Physic informed neural networks for solving direct and inverse problems

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Outline

Introduction to Neural methods for elliptic equations

Objectives

Linear elliptic PDEs

Here we consider elliptic and linear PDEs of the form:

$$\begin{cases} L(u(\mathbf{x})) = -\nabla \cdot (A(\mathbf{x})\nabla u(\mathbf{x})) + \nabla \cdot (\beta(\mathbf{x})u(\mathbf{x})) + c(\mathbf{x})u(\mathbf{x}) = f(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \subset \mathbb{R}^d \\ u(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in \partial\Omega \end{cases}$$

Numerical methods Vs ML regression

Both regression and numerical methods seek to finf function approximations. In both cases, we use parametric functions. One is constrained by the data, the other by the physical equations.

Idea

Use neural networks as parametric models in numerical methods.

Principle of numerical method

- Choose an finite-dimensional approximation space to represent your numerical solution.
- Transform the PDE constrains on the solution into a constrains on the unknowns parameters.
- Solve the problem obtained to find the best parameters.

Approximation space

Linear space

- We choose $f_1, f_2 \in V_n$:

$$f_1(\mathbf{x}) + f_2(\mathbf{x}) = \sum_{i=1}^{N} \theta_i \phi_i(\mathbf{x}) \in V_n$$

- V_n is a vectorial space.

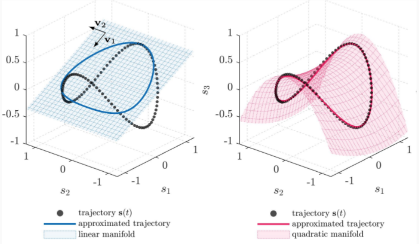
Nonlinear space

- We choose $f_1, f_2 \in M_n$:

$$f_1(\mathbf{x}) + f_2(\mathbf{x}) \not\subset M_n$$

- M_n is not a vectorial space but a manifold.

- Vectorial space Vs Manifold



- **Difficulty**: the projection on a manifold is not unique.

Approximation space II

Examples of linear space

- Fourier spectral functions (global):

$$f(\mathbf{x}) = \sum_{i=k}^{n} \alpha_k \sin(2k\pi x)$$

- Orthogonal polynomiales spectral functions (global):

$$f(\mathbf{x}) = \sum_{i=k}^{n} \alpha_k P_k(\mathbf{x})$$

- Finite element basis (local):

$$f(\mathbf{x}) = \sum_{i=k}^{n} \alpha_k \phi_{h,k}(\mathbf{x})$$

  with $\phi_{h,k}$ piecewise polynomiales functions.
- Radial basis (local):

$$f(\mathbf{x}) = \sum_{i=k}^{n} \alpha_k \phi(\epsilon \mid \mathbf{x} - \mathbf{x}_i \mid)$$

  avec $\phi(r) = e^{-r^2}$, $\phi(r) = \sqrt{(1 + r^2)}$.

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Examples of nonlinear functions

- Tensor methods:
$$f(\mathbf{x})=\sum_{i=1}^{r}\left(\sum_{k=1}^{n}\alpha_{i,k}\phi_k(\mathbf{x}_1)\right)\left(\sum_{k=1}^{n}\beta_{i,k}\phi_k(\mathbf{x}_2)\right)$$
avec $\mathbf{x}=(\mathbf{x}_1,\mathbf{x}_2)$.

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avec $\mathbf{x}=(\mathbf{x}_1,\mathbf{x}_2)$.
- Fourier spectral functions (global):
$$f(\mathbf{x})=\sum_{i=k}^{n}\alpha_k \sin(2\omega_k \pi x)$$
- Radiales basis (global):
$$f(\mathbf{x})=\sum_{i=k}^{n}\alpha_k \phi(\epsilon_k \mid \mathbf{x}-\mathbf{x}_i \mid)$$
- Anisotropic radial basis (global):
$$f(\mathbf{x})=\sum_{i=k}^{n}\alpha_k \phi(\mid \Sigma_k^{-1}(\mathbf{x}-\mathbf{x}_i)\mid)$$
- MLP Neural network (global):
$$f(\mathbf{x})=nn_\theta(\mathbf{x})$$
- KAN neural Network (global):
$$f(\mathbf{x})=kan_\theta(\mathbf{x})$$

Approximation space II

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avec $\phi(r) = e^{-r^2}$, $\phi(r) = \sqrt{(1 + r^2)}$.
- Random networks (global):
$$f(\mathbf{x}) = \sum_{i=k}^{n} \alpha_k nn_{\theta_k}(x)$$
with θ_k are randomly chosen.

