A Few Thoughts on Deep Learning-Based Scientific Computing

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November 20, 2020

Acknowledgment

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Funding

National Science Foundation under the grant award 1945029

Deep Learning for Scientific Computing?

- Good to use?
- How to use?

Outline

- Deep Network Approximation
  - Exponential Convergence
  - Curse of dimensonality
  - Deep network is powerful
- Deep Network Optimization
  - Global convergence for supervised learning
  - Global convergence for solving PDEs
  - Deep learning optimization can be realistic?
- Practical applications in scientific computing
  - Approximate solutions for high-dimensional problems
  - Preconditioners for low-dimensional nonlinear problems
  - Multiple solutions of nonlinear problems

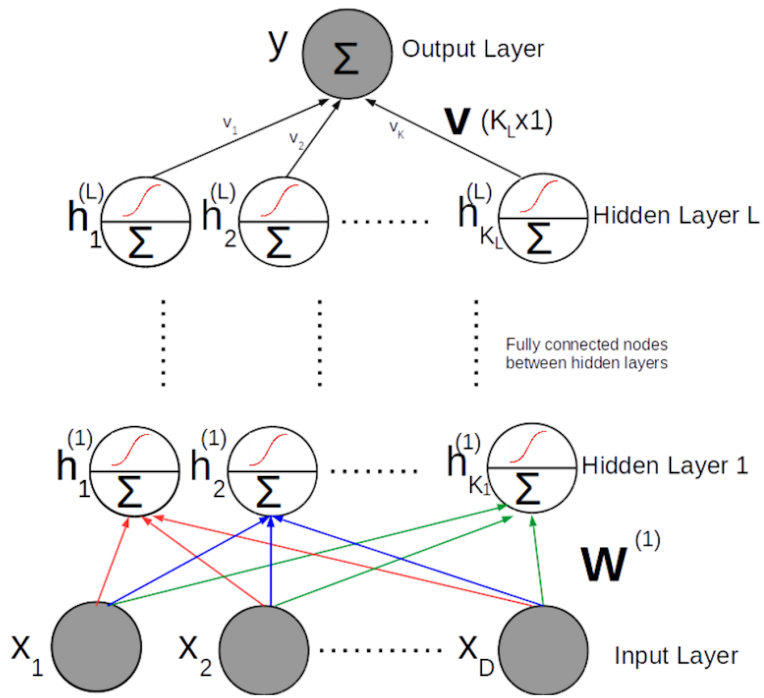
Deep Neural Network

Function composition in the parametrization:

$$y = h(x;\theta) := T \circ \phi(x) := T \circ h^{(L)} \circ h^{(L-1)} \circ \cdots \circ h^{(1)}(x)$$

where

- $h^{(i)}(x) = \sigma({W^{(i)}}^T x + b^{(i)})$;
- $T(x) = V^T x$;
- $\theta = (W^{(1)}, \ldots, W^{(L)}, b^{(1)}, \ldots, b^{(L)}, V)$.



Deep Learning for Solving PDEs

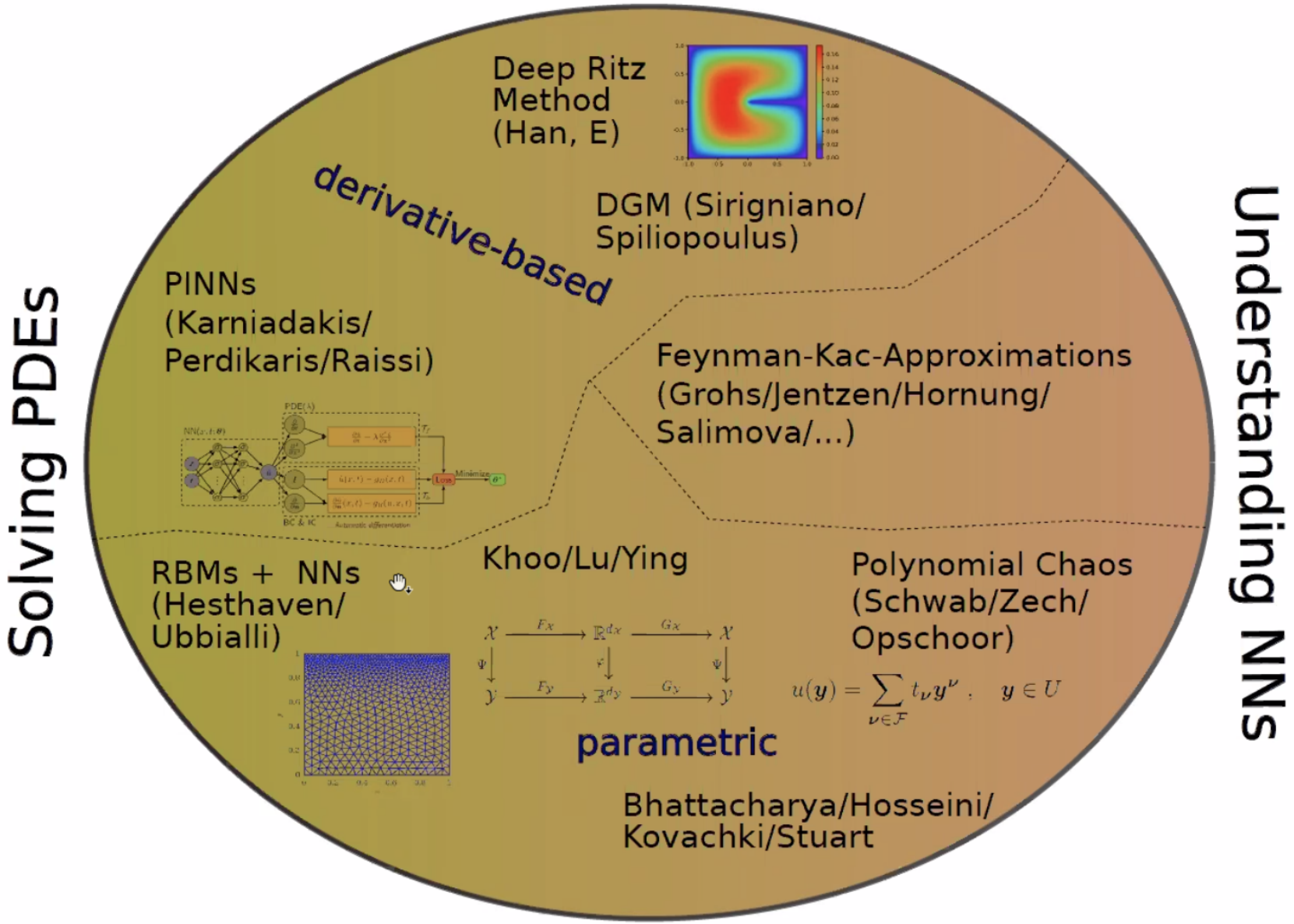


Figure: Figure by Phillip Peterson.

