A Few Thoughts on Deep Learning-Based Scientific Computing

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Deep Learning for Scientific Computing?

Still not a complete story.

Outline

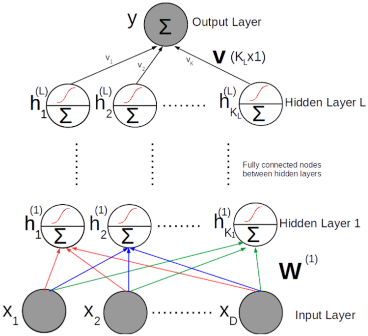
- **Neural Network Approximation**
  - Exponential Approximation Rate
  - Curse of dimensonality
  - Deep network is powerful
- **Neural Network Optimization**
  - Global convergence for supervised learning
  - Global convergence for solving PDEs
  - But assumption is strong
- **Neural Network Generalization**
  - Generalization for supervised learning
  - Generalization for solving PDEs
  - But requires regularization

Deep neural networks

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

where

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



Supervised deep learning

Conditions

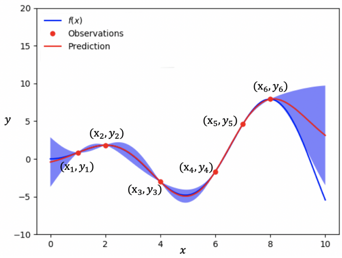
- Given data pairs $\{(x_i, y_i = f(x_i))\}$ from an unknown map $f(x)$ defined on Ω
- $\{x_i\}_{i=1}^n$ are sampled randomly from an unknown distribution $U(x)$ on Ω

Goal

Recover the unknown map $f(x)$

Deep learning

- Design a family of DNNs $\{h(x;\theta)\}_\theta$ of a given size
- Find the best DNN $h(x;\theta) \approx f(x)$ on Ω



Supervised deep learning

Deep learning ideally

- Quantify how good $h(x;\theta) \approx f(x)$ via the population loss:

$$R_D(\theta) \overset{\text{e.g.}}{=} \mathrm{E}_{x\sim U(\Omega)}\left[|h(x;\theta) - f(x)|^2\right]$$

- The best solution is $h(x;\theta_D)$ with

$$\theta_D = \operatorname{argmin} R_D(\theta)$$

- But $U(\Omega)$ is not known

Deep learning in practice

- Only the empirical loss is available:

$$R_S(\theta) := \frac{1}{N}\sum_{i=1}^{N}(h(x_i;\theta) - y_i)^2$$

- The best empirical solution is $h(x;\theta_S)$ with

$$\theta_S = \operatorname{argmin} R_S(\theta)$$

- Numerical optimization to obtain a numerical solution $h(x;\theta_N)$.
- In practice, $\theta_N \neq \theta_S \neq \theta_D$ and how good $R_D(\theta_N)$ is?

Supervised deep learning

A full error analysis of $R_D(\theta_N)$

$$
\begin{aligned}
R_D(\theta_N) &= [R_D(\theta_N) - R_S(\theta_N)] + [R_S(\theta_N) - R_S(\theta_S)] + [R_S(\theta_S) - R_S(\theta_D)] \\
&\quad + [R_S(\theta_D) - R_D(\theta_D)] + R_D(\theta_D) \\
&\le R_D(\theta_D) + [R_S(\theta_N) - R_S(\theta_S)] \\
&\quad + [R_D(\theta_N) - R_S(\theta_N)] + [R_S(\theta_D) - R_D(\theta_D)],
\end{aligned}
$$

A full error analysis of $R_D(\theta_N)$

$$\begin{aligned} R_D(\theta_N) &= [R_D(\theta_N) - R_S(\theta_N)] + [R_S(\theta_N) - R_S(\theta_S)] + [R_S(\theta_S) - R_S(\theta_D)] \\ &\quad + [R_S(\theta_D) - R_D(\theta_D)] + R_D(\theta_D) \\ &\le R_D(\theta_D) + [R_S(\theta_N) - R_S(\theta_S)] \\ &\quad + [R_D(\theta_N) - R_S(\theta_N)] + [R_S(\theta_D) - R_D(\theta_D)], \end{aligned}$$

