d}{d\beta} D_{\beta, v(\beta)} \right]$$

Implicit curriculum learning

Follow the update:

$$\frac{d}{d\beta} \theta(\beta) = \partial_{\theta} (D \circ u_{\theta})_{\beta, u_{\theta(\beta)}}^{\dagger} \left[\frac{d}{d\beta} D_{\beta, u_{\theta(\beta)}} \right]$$

Table: Comparison of the method with Adam on different PDEs

Equation	Method	Metric
Hamilton–Jacobi–Bellman (Relative Error)	Adam	$5.56e-01 \pm 1.99e-01$
	Implicit Curriculum Learning	$3.44e-01 \pm 2.05e-01$
Eikonal (Relative Error)	Adam	$8.02e-01 \pm 9.78e-01$
	Implicit Curriculum Learning	$2.05e-02 \pm 1.09e-02$
Burgers (Evaluation Loss)	Adam	$1.32e-02$
	Implicit Curriculum Learning	$7.21e-03$

Ongoing work : *Collocation points* selection

Reinterpreting ANaGRAM optimal criterion

Remark

$$(x_i)^* = \operatorname{argmin}_{(x_i) \in \Omega^S} \left\| \Pi_{\widehat{T}_{\theta, K}^{\perp}(x_i) \mathcal{M}} \nabla \mathcal{L}|_{u_{\theta_t}} - \nabla \mathcal{L}|_{u_{\theta_t}} \right\|_{L^2} = \operatorname{argmin}_{(x_i) \in \Omega^S} \inf_{\alpha \in \mathbb{R}^S} \left\| \sum_{i=1}^S \alpha_i K_{\theta}(x_i, \cdot) - \nabla \mathcal{L}|_{u_{\theta_t}} \right\|_{L^2}^2$$

Consequence

$(x_i)^*$ can be “learned” by the minimization through natural gradient descent of

$$u : \begin{cases} \Omega^S \times \mathbb{R}^S & \rightarrow L^2(\Omega \rightarrow \mathbb{R}, \mu) \\ ((x_i), \alpha) & \mapsto \sum_{i=1}^S \alpha_i K_{\theta}(x_i, \cdot) \end{cases}$$

Even better: closed form formulas exist !

Proposition

- $\langle \partial_{\alpha_i} u_{\theta}, \partial_{\alpha_j} u_{\theta} \rangle = K_{\theta}(x_i, x_j)$
- $\langle \partial_{x_i} u_{\theta}, \partial_{\alpha_j} u_{\theta} \rangle = \alpha_j \partial_1 K_{\theta}(x_i, x_j)$
- $\langle \partial_{x_i} u_{\theta}, \partial_{x_j} u_{\theta} \rangle = \alpha_i \partial_2 \partial_1 K_{\theta}(x_i, x_j) \alpha_j$
- $\langle \partial_{\alpha_i} u_{\theta}, \nabla \mathcal{L} \rangle = \Pi_{T_{\theta} \mathcal{M}} \nabla \mathcal{L}(x_i) \simeq \nabla \mathcal{L}(x_i)$
- $\langle \partial_{x_i} u_{\theta}, \nabla \mathcal{L} \rangle = \alpha_i \Pi_{T_{\theta} \mathcal{M}} \nabla \mathcal{L}'(x_i) \simeq \alpha_i \nabla \mathcal{L}'(x_i)$