Least Square Methods

Neural networks + least square for PDEs (date back to 1990s),

$$\mathcal{D}(u) = f \quad \text{in } \Omega,$$
$$\mathcal{B}(u) = g \quad \text{on } \partial\Omega.$$

A DNN $\phi(\boldsymbol{x};\boldsymbol{\theta}^*)$ is constructed to approximate the solution $u(\boldsymbol{x})$ via

$$\begin{aligned}
\boldsymbol{\theta}^* &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) \\
&:= \operatorname*{argmin}_{\boldsymbol{\theta}} \|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})\|_2^2 + \lambda \|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})\|_2^2 \\
&= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x}\in\Omega}\left[|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})|^2\right] + \lambda \mathbb{E}_{\boldsymbol{x}\in\partial\Omega}\left[|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})|^2\right].
\end{aligned}$$

Stochastic gradient descent method

- Randomly generate sample sets Ω^r and $\partial\Omega^r$
- Define a random loss function

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}, \Omega^r, \partial\Omega^r) \quad := \quad & \frac{1}{|\Omega^r|} \sum_{\boldsymbol{x}\in\Omega^r} \left[|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})|^2 \right] \\ & + \frac{\lambda}{|\partial\Omega^r|} \sum_{\boldsymbol{x}\in\partial\Omega^r} \left[|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})|^2 \right].\end{aligned}$$

- Update via gradient descent

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}(\boldsymbol{\theta}, \Omega^r, \partial\Omega^r)}{\partial \boldsymbol{\theta}}$$

Main foundation of deep learning

- Approximation theory: how good DNNs approximating functions?
- Optimization algorithms: how can we obtain (nearly) the best parameters?
- Generalization analysis: generalize well to unseen data?

Numerical observation

- Non-uniqueness of powerful network representation.
- Many good local minimizers.
- Fast convergence to approximate solutions.

Gaps between theory and practice.

Deep Network Approximation

Goals

- The curse of dimensionality exist?
- Is exponential convergence available?

Why this goal?

- Computational efficiency
- For example, when we apply DNNs to solve high-dimensional PDEs, it is better to answer the above questions.

Literature Review

A long list with active research directions

- Cybenko, 1989; Hornik et al., 1989; Barron, 1993; Liang and Srikant, 2016; Yarotsky, 2017; Poggio et al., 2017; Schmidt-Hieber, 2017; E and Wang, 2018; Petersen and Voigtlaender, 2018; Chui et al., 2018; Yarotsky, 2018; Nakada and Imaizumi, 2019; Gribonval et al., 2019; Gühring et al., 2019; Chen et al., 2019; Li et al., 2019; Suzuki, 2019; Bao et al., 2019; E et al., 2019; Opschoor et al., 2019; Yarotsky and Zhevnerchuk, 2019; Bölcskei et al., 2019; Montanelli and Du, 2019; Chen and Wu, 2019; Zhou, 2020; Montanelli et al., 2020, etc.
- Functions spaces: continuous functions, smooth functions, functions with integral representations;
- Tools: polynomial approximations, the law of large number, Kolmogorov-Arnold representation theory, bit extraction technology (Bartlett et al., 1998; Harvey et al., 2017).

Our understanding on the literature

ReLU DNNs

- Curse of dimensionality exisits for continuous and smooth functions.
- Exponential convergence is achievable for special function classes.

DNNs with advanced activation functions

- Curse of dimensionality does not exisit and exponential convergence is achievable for (Hölder) continuous functions.
- Require exponentially large computation with high precision.

ReLU DNNs, continuous functions $C([0,1]^d)$

ReLU; Fixed width $O(d)$, varying depth L

- Tight error rate $O(L^{-2/d})$ with L^∞-norm
- Yarotsky, 2018

ReLU; Fixed network width $O(N)$ and depth $O(L)$

- Tight error rate $5\omega_f(8\sqrt{d}N^{-2/d}L^{-2/d})$ simultaneously in N and L with L^∞-norm
- ω_f is the modulas of continuity
- Shen, Y., and Zhang (CiCP, 2020)

Curse of dimensionality exists!

ReLU DNNs, smooth functions $C^s([0,1]^d)$

Does smoothness help?

ReLU; Fixed width $O(d)$, varying depth L

- Tight error rate $O(L^{-2s/d})$ with L^∞-norm
- Yarotsky, 2019

ReLU; Fixed network width $O(N)$ and depth $O(L)$

- Tight rate $85(s+1)^d 8^s \|f\|_{C^s([0,1]^d)} N^{-2s/d} L^{-2s/d}$ simultaneously in N and L with L^∞-norm
- Lu, Shen, Y., and Zhang (preprint, 2020)

The curse of dimensionality exists if s is fixed and smoothness may help a bit

DNNs with advanced activation function

Sine-ReLU; Fixed width $O(d)$, varying depth L

- $\exp(-c_{r,d}\sqrt{L})$ with L^∞-norm for $C^r([0,1]^d)$
- Root exponential convergence achieved
- Curse of dimensionality is not clear
- Yarotsky, 2019

Floor and ReLU activation, width $O(N)$ and depth $O(dL)$, $C([0,1]^d)$

- Error rate $\omega_f(\sqrt{d}N^{-\sqrt{L}}) + 2\omega_f(\sqrt{d})N^{-\sqrt{L}}$ with L^∞-norm
- Merely based on the compositional structure of DNNs
- NO curse of dimensionality for many continuous functions
- Root exponential approximation rate
- Shen, Y., and Zhang (Neural Computation, 2020)

DNNs with advanced activation function

Floor and ReLU activation, width $O(N)$ and depth $O(dL)$, $C([0,1]^d)$

- Error rate $\omega_f(\sqrt{d}N^{-\sqrt{L}}) + 2\omega_f(\sqrt{d})N^{-\sqrt{L}}$ with L^∞-norm
- Merely based on the compositional structure of DNNs
- NO curse of dimensionality for many continuous functions
- Root exponential approximation rate
- Shen, Y., and Zhang (Neural Computation, 2020)

Floor, Sign, and 2^x activation, width $O(N)$ and depth 3, $C([0,1]^d)$

- Error rate $\omega_f(\sqrt{d}2^{-N}) + 2\omega_f(\sqrt{d})2^{-N}$ with L^∞-norm
- Merely based on the compositional structure of DNNs
- NO curse of dimensionality for many continuous functions
- Exponential approximation rate
- Shen, Y., and Zhang (preprint, 2020)

Open problem: How to train these networks efficiently?