- $R_D(\theta_D) = \int_\Omega (h(x;\theta_D) - f(x))^2 d\mu(x) \le \int_\Omega (h(x;\tilde{\theta}) - f(x))^2 d\mu(x)$ can be bounded by a constructive approximation of $\tilde{\theta}$

Supervised deep learning

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- $[R_S(\theta_N) - R_S(\theta_S)]$ is the optimization error

A full error analysis of $R_D(\theta_N)$

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&\le R_D(\theta_D) + [R_S(\theta_N) - R_S(\theta_S)] \\
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\end{aligned}
$$

- $R_D(\theta_D) = \int_\Omega (h(x;\theta_D) - f(x))^2 d\mu(x) \le \int_\Omega (h(x;\tilde{\theta}) - f(x))^2 d\mu(x)$ can be bounded by a constructive approximation of $\tilde{\theta}$
- $[R_S(\theta_N) - R_S(\theta_S)]$ is the optimization error
- Other two terms are the generalization error

Deep Learning for Solving PDEs

Goals

Learning the solutions of high-dimensional and highly nonlinear PDEs

Challenges for traditional methods

- curse of dimensionality

Machine learning for PDEs

- Owens and Filkin, 1989; Lee and Kang, 1990; Dissanayake and Phan-Thien, 1994
- RBM, Quantum Many-Body Problem, Giuseppe Carleo, Matthias Troyer, 2016
- BSDE, Han et al, 2017
- DGM, Sirignano and Spiliopoulos, 2017
- Deep Ritz, E and Yu, 2017
- PINN, Raissi, Perdikaris, and Karniadakis, 2017

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

$$\begin{aligned}\boldsymbol{\theta}^* &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) \\ &:= \operatorname*{argmin}_{\boldsymbol{\theta}} \|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})\|_2^2 + \lambda\|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})\|_2^2\end{aligned}$$

Least Square Methods

We aim at the full error analysis:

- Approximation theory
- Optimization theory
- Generalization theory

Deep Network Approximation

Goals

- The curse of dimensionality exist? e.g., # parameters not $(\frac{1}{\epsilon})^d$
- Is exponential approximation rate available? e.g., # parameters $\log(\frac{1}{\epsilon})$

Why this goal?

- Computational efficiency especially in high dimension

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.

Literature Review

Functions spaces

- Continuous functions
- Smooth functions
- Functions with integral representations

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

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

- Nearly tight error rate $5\omega_f(8\sqrt{d}N^{-2/d}L^{-2/d})$ simultaneously in N and L with L^∞-norm. Shen, Y., and Zhang (CiCP, 2020)
- ω_f is the modulas of continuity
- Improved to a tight rate $O\left(\sqrt{d}\,\omega_f\left(\left(N^2L^2\log_3(N+2)\right)^{-1/d}\right)\right)$. Shen, Y., and Zhang (J Math Pures Appl, 2021)

Curse of dimensionality exists!

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

Does smoothness help?

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

- Nearly 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 (SIMA 2021)

The curse of dimensionality exists if s is fixed.

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 approximation rate achieved
- Curse of dimensionality is not clear
- arotsky and Zhevnerchuk, NeurIPS 2020

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

What if we use more activation functions?

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 (Neural Networks, 2021)

Further interpretation of our result

Explicit error bound

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

- Error rate $3\lambda(2\sqrt{d})^\alpha 2^{-\alpha N}$ with L^∞-norm
- NO curse of dimensionality
- Exponential approximation rate
- Shen, Y., and Zhang (Neural Networks, 2021)

Further interpretation of our result

Realistic consideration

- Constructive approximation requires f or exponentially many samples given
- Constructed parameters require high precision computation
- Floor and Sign are discontinuous functions leading to gradient vanishing
- The network size has to be increased when $\epsilon \to 0$

DNNs with advanced activation function

Elementary universal activation function (EUAF)

A continuous activation function without gradient vanishing

$$\sigma_1(x) = \left|x - 2\lfloor \tfrac{x+1}{2} \rfloor\right|,$$

$$\sigma_2(x) := \frac{x}{|x| + 1},$$

$$\sigma(x) := \begin{cases} \sigma_1(x) & \text{for } x \in [0, \infty), \\ \sigma_2(x) & \text{for } x \in (-\infty, 0). \end{cases}$$

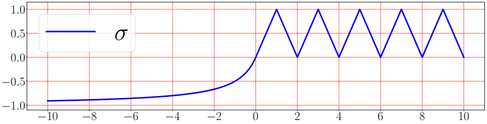


Figure: An illustration of σ on $[-10, 10]$.