Examples of nonlinear functions

- Tensor methods:
$$f(\mathbf{x}) = \sum_{i=1}^{r} \left(\sum_{k=1}^{n} \alpha_{i,k} \phi_k(\mathbf{x}_1) \right) \left(\sum_{k=1}^{n} \beta_{i,k} \phi_k(\mathbf{x}_2) \right)$$
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Approximation methods

- We want solve the problem $L(u(\mathbf{x})) = f(\mathbf{x})$ on Ω.
- The solution of the this PDE is solution of minimization problem

$$u(\mathbf{x}) = \min_{v \in H} \int_{\Omega} \mid L(v) - f \mid^2, \qquad \text{or } u(\mathbf{x}) = \min_{v \in H} \left(\int_{\Omega} \mid \nabla v \mid^2 - f(x) v \right)$$

Linear spaces

- Ritz-Galerkin:

$$\theta^* = \min_{v \in V_n} \left(\int_{\Omega} \mid \nabla v \mid^2 - f(x) v \right)$$

- Least square Galerkin:

$$\theta^* = \min_{v \in V_n} \int_{\Omega} \mid L(v) - f \mid^2$$

Nonlinear spaces

- Deep-Ritz:

$$\theta^* = \min_{v \in M_n} \left(\int_{\Omega} \mid \nabla v \mid^2 - f(x) v \right)$$

- PINNs:

$$\theta^* = \min_{v \in M_n} \int_{\Omega} \mid L(v) - f \mid^2$$

- The idea is the same. We restrict the functions to be minimized to the approximation space.
- The difference between classical and neural methods is the approximation space.
- The choice of integral approximation and resolution follows from this.

Integration

- To calculate the previous minimization problems, we need to integrate over the domain. Integration depends on the choice of space. In many cases we use quadrature formula.
- We're going to look here at the case of nonlinear spaces, in particular based on neural networks whose characteristics are:
  - Global models which not use meshes.
  - Good approximation properties in large dimension.

Integration

Given the qualities of NNs, the most suitable integration method is Monte Carlo.

$$\int_\Omega \|u_\theta(\mathbf{x}) - u(\mathbf{x})\|_2^2 dx = \mathbb{E}_{\mathcal{U}(\Omega)}[\|u_\theta(\mathbf{x}) - u(\mathbf{x})\|_2^2]$$

with $\mathcal{U}(\Omega)$ a uniform law on Ω. Applying the law of large numbers, we have

$$\int_\Omega \|u_\theta(\mathbf{x}) - u(\mathbf{x})\|_2^2 d\mathbf{x} \approx \frac{1}{N}\sum_{i=1}^{N} \|u_\theta(\mathbf{x}_i)) - u(\mathbf{x}_i)\|_2^2$$

Integration and complex geometries

Level-set function

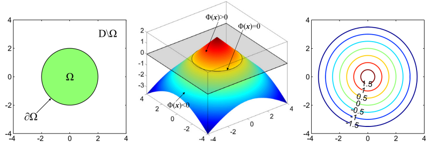
Given an Ω domain with Γ boundary, we call a level function a ϕ function such that

$$\phi(x) = \begin{cases} < 0, & \mathbf{x} \in \Omega \\ = 0, & \mathbf{x} \in \Gamma \\ > 0, & \mathbf{x} \in \mathbb{R}^d/\Omega \end{cases}$$

- How to sample ?
  - We draw a point randomly in $[a, d]^d$ such that Ω is included.
  - If $\phi(\mathbf{x}) < 0$ we keep the point otherwise we start again.
- No level function uniqueness. Example: the disk:

$$\phi_1(\mathbf{x}) = \sqrt{x_1^2 + x_2^2} - r, \quad \phi_1(\mathbf{x}) = x_1^2 + x_2^2 - r^2$$

- The first is called The signed distance function because it gives the distance between each point and Γ. It is a C^0 function, not a C^1 one.



(a) A circular domain Ω embedded in a domain D.
(b) Higher-dimensional LSF of the circular domain Ω.
(c) Iso-contours of the LSF.

- **Domains sum**: $\phi_1(\mathbf{x}) < 0$ ou $\phi_2(\mathbf{x}) < 0$
- **Domains intersection**: $\phi_1(\mathbf{x}) < 0$ et $\phi_2(\mathbf{x}) < 0$
- **Domains with holes**: $\phi_d(\mathbf{x}) < 0$ et $\phi_h(\mathbf{x}) > 0$

Boundary conditions

- For classical numerical methods we can impose BC weakly (we speak about penalization method) or strongly in the approximation space. It is the same for the NNs based methods.