Key ideas of our approximation

For $\boldsymbol{x} \in Q_{\boldsymbol{\beta}}$:
$\boldsymbol{x} \to \phi_1(\boldsymbol{x}) = \boldsymbol{\beta} \to \phi_2(\boldsymbol{\beta}) = k_{\boldsymbol{\beta}} \to \phi_3(k_{\boldsymbol{\beta}}) = f(\boldsymbol{x}_{\boldsymbol{\beta}}) \approx f(\boldsymbol{x})$

- Piecewise constant approximation:
  $f(\boldsymbol{x}) \approx f_p(\boldsymbol{x}) \approx \phi_3 \circ \phi_2 \circ \phi_1(\boldsymbol{x})$
- N pieces per dim and N^d pieces with accuracy $\frac{1}{N}$
- Floor NN $\phi_1(\boldsymbol{x})$ s.t. $\phi_1(\boldsymbol{x}) = \boldsymbol{\beta}$ for $\boldsymbol{x} \in Q_{\boldsymbol{\beta}}$.
- Linear NN ϕ_2 mapping $\boldsymbol{\beta}$ to an integer
  $k_{\boldsymbol{\beta}} \in \{1, \ldots, N^d\}$
- Key difficulty: Floor ReLU NN ϕ_3 of width $O(N)$ and depth $O(dL)$ fitting N^d samples in 1D with accuracy $O(N^{-L})$
- ReLU NN fails

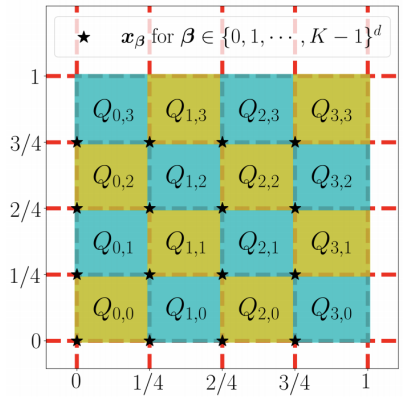


Figure: Uniform domain partitioning.

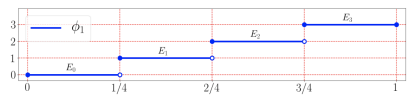


Figure: Floor function.

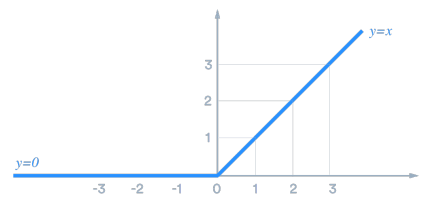


Figure: ReLU function.

Summary

- Deep Neural Networks are powerful
- How to identify these networks via optimization?

Why Deep Neural Netwokrs?

From the point of view of optimization.

Conjectures

- When network is sufficiently large, local minimizers are usually good minimizers.

Reality

- No practical theory and even efficient algorithm.

Neural tangent kernel/Lazy training

- Jacot et al. 2018; Du et al. 2019a; Allen-Zhu et al. 2019b; Du et al. 2019b; Zou et al. 2018; Chizat et al. 2019, etc.
- Idea: in the limit of infinite width, DNN becomes kernel methods

Mean-field analysis

- Chizat and Bach 2018; Mei et al. 2018; Mei et al. 2019, Lu et al. 2020
- Idea:
  1) a two-layer neural network can be seen as an approximation to an infinitely wide neural network with parameters following a distribution p_t;
  2) understanding network training via the evolution of p_t.

Key Analysis of Neural Tangent Kernel

Simplifying the residual dynamic via approximation:

$$\begin{aligned}
\phi(\boldsymbol{X};\boldsymbol{\theta}_{t+1}) - f(\boldsymbol{X}) &\approx [\boldsymbol{I} - \tfrac{m\eta}{n}\boldsymbol{H}_t](\phi(\boldsymbol{X};\boldsymbol{\theta}_t) - f(\boldsymbol{X})) && \text{(NN dynamic)} \\
&\approx [\boldsymbol{I} - \tfrac{m\eta}{n}\boldsymbol{H}_0](\phi(\boldsymbol{X};\boldsymbol{\theta}_t) - f(\boldsymbol{X})) && \text{(lazy training)} \\
&\approx [\boldsymbol{I} - \tfrac{m\eta}{n}\boldsymbol{H}](\phi(\boldsymbol{X};\boldsymbol{\theta}_t) - f(\boldsymbol{X})) && \text{(NTK dynamic)}
\end{aligned}$$

- Training samples $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]^T$;
- Learning rate η;
- Width m;
- Gram matrix $\boldsymbol{H}_t := (\frac{1}{m}\langle \nabla\phi(\boldsymbol{x}_i;\boldsymbol{\theta}_t), \nabla\phi(\boldsymbol{x}_j;\boldsymbol{\theta}_t)\rangle)_{n\times n}$;
- NTK $\boldsymbol{H} = \lim_{m\to\infty} \boldsymbol{H}_0$;
- $\approx$ valid when $\boldsymbol{\theta}_{t+1} \approx \boldsymbol{\theta}_t \leftarrow \eta \approx 0$;
- $\approx$ valid when $\boldsymbol{\theta}_t \approx \boldsymbol{\theta}_0 \leftarrow \eta \approx 0$;
- $\approx$ valid when $m \to \infty$ by the law of large numbers.

Optimization for PDE Solvers

Question: can we apply existing optimization analysis for PDE solvers?