DNNs with advanced activation function

Theorem (EUAF approximation in d-dimensions)

Arbitrarily small error with a fixed number of neurons for $C([0,1]^d)$.

- *For any* $\epsilon > 0$, *there exists* ϕ *of width* $36d(2d+1)$ *and depth* 11 *s.t.*

$$\|f(x) - \phi(x)\|_{L^\infty([0,1]^d)} \leq \epsilon$$

- *Shen, Y., and Zhang (arXiv:2107.02397)*

DNNs with advanced activation function

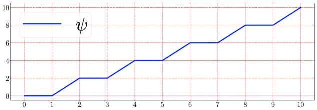
Theorem (EUAF representation in d-dimensions)

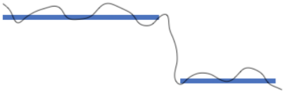
Exact representation with a fixed number of neurons for classification functions.

- *For any classification function* $f(x)$ *with* K *classes, there exists* ϕ *of width* $36d(2d+1)$ *and depth* 12 *s.t.*

$$f(x) = \phi(x)$$

  on the supports of each class.
- *Shen, Y., and Zhang (arXiv:2107.02397)*





DNNs with advanced activation function

Two main ideas

- Theorem (Kolmogorov-Arnold Superposition Theorem)
  $\forall f(\mathbf{x}) \in C([0,1]^d)$, there exist $\psi_p(x)$ and $\phi(x)$ in $C(\mathbb{R})$ and $b_{pq} \in \mathbb{R}$ s.t.
  $$f(\mathbf{x}) = \sum_{q=1}^{2d+1} a_q \phi(\sum_{p=1}^{d} b_{pq}\psi_p(x_p)).$$

- Lemma (EUAF approximation in 1D (Shen, Y., and Zhang (arXiv:2107.02397))
  NNs with width 36 and depth 5 constructed with EUAF is dense in $C([0,1])$.

Other EUAF

- C^s EUAF
- Sigmod EUAF

Summary

- Deep Neural Networks are powerful
- Quantitative approximation results are available
- How to quantify deep learning optimization and generalization errors?

Optimization and Generalization of Deep Learning

In the setting of supervised learning:

Mean-field analysis

- Chizat and Bach 2018; Mei et al. 2018; Mei et al. 2019, Lu et al. 2020, etc.
- 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.

In the setting of solving PDEs: vastly open

Optimization and Generalization of Deep Learning

In the setting of supervised learning:

Neural tangent kernel/Lazy training

- Idea: in the limit of infinite width, deep learning becomes kernel methods
- Global optimization convergence:
  - Jacot et al. 2018 (two layers);
  - Du et al. 2019 (L layers, DNN);
  - Z Allen-Zhu, Y Li, Z Song 2018 (L layers, DNN, RNN);
  - D Zou*, Y Cao*, D. Zhou, and Q Gu 2018 (L layers, DNN, milder conditions)
  - Chizat et al. 2018
- Generalization theory
  - Y Cao and Q Gu, 2019a (GD)
  - Y Cao and Q Gu, 2019b (SGD)
- Consistent optimization and generalization for classification
  - Z Ji and M Telgarsky 2020
  - Z Chen*, Y Cao*, D Zou, and Q Gu 2020 (SOTA)

In the setting of solving PDEs: vastly open

Neural Tangent Kernel of Deep Learning Optimization

- **Optimization objective function**:

$$R_S(\boldsymbol{\theta}) := \frac{1}{N}\sum_{i=1}^{N}(h(\boldsymbol{x}_i;\boldsymbol{\theta}) - f(\boldsymbol{x}_i))^2$$