Weak BC for neural based methods

The minimization problem becomes

$$\min_{u_\theta \in W_n}\left(\mathcal{J}r(u_\theta) + \lambda_{bc}\int_\Omega \| B(u_\theta) \|_2^2 \, d\mathbf{x}\right)$$

- **Fails**:If $\| \nabla_\theta \mathcal{J}_r(u_\theta) \|_{L^\infty} >> \| \nabla_\theta \mathcal{J}_{bc}(u_\theta) \|_{L^\infty}$ the training can learn mainly the PDE, ignore the BC and compute trivial solution.

Dirichlet BC

To impose $g(\mathbf{x})$ at the bc we use the space

$$M_n = \{g(\mathbf{x}) + \phi(\mathbf{x}) nn_\theta(\mathbf{x}), \quad \theta \in \Theta \subset \mathbb{R}^d\}$$

- Possible to impose strongly other BC.
- Since the model is plug in the residual we need that ϕ is a regular function. Not always the case. We can learn smooth level set.

How compute solve the minimization problem

Linear spaces

- **Gradient computation**: analytic
- **Solving of $\nabla J = 0$**: normal equation.
  - In the linear case we have:

$$\nabla J = 0 \longleftrightarrow A\theta - \mathbf{b} = 0$$

  - We solve a linear system with LU, CG, GMRES.
- **Computation of the model derivatives**: analytic

Nonlinear space

- **Gradient computation**: Automatic differentiation.
- **Solving of $\nabla J = 0$**: Gradient method to begin and quasi-Newton method to finish.
- **Computation of the model derivatives**: Automatic differentiation.

- The main difference is that in the classical case (linear methods) a large part of the optimisation problem can be solved analytically

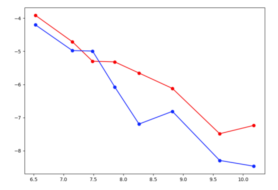
Advantages and disadvantages

Disadvantages

The main disadvantage of the Neural approach are the difficulty to obtain a good accuracy, and the fact that only asymptotic convergence results are available.

- Consider a 2D Laplacian solves with a 5-layer neural network and increase the size (685 weights for the smallest network and 26300 weights for the largest).

- Two learning rates:



FE	N_{dof}	Error
1D	100	-
2D	$1E^4$	$\approx 2E^{-3}$
3D	$1E^6$	$\approx 2E^{-3}$

Advantage

Mesh-free and ratio accuracy/degree of freedom less sensitive to the dimension.

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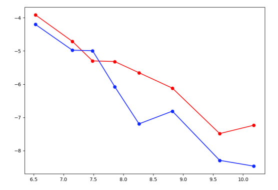


PINNs	N_{dof}	Error
1D	5081	$3E^{-4}$-$6E^{-4}$
2D	5121	$4E^{-4}$-$2E^{-3}$
3D	5161	$1E^{-3}$-$4E^{-3}$

Advantage

Mesh-free and ratio accuracy/degree of freedom less sensitive to the dimension.

Parametric problems

- In optimization, uncertainty propagation etc., we want to solve problems such as
$$L_\alpha(u(\mathbf{x})) - f(\mathbf{x}, \beta)$$
with $\mu = (\alpha, \beta)$ parameters that live in a space V_μ.
- A large part of usual methods are too expensive in high dimension so we don't solve this problem in V_μ space.
- In general, we run simulations for different μ and build a reduced model.

Parametric neural methods

Since neural network spaces are more efficient in high dimensions, we can try to solve in V_μ space.

- In this case the restriction operator is defined by
$$\theta^* = \min_\theta \int_{V_\mu} \int_\Omega \mid u(\mathbf{x}, \mu) - nn_\theta(\mathbf{x}, \mu) \mid^2 dx,$$
- The PINNs method becomes:
$$\theta^* = \min_\theta \int_{V_\mu} \int_\Omega \mid L_\alpha(u(\mathbf{x}, \mu)) - f(\mathbf{x}, \beta) \mid^2 dx,$$

Greedy approaches

Greedy Method

Objectives

Solve, with good accuracy, large-dimensional parametric elliptic problems. We wish to use an approach with only neural networks. How to increase the accuracy ?

Idea

Correct the first network with a second one, iterate (multistage, multlevel PINNs).

- We can write that as a greedy algorithm.
  - We consider the following submanifold approximation $\mathcal{M}_i, \quad 1 \leqslant i \leqslant d$
  - We initialize the greedy basis: $\mathcal{B} = \emptyset$, $u_h(x,\mu) = 0$
  - While $k < K$ and $\mid R(u_h) \mid > \epsilon$
    - We solve
$$\text{argmin}_{\theta_k}\left(\int_{\mathcal{P}}\int_{\Omega} R(u_h(x,\mu) + u_k(x,\mu))dx + \lambda \int_{\mathcal{P}}\int_{\partial\Omega} B(u_h(x,\mu) + u_k(x,\mu))dx\right)$$
    - We compute $(\alpha_0, \dots . \alpha_k)$ with a Galerkin projection or with a estimation of α_k.
    - Gives global approximation $u_h(x,\mu) = \sum_{i=0}^{k} \alpha_i u_i(x,\mu)$.