A simple example

- Two-layer network: $\phi(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{k=1}^{N} a_k \sigma(\boldsymbol{w}_k^T \boldsymbol{x})$.
- A second order differential equation: $\mathcal{L}u = f$ with

$$\mathcal{L}u = \sum_{\alpha,\beta=1}^{d} A_{\alpha\beta}(\boldsymbol{x}) u_{x_\alpha x_\beta}.$$

- $f(\boldsymbol{x};\boldsymbol{\theta}) := \mathcal{L}\phi(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{k=1}^{N} a_k \boldsymbol{w}_k^T A(\boldsymbol{x}) \boldsymbol{w}_k \sigma''(\boldsymbol{w}_k^T \boldsymbol{x})$ to fit $f(\boldsymbol{x})$
- Much more difficult nonlinearity in $\boldsymbol{x}$ and $\boldsymbol{w}$ in the fitting than the original NN fitting.

Optimization for PDE Solvers

Assumption

- Two-layer network: $\phi(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{k=1}^{N} a_k \sigma(\boldsymbol{w}_k^T \boldsymbol{x})$.
- A second order differential equation: $\mathcal{L}u = f$ with

$$\mathcal{L}u = \sum_{\alpha,\beta=1}^{d} A_{\alpha\beta}(\boldsymbol{x}) u_{x_\alpha x_\beta} + \sum_{\alpha=1}^{d} b_\alpha(\boldsymbol{x}) u_{x_\alpha} + c(\boldsymbol{x}) u.$$

- Fixed n samples in the PDE domain.
- Empirical loss

$$\min_{\boldsymbol{\theta}} \frac{1}{n} \sum_{\{\boldsymbol{x}_i\}_{i=1}^n} |\mathcal{L}\phi(\boldsymbol{x}_i;\boldsymbol{\theta}) - f(\boldsymbol{x}_i)|^2.$$

Theorem: optimization convergence (T. Luo and Y., preprint, 2020)

Under the assumption of over-parametrization, with a high probability over random initialization, gradient descent dynamics makes the empirical loss function linearly converge to zero.

Summary

- Deep network approximation is powerful
- Deep network optimization for scientific computing is challenging with few theories
  - Finite width and finite depth: open problem
  - SGD instead of gradient flow analysis: open problem
  - Nonlinear PDEs: open problem

Next question: Where to apply deep learning in scientific computing?

Deep learning for solving PDEs

Problem

$$\mathcal{D}(u) = f \quad \text{in } \Omega,$$
$$\mathcal{B}(u) = g \quad \text{on } \partial\Omega.$$

Continuous method

A DNN $\phi(\boldsymbol{x}; \boldsymbol{\theta}^*)$ is constructed to approximate the solution $u(\boldsymbol{x})$ via

$$\begin{aligned} \boldsymbol{\theta}^* &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) \\ &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x}\in\Omega}\left[|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})|^2\right] + \lambda \mathbb{E}_{\boldsymbol{x}\in\partial\Omega}\left[|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})|^2\right]. \end{aligned}$$

Our philosophy

- Non-uniqueness of network representation.
- Many good local minimizers.
- Fast convergence to good approximate solutions.

Example 1: Solving High-Dimensional PDEs

Previous successes

Han et al., Sirignano et al., Berg et al., Khoo et al., Maissi et al., etc.

SelectNet: Self-Paced Learning for High-dimensional Partial Differential Equations

- Gu, Y., and Zhou (preprint, 2019)
- Importance sampling
- Faster convergence
- Better local minimizers

SelectNet

Given a PDE problem,

$$\begin{aligned}\mathcal{D}(u) &= f \quad \text{in } \Omega,\\ \mathcal{B}(u) &= g \quad \text{on } \partial\Omega.\end{aligned}$$

- First DNN $\phi(\boldsymbol{x};\boldsymbol{\theta})$ is constructed to approximate the solution $u(\boldsymbol{x})$;
- Second DNN $\phi_s(\boldsymbol{x};\boldsymbol{\theta}_s) \in [m_1, m_2]$ for weighting.

$$\begin{aligned}\min_{\boldsymbol{\theta}} \max_{\boldsymbol{\theta}_s} \mathcal{L}(\boldsymbol{\theta},\boldsymbol{\theta}_s) : \quad = \quad & \mathrm{E}_{\boldsymbol{x}\in\Omega}\left[\phi_s(\boldsymbol{x};\boldsymbol{\theta}_s)\,|\mathcal{D}(\phi(\boldsymbol{x};\boldsymbol{\theta})) - f(\boldsymbol{x})|^2\right]\\ & +\lambda \mathrm{E}_{\boldsymbol{x}\in\partial\Omega}\left[\phi_s(\boldsymbol{x};\boldsymbol{\theta}_s)\,|\mathcal{B}(\phi(\boldsymbol{x};\boldsymbol{\theta})) - g(\boldsymbol{x})|^2\right]\\ & -\varepsilon^{-1}\left(\frac{1}{|\Omega|}\int_{\Omega}\phi_s(\boldsymbol{x};\boldsymbol{\theta}_s) - 1\right)^2\\ & -\varepsilon^{-1}\left(\frac{1}{|\partial\Omega|}\int_{\partial\Omega}\phi_s(\boldsymbol{x};\boldsymbol{\theta}_s) - 1\right)^2\end{aligned}$$

Nonlinear Elliptic Equations

- PDE

$$-\nabla \cdot (a(x)\nabla u) + |\nabla u|^2 = f(x), \quad \text{in } \Omega := \{\boldsymbol{x} : |\boldsymbol{x}| < 1\},$$
$$u = g(x), \quad \text{on } \partial\Omega,$$

  with $a(x) = 1 + \frac{1}{2}|\boldsymbol{x}|^2$.