- Introduce $\mathcal{X} := [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N]^T \in \mathbb{R}^{N\times d}$, then
  - $h(\mathcal{X};\boldsymbol{\theta}(t)) := [h(\boldsymbol{x}_i;\boldsymbol{\theta}(t))] \in \mathbb{R}^N$
  - $\nabla_{\boldsymbol{\theta}} h(\mathcal{X};\boldsymbol{\theta}(t)) := [\nabla_{\boldsymbol{\theta}_j} h(\boldsymbol{x}_i;\boldsymbol{\theta}(t))] \in \mathbb{R}^{N\times W}$
  - $\nabla_{h(\mathcal{X};\boldsymbol{\theta}(t))} R_S := \frac{2}{N}(h(\mathcal{X};\boldsymbol{\theta}(t)) - f(\mathcal{X})) := [\frac{2}{N}(h(\boldsymbol{x}_i;\boldsymbol{\theta}(t)) - f(\boldsymbol{x}_i))] \in \mathbb{R}^N$
- **Gradient descent**

$$\begin{aligned}\boldsymbol{\theta}(t+1) &= \boldsymbol{\theta}(t) - \tau\frac{2}{N}\sum_{i=1}^{N}(h(\boldsymbol{x}_i;\boldsymbol{\theta}(t)) - f(\boldsymbol{x}_i))\nabla_{\boldsymbol{\theta}(t)} h(\boldsymbol{x}_i;\boldsymbol{\theta}) \\ &= \boldsymbol{\theta}(t) - \tau\nabla_{\boldsymbol{\theta}} h(\mathcal{X};\boldsymbol{\theta}(t))^T \nabla_{h(\mathcal{X};\boldsymbol{\theta}(t))} R_S,\end{aligned}$$

- **Gradient flow**

$$\partial_t \boldsymbol{\theta}(t) = -\nabla_{\boldsymbol{\theta}} h(\mathcal{X};\boldsymbol{\theta}(t))^T \nabla_{h(\mathcal{X};\boldsymbol{\theta}(t))} R_S,$$

Neural Tangent Kernel of Deep Learning Optimization

- **Gradient flow**

$$\partial_t \boldsymbol{\theta}(t) = -\nabla_{\boldsymbol{\theta}} h(\mathcal{X}; \boldsymbol{\theta}(t))^T \nabla_{h(\mathcal{X};\boldsymbol{\theta}(t))} R_S,$$

- **DNN evolution**

$$\partial_t h(\mathcal{X}; \boldsymbol{\theta}(t)) = \nabla_{\boldsymbol{\theta}} h(\mathcal{X}; \boldsymbol{\theta}(t)) \partial_t \boldsymbol{\theta}(t) = -\hat{\Theta}_t(\mathcal{X}, \mathcal{X}) \nabla_{h(\mathcal{X};\boldsymbol{\theta}(t))} R_S$$

  with the neural tangent kernel (NTK)

$$\hat{\Theta}_t = \nabla_{\boldsymbol{\theta}} h(\mathcal{X}; \boldsymbol{\theta}(t)) \nabla_{\boldsymbol{\theta}} h(\mathcal{X}; \boldsymbol{\theta}(t))^T.$$

- Nonlinear ODEs and challenging to analyze

- **Linearization**

  $h^{\text{lin}}(\boldsymbol{x};\theta(t)) := h(\boldsymbol{x};\theta(0)) + \nabla_{\theta} h(\boldsymbol{x};\theta(0))(\theta(t)-\theta(0)) \approx h(\boldsymbol{x};\theta(t)),$

- **Approximate DNN evolution**

$$\begin{aligned}\partial_t h^{\text{lin}}(\boldsymbol{x};\theta(t)) &= -\hat{\Theta}_0(\boldsymbol{x},\mathcal{X})\nabla_{h^{\text{lin}}(\boldsymbol{x};\theta(t))} R_S \\ &= -\hat{\Theta}_0(\boldsymbol{x},\mathcal{X})\frac{2}{N}(h^{\text{lin}}(\boldsymbol{x};\theta(t)) - f(\mathcal{X}))\end{aligned}$$