First results for collocation learning in Fourier space

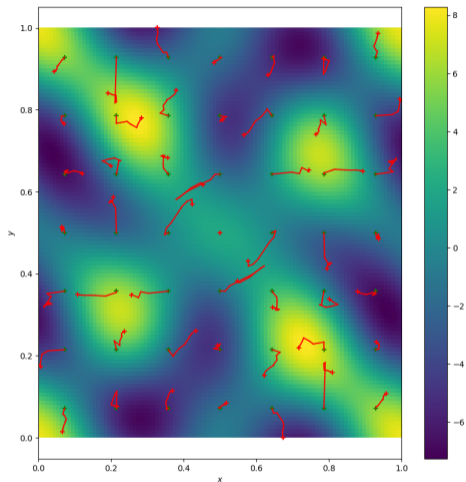


Figure: Points learning dynamic

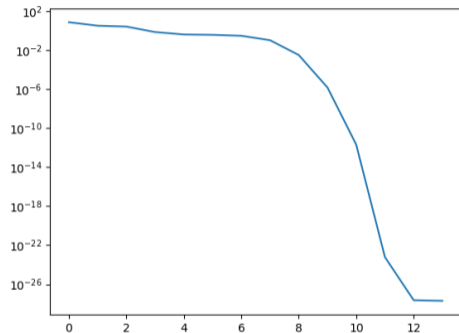


Figure: $\left\| \Pi_{\hat{\mathcal{T}}_{\theta, K}^{(x_i)} \mathcal{M}}^\perp \nabla \mathcal{L}|_{u_{\theta_t}} - \nabla \mathcal{L}|_{u_{\theta_t}} \right\|_{L^2}$ wrt (x_i)
learning steps

Ongoing work : Connection to Galerkin's method

Strong formulation

Find $u \in H^2(\Omega)$ such that

$$\begin{cases} \Delta u = f \in L^2(\Omega) & \text{in } \Omega \\ u = 0 \in L^2(\partial\Omega) & \text{on } \partial\Omega \end{cases}.$$

Weak formulation

Find $u \in H_0^1(\Omega)$ such that: $\forall v \in H_0^1(\Omega)$,

$$\langle \nabla u, \nabla v \rangle_{L^2(\Omega \rightarrow \mathbb{R}^d)} = \langle v, -f \rangle_{L^2(\Omega)}.$$

Galerkin method

Fixing a finite dimensional space

$$H_n \subset H_0^1(\Omega).$$

Find $u \in H_n$ such that: $\forall v \in H_n$,

$$\langle \nabla u, \nabla v \rangle_{L^2(\Omega \rightarrow \mathbb{R}^d)} = \langle v, -f \rangle_{L^2(\Omega)}.$$

Kernelization of Galerkin's Method

Kernelization of Galerkin

Let $(v_i^n)_{i=1}^n$ be a basis of H_n .

$$\mathcal{T}_{H_n} : \theta \in \mathbb{R}^n \mapsto \sum_{i=1}^n \theta_i v_i^n \in H_n.$$

$$\text{NNTK}_s(x, y) = \sum_{1 \leq p, q \leq n} \partial_p \mathcal{T}_{H_n} G_{sp, q}^\dagger \partial_q \mathcal{T}_{H_n}.$$

Strong formulation

$$G_{2p, q} = \langle \Delta \partial_p \mathcal{T}_{H_n}, \Delta \partial_q \mathcal{T}_{H_n} \rangle_{L^2(\Omega)}.$$

$$u_n = \langle \Delta \text{NNTK}_2(x, \cdot), f \rangle_{L^2(\Omega)}.$$

Weak formulation

$$G_{1p, q} = \langle \nabla \partial_p \mathcal{T}_{H_n}, \nabla \partial_q \mathcal{T}_{H_n} \rangle_{L^2(\Omega \rightarrow \mathbb{R}^d)}.$$

$$u_n = \langle \text{NNTK}_1(x, \cdot), -f \rangle_{L^2(\Omega)}.$$

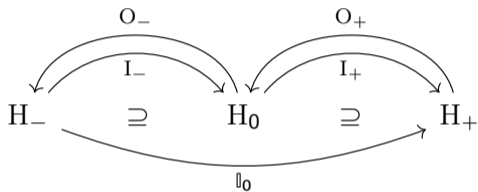


Figure: Schematic diagram of the basic structure of a Hilbert Rigging (a.k.a. Gelfand triple), adapted from Berezansky et al. (1996).

O_+ : embedding of H_+ into H_0

$$I_+ := O_+^* : H_0 \rightarrow H_+$$

$$\langle \cdot, \cdot \rangle_- : (u, v) \in H_0^2 \mapsto \langle I_+ u, I_+ v \rangle_{H_+}$$

$$H_- := \overline{H_0}^{\|\cdot\|_-} \simeq H'_+$$

$$\mathbb{I}_0 := \overline{I_+} : H_- \rightarrow H_+$$

O_- : embedding of H_0 into H_-

$$I_- := O_-^* : H_- \rightarrow H_0$$

$$\mathbb{I}_0 O_- = I_+; \quad O_+ \mathbb{I}_0 = I_-$$

Weak-Strong equivalence

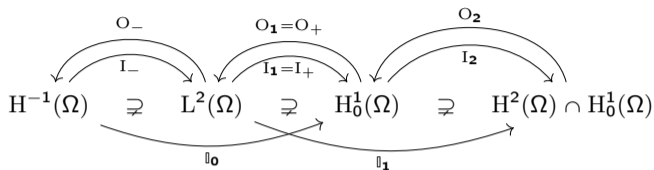


Figure: Schematic representation of the Hilbert rigging chain unifying the weak and strong formulations. Adapted from Berezansky et al. (1996).