- Example:

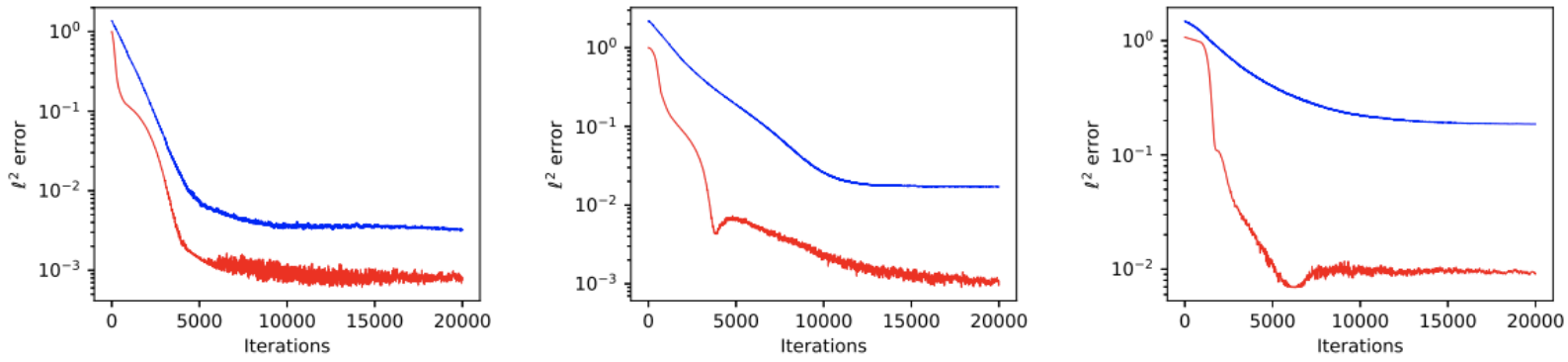
$$u(\boldsymbol{x}) = \sin(\frac{\pi}{2}(1 - |\boldsymbol{x}|)^{2.5})$$

  in $\Omega = \{\boldsymbol{x} : |\boldsymbol{x}| < 1\}$.

dimension	SelectNet	Basic
$d = 10$	7.9×10^{-4}	3.2×10^{-3}
$d = 20$	9.6×10^{-4}	1.7×10^{-2}
$d = 100$	9.3×10^{-3}	1.9×10^{-1}

Table: The minimal relative L^2 errors obtained by various methods in the nonlinear elliptic example.

Nonlinear Elliptic Equations



(a) $d = 10$ (b) $d = 20$ (c) $d = 100$

Fig. 6.2: *ℓ^2 errors v.s. iterations in the nonlinear elliptic example (Red: SelecNet model; Blue: the basic model).*

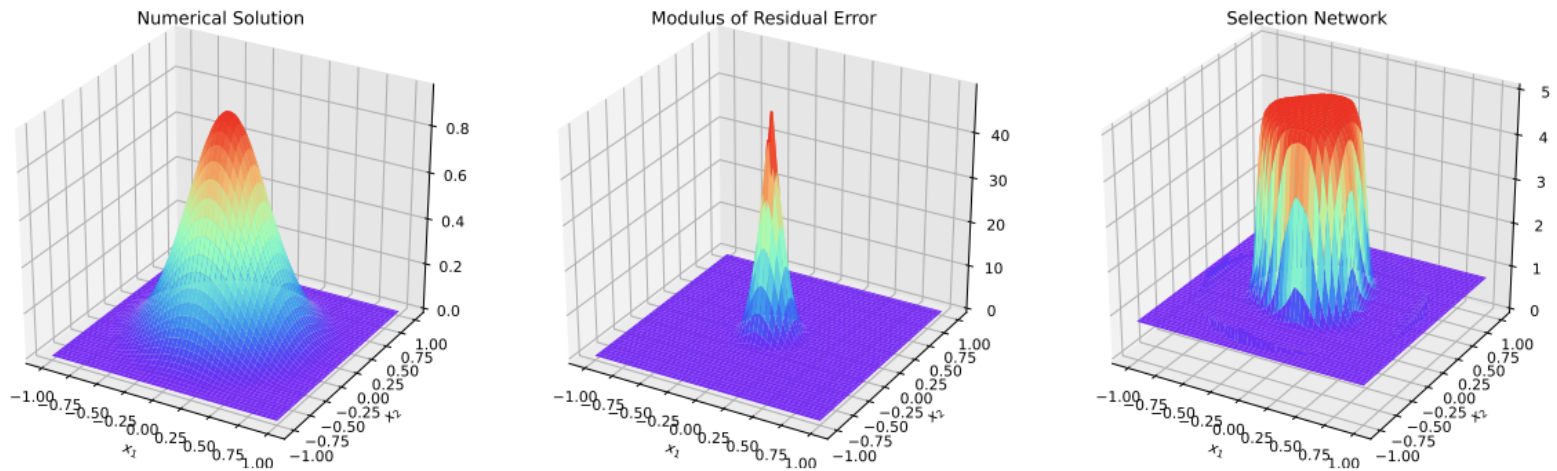


Fig. 6.3: *The (x_1, x_2)-surfaces of the numerical solution, modulus of residual error and selection network by SelectNet (d=20) in the nonlinear elliptic example.*

Parabolic Equations

- PDE

$$\begin{aligned} \partial_t u(x,t) - \Delta u(x,t) &= f(x,t), \quad \text{in } Q := \Omega \times (0,1), \\ u(x,t) &= g(x), \quad \text{on } \partial\Omega \times (0,1), \\ u(x,0) &= h(x), \quad \text{in } \Omega, \end{aligned}$$

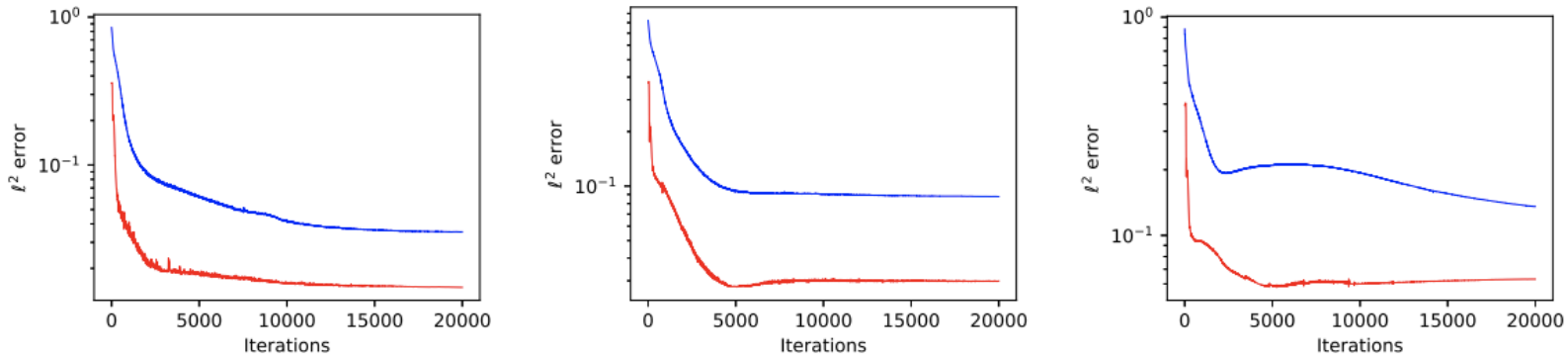
  with $\Omega := [-1,1]^d$.