Remarks

Interesting point: each approximation space $\mathcal{M}_i$ can be different. Examples: NNs, FE etc.
Can we prove the convergence and compute the hyper-parameters ? (work in PEPR PDE-IA).

Full NN greedy method I

Full NN approach

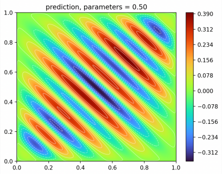
How choose the model at each step:

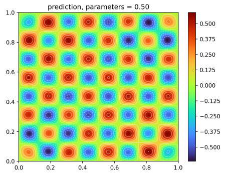
- One layer hidden-NN where we double the number of parameters at each step.
- Deep NN at each step with increase ability to capture high frequencies.

Spectral bias

MLPs first learn low frequencies, before learning the high frequencies (with difficulty).

- We solve $-\Delta u = 128 \sin(8\pi x)\sin(8\pi y)$. First try (left figure): classical MLP vs Fourier NNs.

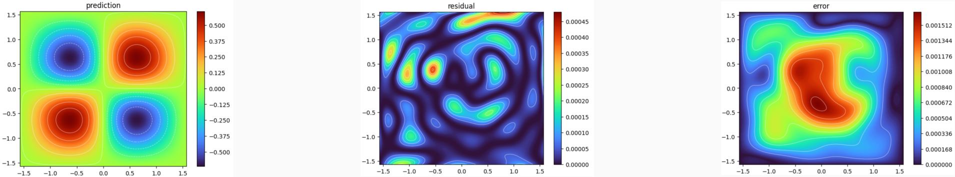




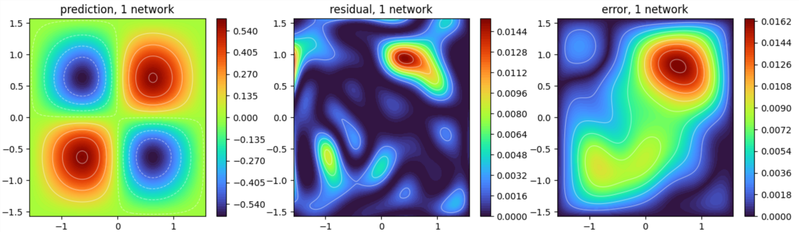
- FNN: we add Fourier features. We replace $NN_\theta(x)$ by $NN_\theta(x, \sin(2\pi k_1 x), ..., \sin(2\pi k_n x))$ with $(k_1, ...k_n)$ trainable parameters.

Full NN greedy method II

- Test: 4D problem (2D spatial + 2 parameters).
- Classical network ($\approx$ 9k parameters). 4000 epochs. 25k points. 45 min CPU.



- Greedy network (4 sub-networks) (2 MLPs, 2 Fourier MLPs). 1k, 1k, 3k and 4k parameters (total: 9k). Each trained for 1000 epochs. 5k, 5k, 25k and 50k points by epoch (1h05 CPU).



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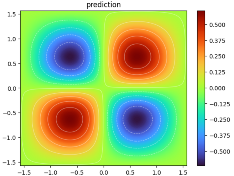

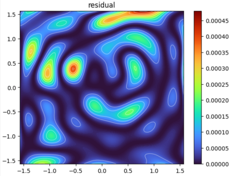

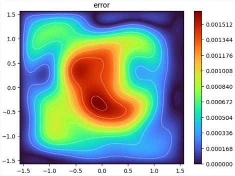

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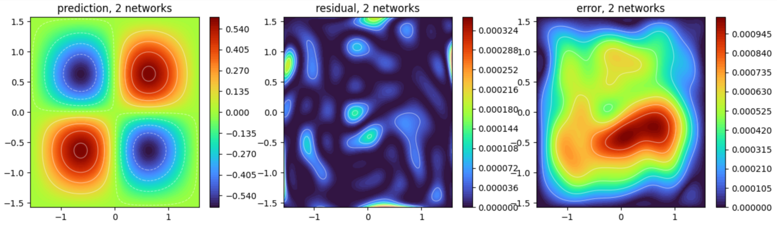