Proposition (Green's Identity)

$$\langle \Delta u, O_1 v \rangle_{L^2(\Omega)} = - \int_{\Omega} \langle \nabla u, \nabla v \rangle_{\mathbb{R}^d} = - \langle O_2 u, v \rangle_{H_0^1(\Omega)}.$$

Proposition

$$\Delta_2 := \Delta = -\mathbb{I}_1^* : H^2(\Omega) \cap H_0^1(\Omega) \rightarrow L^2(\Omega)$$

$$\Delta_1 := \overline{\Delta}^{H_0^1(\Omega)} = -\mathbb{I}_0^* : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$$

Test form of the Strong formulation

Find $u \in H^2(\Omega) \cap H_0^1(\Omega)$ s.t.,
 $\langle \Delta u, v \rangle_{H_0^1(\Omega)} = - \langle f, v \rangle_{H_0^1(\Omega)},$
 $\forall v \in H^2(\Omega) \cap H_0^1(\Omega).$

Least-squares form of the Weak formulation

Find $u \in H_0^1(\Omega)$ s.t $\Delta_1[u] = O_- f$
 or even $\Delta_1[u] = \alpha \in H^{-1}(\Omega).$

Proposition

$$u_{\text{weak}} = -I_1 f = O_2 u_{\text{strong}}$$

Formulation \ Form	Weak formulation	Strong formulation
Test form	$ \begin{aligned} & -O_1[\text{NNTK}_{1,n}(\mathbf{x}, \cdot)] \\ & \simeq -\text{NNTK}_{1,n}(\mathbf{x}, \cdot) \\ & \in L^2(\Omega) \end{aligned} $	$ \begin{aligned} & -O_2[\text{NNTK}_{2,n}(\mathbf{x}, \cdot)] \\ & \simeq -\text{NNTK}_{2,n}(\mathbf{x}, \cdot) \\ & \in H_0^1(\Omega) \end{aligned} $
Least-squares form	$ \begin{aligned} & -\mathbb{I}_0^*[\text{NNTK}_{1,n}(\mathbf{x}, \cdot)] \\ & = \Delta_1[\text{NNTK}_{1,n}(\mathbf{x}, \cdot)] \\ & \in H^{-1}(\Omega) \end{aligned} $	$ \begin{aligned} & -\mathbb{I}_1^*[\text{NNTK}_{2,n}(\mathbf{x}, \cdot)] \\ & = \Delta_2[\text{NNTK}_{2,n}(\mathbf{x}, \cdot)] \\ & \in L^2(\Omega) \end{aligned} $

N.B: While those approximations yield the same asymptotic solution, the approximations (*i.e.* solutions on H_n) differ.

Table: Summary of the Green's functions associated with each combination of formulation and form, computed over a finite-dimensional subspace H_n of functions, with $\mathbf{x} \in \Omega$.

Illustration of natural gradient dynamics

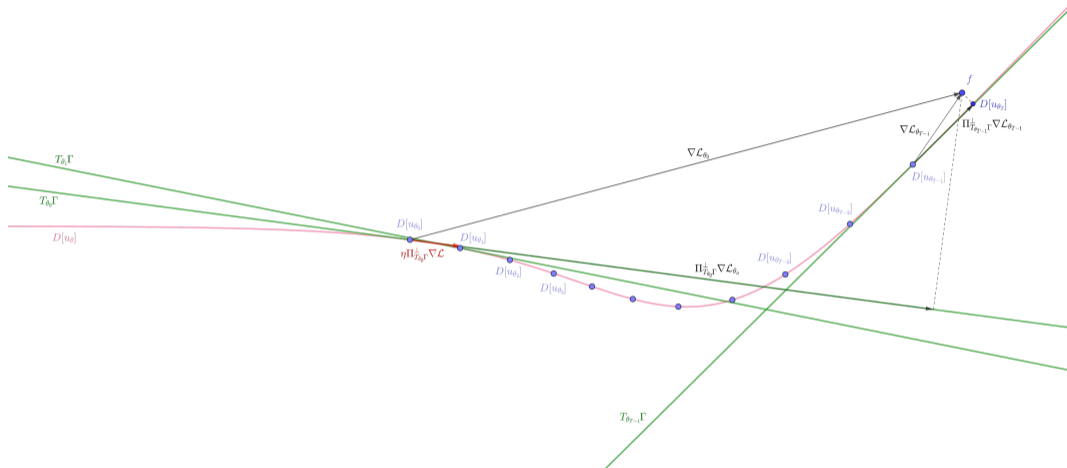


Figure: Illustration of PINNs learning process under natural gradient, as successive applications of Green's function