- Example: $u(x,t) = e^{-t}\sin(\frac{\pi}{2}(1-|x|)^{2.5})$.

dimension	SelectNet	Basic
$d = 10$	1.5×10^{-2}	3.5×10^{-2}
$d = 20$	3.0×10^{-2}	8.7×10^{-2}
$d = 100$	6.3×10^{-2}	1.4×10^{-1}

Table: The minimal relative L^2 errors obtained by various methods in the parabolic example.

Parabolic Equations



(a) $d = 10$ (b) $d = 20$ (c) $d = 100$

Fig. 6.4: *ℓ^2 errors v.s. iterations in the first parabolic example (Red: SelecNet model; Blue: the basic model).*

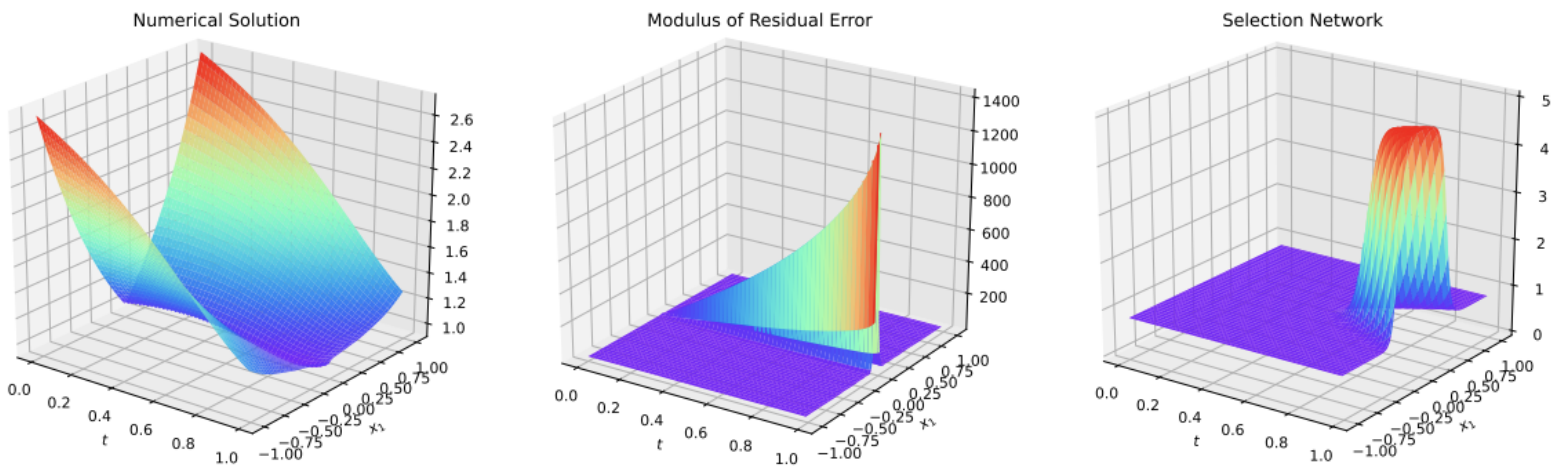
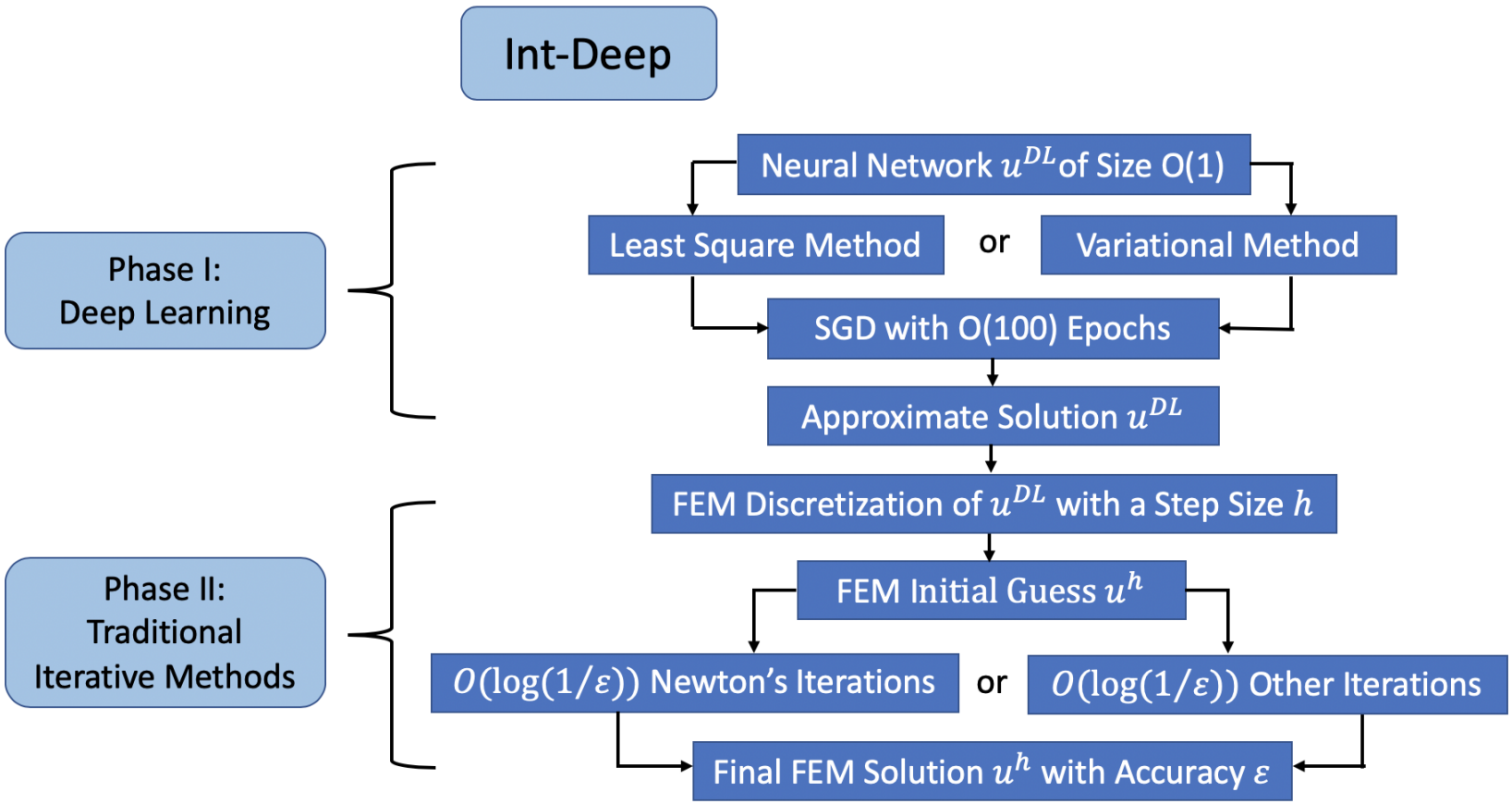