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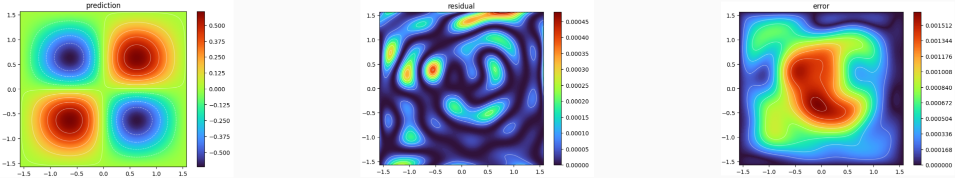

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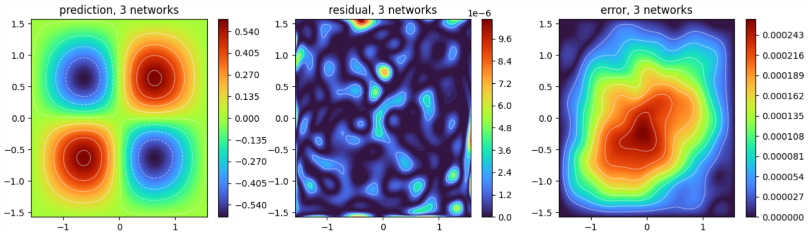

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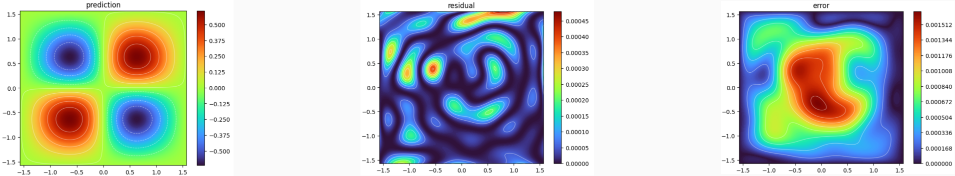

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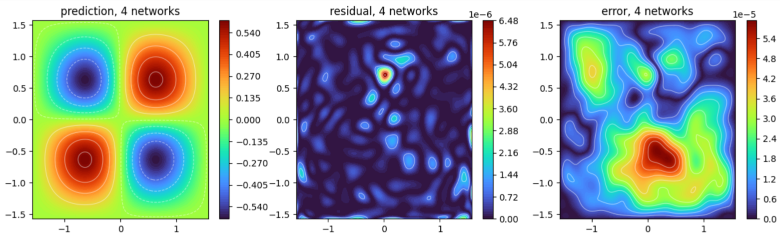


Prediction-correction method

Hybrid methods

In this context, hybrid methods combine classical numerical methods and numerical methods based on neural representations.

Objectives

Taking the best of both worlds: the accuracy of classical numerical methods, and the mesh-free large-dimensional capabilities of neural-based numerical methods.

General Idea

- **Offline/Online process**: train a Neural Network (PINNs, NGs, or NOs) to obtain a large family of approximate solutions.
- **Online process**: correct the solution with a numerical method.
- Can be view as a two step Greedy method. The first with NNs on $\Omega \times V_\mu$ and the second with finite element on $\Omega \times \{\mu_1, ..., \mu_n\}$.

Predictor-corrector method

- We consider the following elliptic problem:

$$\begin{cases} Lu(\mathbf{x}) = -\nabla\cdot(A(\mathbf{x}\nabla u(\mathbf{x})) + \mathbf{v}\cdot\nabla u(\mathbf{x}) + ru(\mathbf{x}) = f(\mathbf{x}), & \forall \mathbf{x}\in\Omega \\ \partial_{\mathbf{n}} u(\mathbf{x}) + \beta u(\mathbf{x}) = g(\mathbf{x}), & \forall x\in\partial\Omega \end{cases}$$

- We assume that we have a continuous prior given by a parametric PINN $u_\theta(x;\mu)$
- We propose the following approximation: $u_h(\mathbf{x}) = u_\theta(\mathbf{x};\mu) + p_h(\mathbf{x})$ with $p_h(\mathbf{x})$ a perturbation discretized using P_k Lagrange finite element.
- For the **first approach**, we solve in practice:

$$\begin{cases} Lp_h(\mathbf{x}) = f(\mathbf{x}) - Lu_\theta(x;\mu), & \forall \mathbf{x}\in\Omega \\ \partial_{\mathbf{n}} p_h(\mathbf{x}) + \beta p_h(\mathbf{x}) = g(\mathbf{x}) - u_\theta(\mathbf{x};\mu), & \forall \mathbf{x}\in\partial\Omega \end{cases}$$

Error

We note $I_h()$ the interpolator operator on the finite element space. The error of the predictor-corrector method is given by

$$\| u - u_h \|_{H^m} \leqslant \frac{M}{\alpha} C h^{k+1-m} \underbrace{\left(\frac{|u-u_\theta|_{H^m}}{|u|_{H^m}} \right)}_{gain} |u|_{H^m}$$

- **Test 1**:

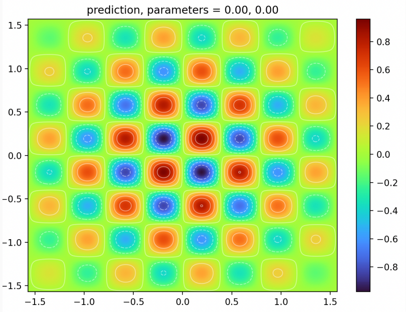
$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = g, & \text{on } \Gamma. \end{cases}$$

We define Ω by the square $\Omega = [-0.5\pi, 0.5\pi]^2$. For the test case the solution u_{ex} is given by

$$u_{ex}(x, y) = \sin(8x)\ \sin(8y)\ \times 10^{-\frac{1}{2}((x-\mu_1)^2+(y-\mu_2)^2)},$$

with homogeneous BC on Ω (i.e. $g = 0$) and $\mu_1, \mu_2 \sim \mathcal{U}(-0.5, 0.5)$.

- Example of solution



Results I

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with homogeneous BC on Ω (i.e. $g = 0$) and $\mu_1, \mu_2 \sim \mathcal{U}(-0.5, 0.5)$.

- Gain at fixed size

	Gains on PINNs				Gains on FEM			
N	min	max	mean	std	min	max	mean	std
20	9.17	36.13	19.79	6.63	112.2	454.43	349.41	82.75
40	26.14	111.44	58.86	19.8	106.01	388.96	308.49	71.81

	Gains on PINNs				Gains on FEM			
N	min	max	mean	std	min	max	mean	std
20	35.47	166.68	87.44	29.18	65.7	206.07	157.83	37.13
40	207.56	1,102.21	524.38	181.75	52.97	141.53	111.17	22.44

	Gains on PINNs				Gains on FEM			
N	min	max	mean	std	min	max	mean	std
20	75.86	499.24	215.89	79.51	28.91	64.9	52.36	8
40	999.27	6,317.61	2,665.31	1,003.72	20.09	42.2	34.3	5.19

Results I

- **Test 1**:

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = g, & \text{on } \Gamma. \end{cases}$$

We define Ω by the square $\Omega = [-0.5\pi, 0.5\pi]^2$. For the test case the solution u_{ex} is given by

$$u_{ex}(x, y) = \sin(8x)\,\sin(8y)\ \times 10^{-\frac{1}{2}((x-\mu_1)^2+(y-\mu_2)^2)},$$

with homogeneous BC on Ω (i.e. $g = 0$) and $\mu_1, \mu_2 \sim \mathcal{U}(-0.5, 0.5)$.

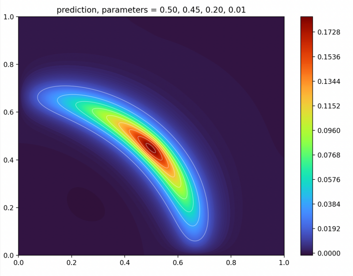
- Gain at fixed error (Finite element P_1)

	N_{dof}	CPU	Error
Pinns	28045	13min	2.4×10^{-2}
Correction 20^2	400	2sec	1.1×10^{-3}
FE 160^2	25600	1min54	7.8×10^{-3}
FE 320^2	102400	7m29	1.95×10^{-3}

- The error is the average error on a set of 10 parameters.
- CPU time for 100 simulations varying parameters: 980sec for our method, 44900 sec for FE. CPU divided by 45.8.
- CPU time for 1000 simulations varying parameters: 2780sec for our method, 449000 sec for FE. CPU divided by 161.
- Using a more FEM library this ratio will be less good.

Results II

- **Test 2** (6D problem):
$$\begin{cases} -\nabla \cdot (\mathbb{K}\nabla u) = f, & \text{in } \Omega, \\ u = 0, & \text{on } \Gamma. \end{cases}$$
We define Ω by the square $\Omega = [-0.5\pi, 0.5\pi]^2$. The source is given by
$$f(x,y) = 10\exp(-((x1 - c1)^2 + (x2 - c2)^2)/(0.025\sigma^2))$$
and the anisotropy matrix is given by
$$K = \begin{pmatrix} \epsilon x^2 + y^2 & (\epsilon - 1)xy \\ (\epsilon - 1)xy & x^2 + \epsilon y^2 \end{pmatrix}$$
with $c_1, c_2 \sim \mathcal{U}(-0.4, 0.6)$, $\sigma \sim \mathcal{U}(0.1, 0.8)$ and $\epsilon \sim \mathcal{U}(0.01, 0.9)$.
- Example of solution (no analytic solution: we will compare with a fine solution)



- Better results for smaller parameters domain.