In the population limit, the natural gradient of PINNs is the update:

$$\theta_{t+1} \leftarrow \theta_t - \eta d((D, B) \circ u)_{\theta_t}^\dagger \left(\Pi_{T_{\theta_t}^\perp \Gamma} \nabla \mathcal{L}|_{u_{\theta_t}} \right)$$

Corollary

The kernel of $\Pi_{T_\theta \Gamma}$ is: for all $x, y \in (\Omega \times \partial\Omega)^2$

$$\begin{aligned} NNTK_\theta(x, y) &= \sum_{1 \leq p, q \leq P} \partial_p(D, B)[u_\theta](x) G_{\theta_{p,q}}^\dagger \partial_q(D, B)[u_\theta](y) \\ &= \sum_{1 \leq p, q \leq P} (\partial_p D[u_\theta](x_1), \partial_p B[u_\theta](x_2)) G_{\theta_{p,q}}^\dagger (\partial_q D[u_\theta](y_1), \partial_q B[u_\theta](y_2)), \end{aligned}$$

where for all $1 \leq p, q \leq P$

$$\begin{aligned} G_{\theta_{p,q}} &:= \langle \partial_p(D, B)[u_\theta], \partial_q(D, B)[u_\theta] \rangle_{L^2(\Omega \rightarrow \mathbb{R}, \mu) \times L^2(\partial\Omega \rightarrow \mathbb{R}, \sigma)} \\ &= \langle \partial_p D[u_\theta], \partial_q D[u_\theta] \rangle_{L^2(\Omega \rightarrow \mathbb{R}, \mu)} + \langle \partial_p B[u_\theta], \partial_q B[u_\theta] \rangle_{L^2(\partial\Omega \rightarrow \mathbb{R}, \sigma)}. \end{aligned}$$

Corollary

The kernel of $\Pi_{\hat{T}_{\theta}\Gamma}$ is: for all $x, y \in (\Omega \times \partial\Omega)^2$

$$\hat{k}(x, y) = \sum_{1 \leq i, j \leq S} \text{NNTK}_{\theta}(x, x_i) \hat{G}_{\theta i, j}^{\dagger} \text{NNTK}_{\theta}(x_j, y), \text{ where}$$

$$G_{\theta i, j} := \langle \text{NNTK}_{\theta}(\cdot, x_i), \text{NNTK}_{\theta}(x_j, \cdot) \rangle_{L^2(\Omega \rightarrow \mathbb{R}, \mu) \times L^2(\partial\Omega \rightarrow \mathbb{R}, \sigma)} = \text{NNTK}_{\theta}(x_i, x_j)$$

Theorem (ANaGRAM for PINNs)

Under mild assumptions, the empirical natural gradient update:

$$\theta_{t+1} \leftarrow \theta_t - \eta d((D, B) \circ u)_{\theta_t}^{\dagger} \left(\Pi_{\hat{T}_{\theta_t}\Gamma}^{\perp} \nabla \mathcal{L}|_{u_{\theta_t}} \right),$$

does not require to estimate a Gram matrix. More precisely, we have:

$$d((D, B) \circ u)_{\theta_t}^{\dagger} \left(\Pi_{\hat{T}_{\theta_t}\Gamma}^{\perp} \nabla \mathcal{L}|_{u_{\theta_t}} \right) = \hat{\phi}_{\theta_t}^{\dagger} \widehat{\nabla \mathcal{L}}_{\theta_t},$$

where: for all $1 \leq p \leq P, 1 \leq i \leq S$

- $\hat{\phi}_{\theta_t i, p} := (\partial_p D[u_{\theta_t}](x_{i1}), \partial_p B[u_{\theta_t}](x_{i2}))$
- $\widehat{\nabla \mathcal{L}}_{\theta_t i} := \nabla \mathcal{L}|_{u_{\theta_t}}(x_i)$