Fig. 6.5: *The (t, x_1)-surfaces of the numerical solution, modulus of residual error and selection network by SelectNet (d=20) in the first parabolic example.*

Example 2: Preconditioning

Int-Deep: A Deep Learning Initialized Iterative Method for Nonlinear Problems. Huang, Wang, and Y. (JCP, 2020)

- Idea: DL for initial guesses in traditional iterative methods



Semilinear elliptic equations

- PDE

$$\begin{cases} -\Delta u - (u-1)^3 + (u+2)^2 = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

  where $\Omega = (0,1)^d$.
- Example: $u(x) = 3\sin(2\pi x)$ for $d = 1$

Table: The performance of Int-Deep in 1D with different mesh sizes h with linear polynomials in FEM.

h	e_{h^2}	# Epoch	e^{DL}	#K	e^h	order
2^{-7}	6.1e-5	200	3.0e-1	5	1.2e-3	-
2^{-8}	1.5e-5	200	3.0e-1	5	2.9e-4	2.0
2^{-9}	3.8e-6	200	3.0e-1	5	7.3e-5	2.0
2^{-10}	9.5e-7	200	3.0e-1	5	1.8e-5	2.0
2^{-11}	2.4e-7	200	3.0e-1	5	4.6e-6	2.0
2^{-12}	6.0e-8	200	3.0e-1	5	1.1e-6	2.0
2^{-13}	1.5e-8	200	3.0e-1	5	2.8e-7	2.0
2^{-14}	3.7e-9	200	3.0e-1	5	7.1e-8	2.0

Semilinear elliptic equations

- PDE

$$\begin{cases} -\Delta u - (u-1)^3 + (u+2)^2 = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

  where $\Omega = (0,1)^d$.
- Example: $u(x) = 3\sin(2\pi x)$ for $d = 1$

Table: The performance of Int-Deep in 1D with different DNN width N and depth L when $h = \frac{1}{1024}$. T^{DL} denotes the running time of GPU for deep learning training in Pytorch.

L \ N	10				30				50			
	e_0^h	e^h	#K	T^{DL}	e_0^h	e^h	#K	T^{DL}	e_0^h	e^h	#K	T^{DL}
2	3.7e+0	1.8e-5	8	42.0s	2.3e-1	1.8e-5	5	42.0s	5.2e-2	1.8e-5	4	46.9s
4	1.1e-1	1.8e-5	4	48.1s	1.6e-2	1.8e-5	3	49.0s	1.5e-2	1.8e-5	3	48.7s
6	9.8e-2	1.8e-5	4	45.1s	8.5e-3	1.8e-5	3	50.4s	5.3e-3	1.8e-5	3	51.8s

Nonlinear Schrodinger Equation

$$\begin{cases} -\Delta u + V(x)u + 10u^3 = \lambda u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

where $V(x)$ is two Gaussian wells, $\Omega = [0, 1]$.

Table: The performance of Int-Deep in 1D with different mesh sizes h.

h	#epoch	res^{DL}	e^{DL}	λ^{DL}	#K	res^{h}	e^{h}	λ^{h}
2^{-5}	500	6.6e+0	6.3e-2	24.3	4	4.6e-2	3.9e-3	25.1
2^{-6}	500	8.2e+0	6.4e-2	24.3	5	1.2e-2	3.3e-3	25.1
2^{-7}	500	17.5e+0	6.4e-2	24.3	6	3.0e-3	2.2e-3	25.1
2^{-8}	500	34.7e+0	6.4e-2	24.3	7	8.2e-4	1.1e-3	25.1
2^{-9}	500	50.2e+0	6.4e-2	24.3	7	4.2e-4	7.0e-4	25.1

Nonlinear Schrodinger Equation

$$\begin{cases} -\Delta u + V(x)u + 10u^3 = \lambda u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

where $V(x)$ is two Gaussian wells, $\Omega = [0, 1]$.

Table: The performance of Int-Deep in 1D with different DNN width N and depth L when $h = \frac{1}{512}$. T^{DL} denotes the running time of GPU for deep learning training in Pytorch.

L \ N	30				40				50			
	e^h	res^h	#K	T^{DL}	e^h	res^h	#K	T^{DL}	e^h	res^h	#K	T^{DL}
2	3.2e-2	2.7e-3	7	65.4s	2.1e+0	3.8e-3	7	64.9s	2.2e-3	9.2e-3	7	64.9s
4	2.1e+0	6.2e-3	7	68.0s	1.7e-1	3.8e-2	7	68.2s	7.8e-2	2.4e-3	7	68.5s
6	7.0e-2	3.4e-3	7	70.4s	5.2e-2	2.5e-3	7	69.5s	1.2e-3	3.0e-4	7	69.9s

Example 3: Identify Multiple Solutions

NND: Structure Probing Neural Network Deflation. Gu, Wang, and Y. (Submitted, 2020)

- Idea: leverage the power of NN representation for multiple solutions of nonlienar PDEs

Our philosophy

- Non-uniqueness of network representation.
- Many good local minimizers.