Results II

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- Gain at fixed error:

	N_{dof}	CPU	Error
Pinns		30min	2.86×10^{-2}
Correction 20^2	400	1sec	1.40×10^{-3}
Correction 40^2	400	3sec	3.3×10^{-4}
FE 80^2	6400	6sec	2.13×10^{-3}
FE 240^2	57600	55sec	2.38×10^{-4}

- CPU time for 100 simulations varying parameters (precision $\approx 2 \times 10^{-4}$): 2100sec for our method, 5500 sec for FE. CPU divided by 2.62.
- CPU time for 1000 simulations varying parameters (precision $\approx 2 \times 10^{-4}$): 4800sec for our method, 55000 sec for FE. CPU divided by 11.5.
- Better results for smaller parameters domain.

Shape Optimization

Problem solved

PINNs and inverse problem

One of the advantages often mentioned is their ability to easily handle inverse problems and optimal control problems, since we're already solving a nonlinear optimization problem.

- Here we consider Shape optimization problems (work done in PEPR Numpex):
- **Energy Dirichlet**:

$$\mathcal{E}(\Omega) := \inf_{u \in H_0^1(\Omega)} \frac{1}{2} \int_\Omega \left(|\nabla u|^2 - fu \right) d\mathbf{x}$$

- **Problem solved**:

$$\inf\{\mathcal{E}(\Omega), \Omega \text{ bounded open set of } \mathbb{R}^n, \text{ such that } |\Omega| = V_0\}$$

- it is equivalent to solve:

$$\inf_\Omega \left(\frac{1}{2} \int_\Omega \left(|\nabla u|^2 - fu \right) d\mathbf{x} \right), \quad \text{with the constrains} \begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

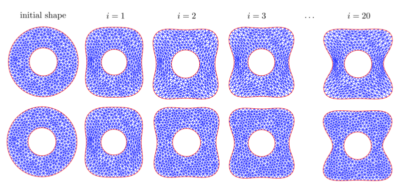
Classical method

- Here we details the classical methods to solve this problem.

One step of the algorithm

- We solve the PDE problem a Finite element or orher method on the mesh Ω_h
- We solve the adjoint PDE problem a Finite element or other method on the mesh Ω_h
- We compute the shape derivative using the primal and adjoint state.
- We use this shape derivative to move the boundary of the shape
- If the mesh becomes too degenerate we remesh.

- Picture of *Parameter-Free Shape Optimization: Various Shape Updates for Engineering Applications*.



- Immersed boundary finite element method avoid the remeshing but need to compute the shape derivative computing level set moving.

PINNs method

- Our approach:
  - We use **two networks**: $u_\theta(\mathbf{x}, \boldsymbol{\mu})$ for the parametric solution of the PDE and $\phi_{\theta_f}(\Omega_0)$ a diffeomorphism which deform the original space.
  - We solve:

$$\min_{\theta,\theta_f}\left(\int_{\phi_{\theta_f}(\Omega)\times\mathbb{M}}\left(\frac{1}{2}|\nabla u_\theta(\mathbf{x};\boldsymbol{\mu})|^2 - f(\mathbf{x};\boldsymbol{\mu})u_\theta(\mathbf{x};\boldsymbol{\mu})\right)\mathrm{d}x\,\mathrm{d}\boldsymbol{\mu}\right)$$

    with $\mathbb{M}$ the parameter space.
  - By a change of variable we find a equivalent problem to solve on Ω_0. We sample on Ω_0.
- Difficulties:
  - How obtain a invertible neural network ?
  - How treat the volume constrains ?

Advantages

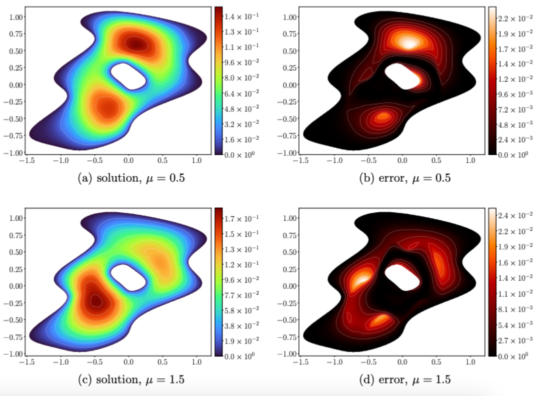
One single loss function to consider.

- A penalization loss for the volume does not work.
- So we propose to impose in hard in the network: invertibility and volume preservation. For that we use neural network which mimic Hamiltonian mechanics called Symplectic NNs.

Results I

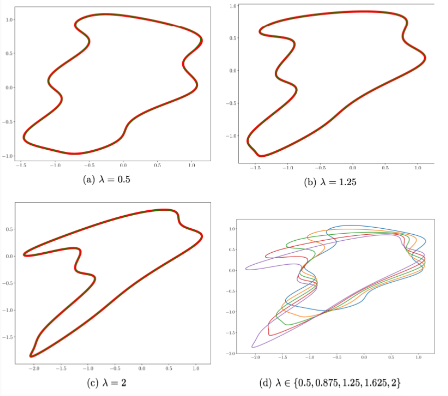
- **Left**: We solve a parametric problem $-\Delta u = f(x_1, x_2; \mu) = \exp\left(1 - \left(\frac{x_1}{\mu}\right)^2 - \left(\frac{x_2}{\mu_2}\right)^2\right)$ on a domain obtain applying a analytic symplectic map:
- **Right**: We learn a parametric symplectic map:

$$\begin{cases} \mathcal{S}_\lambda^1 : (x_1, x_2) \mapsto \left(x_1 - \lambda x_2^2 + 0.3 \sin\left(\frac{x_2}{\lambda}\right) - 0.2 \sin(8x_2), x_2\right), \\ \mathcal{S}_\lambda^2 : (x_1, x_2) \mapsto (x_1, x_2 + 0.2\lambda x_1 + 0.12 \cos(x_1)). \end{cases}$$



(a) solution, $\mu = 0.5$ (b) error, $\mu = 0.5$

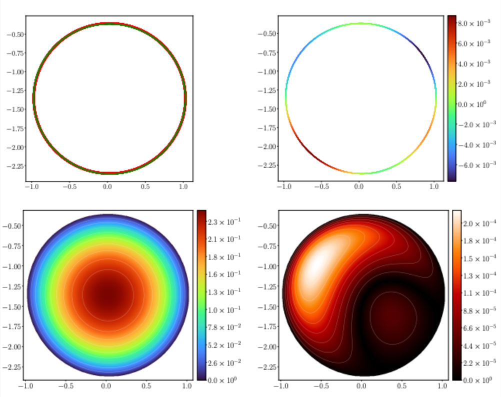
(c) solution, $\mu = 1.5$ (d) error, $\mu = 1.5$



(a) $\lambda = 0.5$ (b) $\lambda = 1.25$

(c) $\lambda = 2$ (d) $\lambda \in \{0.5, 0.875, 1.25, 1.625, 2\}$

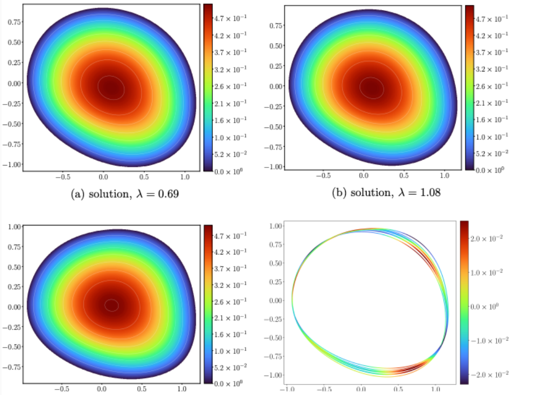
- Optimization problem with $f = 1$ and Ω_0 an ellipse.



method	FEM ($R = 100$)	FEM ($R = 250$)	FEM ($R = 500$)	GeSONN
Computational time (s)	53.3	509	3020	22.5
ℓ^2 error	7.20×10^{-2}	2.83×10^{-2}	2.21×10^{-2}	1.99×10^{-3}

Result III

- Optimization problem with $f(x, y; \lambda) = \exp\left(1 - \|\mathcal{T}_\lambda(x, y)\|^2\right)$ with $\mathcal{T}$ is a the previous symplectic map and Ω_0 is an ellipse.



(a) solution, $\lambda = 0.69$

(b) solution, $\lambda = 1.08$

(c) solution, $\lambda = 1.82$

(d) deviation from the average of the optimality condition

Conclusion

Conclusion

PINNs

PINNs look like a Least-Square Galerkin method on finite dimension submanifold. It is global model (no need mesh) able to tackle large dimensional smooth problems.

Time problems

Two approaches (PINNs): $u(t,\mathbf{x}) = nn(t,\mathbf{x};\theta)$ or ODE based methods (Discrete PINNs, Neural Galerkin): $u(t,\mathbf{x}) = nn(\mathbf{x};\theta(t))$.

Greedy approaches

allow to increase the accuracy of the PINNs. Using a two step greedy method coupling PINNs and FE we can obtain a convergent method more accurate for parametric problems.

Optimization

Since we use nonlinear optimization it is a natural framework for inverse problem and control. NNs are also very useful to parametrize geometries (mapping, signed distance function) and avoid mesh in shape optimization.