Conventional methods

- Functional deflation methods (Ferrell et al.)
- Numerical continuation or homopoty (Sommese and Morgan; Hao et al.; Liao)
- Davidenko differential equation (Branin; Davidenko)

Structure Probing Neural Network Deflation

Deflation

$$\min_{\boldsymbol{\theta}} \mathcal{L}_{\text{NND}} := \Big(\sum_{k=1}^{K} \frac{1}{\|u(\boldsymbol{x};\boldsymbol{\theta}) - u_k(\boldsymbol{x})\|_{L^2(\Omega)}^{p_k}} + \alpha\Big)\mathcal{L}(u(\boldsymbol{x};\boldsymbol{\theta})),$$

- $\mathcal{L}(u(\boldsymbol{x};\boldsymbol{\theta}))$ is the loss function in the least square method
- p_k is a positive power of the deflated solutions u_k
- $\alpha > 0$ is a shift constant to exclude spurious solutions

Structure Probing

$$u_J(\boldsymbol{x};\boldsymbol{\theta}_J) = u(\boldsymbol{x};\boldsymbol{\theta}) + \sum_{j=1}^{J} c_j \xi_j(\boldsymbol{x}),$$

- $\boldsymbol{\theta}_J := \{\boldsymbol{\theta}, \{c_j\}_{j=1}^{J}\}$ is trainable after initialization
- Structure probing functions $\xi_j(\boldsymbol{x})$
  - e.g., $\{\xi_j(\boldsymbol{x}) = e^{\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{x}}, |\boldsymbol{k}_j| = j, j = 1, \cdots, J\}$ with $\boldsymbol{k}_j$ randomly selected
  - e.g., $\{\xi_j(\boldsymbol{x}) = \sin(j\pi|\boldsymbol{x}|), j = 1, \cdots, J\}$

We consider 2-D Yamabe's equation that seeks u such that

$$\begin{aligned} -8\Delta u - 0.1u + \frac{u^5}{|\boldsymbol{x}|^3} &= 0, \quad \text{in } \Omega = \{\boldsymbol{x} \in \mathbb{R}^2 : r < |\boldsymbol{x}| < R\}, \\ u &= 1, \quad \text{on } \partial\Omega, \end{aligned}$$

where r and R are set as 1 and 100.

- 9 solutions by using non-network deflation techniques and various initial guesses in (Farrell et al.)
- We got 14 solutions.

2-D Yamabe's equation

$$-8\Delta u - 0.1u + \frac{u^5}{|\boldsymbol{x}|^3} = 0, \quad \text{in } \Omega = \{\boldsymbol{x} \in \mathbb{R}^2 : r < |\boldsymbol{x}| < R\},$$

$$u = 1, \quad \text{on } \partial\Omega,$$

where r and R are set as 1 and 100.

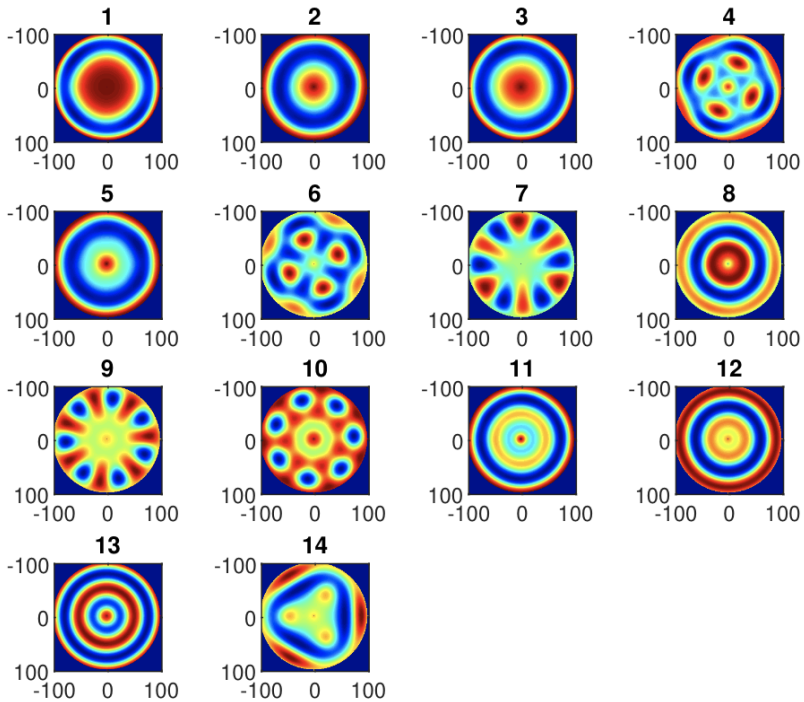


Figure: 14 solutions of the 2D problem.

The 6-dimensional Yamabe's equation

$$-\frac{4(d-1)}{(d-2)}\Delta u - 0.125u + \frac{u^{\frac{d+2}{(d-2)}}}{|\boldsymbol{x}|^3} = 0, \quad \text{in } \Omega = \{1 < |\boldsymbol{x}| < 100\},$$

$$u = 1, \quad \text{on } \partial\Omega,$$

where $d \geq 3$ is the dimension of the problem.

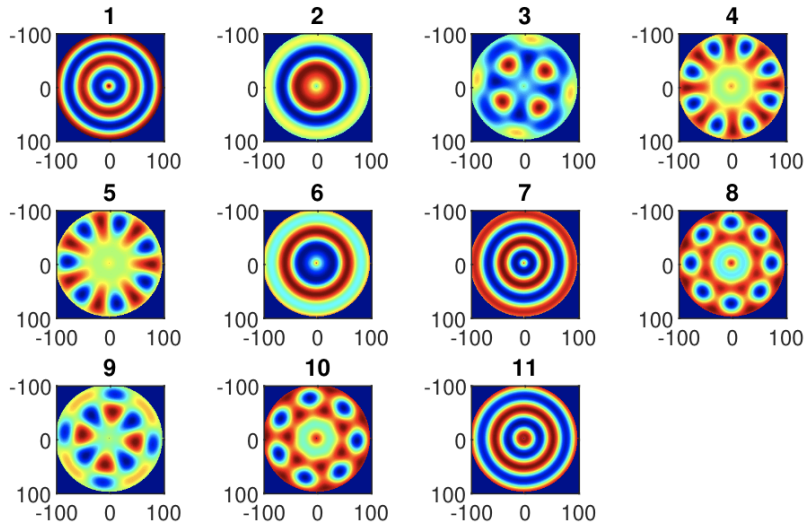


Figure: 11 solutions of the 6D problem.