- **Linear ODE with a solution**

  $h^{\text{lin}}(\boldsymbol{x};\theta(t)) = h(\boldsymbol{x};\theta(0)) - \hat{\Theta}_0(\boldsymbol{x},\mathcal{X})\hat{\Theta}_0^{-1}\left(I - e^{-\hat{\Theta}_0 t}\right)(h(\mathcal{X};\theta(0)) - \mathcal{Y})$

  and

$$h^{\text{lin}}(\mathcal{X};\theta(t)) = \left(I - e^{-\hat{\Theta}_0 t}\right)\mathcal{Y} + e^{-\hat{\Theta}_0 t} h(\mathcal{X};\theta(0)).$$

  with $\mathcal{Y} := [y_1,\ldots,y_N]^T \in \mathbb{R}^N$.

Approximate DNN evolution

$$h^{\text{lin}}(\boldsymbol{x};\boldsymbol{\theta}(t)) = h(\boldsymbol{x};\boldsymbol{\theta}(0)) - \hat{\Theta}_0(\boldsymbol{x},\mathcal{X})\hat{\Theta}_0^{-1}\left(I - e^{-\hat{\Theta}_0 t}\right)(h(\mathcal{X};\boldsymbol{\theta}(0)) - \mathcal{Y})$$

and

$$h^{\text{lin}}(\mathcal{X};\boldsymbol{\theta}(t)) = \left(I - e^{-\hat{\Theta}_0 t}\right)\mathcal{Y} + e^{-\hat{\Theta}_0 t} h(\mathcal{X};\boldsymbol{\theta}(0))$$

Insight for numerical performance

- Spectral bias of deep learning (Rahaman et al, 2018; Xu et al, 2018, Cao et al, 2019)
- sin activation to lessen spectral bias (Tancik et al, 2020; Sitzmann et al, 2020)
- Wendland activation for non-singular NTK (Benson, Damle, and Townsend, 2020)
- Reproducing activation function to reduce the condition number of NTK (Liang, Lyu, Wang, **Y.**, 2021)

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: $\phi(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{k=1}^{N} a_k \sigma(\boldsymbol{w}_k^T \boldsymbol{x})$ on $[0,1]^d$.
- A second order differential equation: $\mathcal{L}u = f$ with

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

- $\mathcal{L}$ satisfies the condition: there exists $M \geq 1$ such that for all $\boldsymbol{x} \in \Omega = [0,1]^d$, $\alpha, \beta \in [d]$, we have $A_{\alpha\beta} = A_{\beta\alpha}$

$$|A_{\alpha\beta}(\boldsymbol{x})| \leq M, \quad |b_\alpha(\boldsymbol{x})| \leq M, \quad \text{and} \quad |c(\boldsymbol{x})| \leq M.$$

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

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

and population loss

$$R_{\mathcal{D}}(\boldsymbol{\theta}) = \frac{1}{2} \mathbb{E}_{\boldsymbol{x}\sim\mathcal{D}} \left[|\mathcal{L}\phi(\boldsymbol{x}_i;\boldsymbol{\theta}) - f(\boldsymbol{x}_i)|^2 \right]$$

with ϕ satisfying boundary conditions.

Luo and Y., preprint, 2020

Theorem (Linear convergence rate)

Let $\boldsymbol{\theta}^0 := \mathrm{vec}\{a_k^0, \boldsymbol{w}_k^0\}_{k=1}^N$ be the GD initialization, where $a_k^0 \sim \mathcal{N}(0, \gamma^2)$ and $\boldsymbol{w}_k^0 \sim \mathcal{N}(\mathbf{0}, \mathbb{I}_d)$ with any $\gamma \in (0, 1)$. Let $C_d := \mathbb{E}\|\boldsymbol{w}\|_1^{12} < +\infty$ with $\boldsymbol{w} \sim \mathcal{N}(\mathbf{0}, \mathbb{I}_d)$ and λ_S be a positive constant. For any $\delta \in (0, 1)$, if width

$$N \geq \max\left\{\frac{512 n^4 M^4 C_d}{\lambda_S^2 \delta}, \frac{200\sqrt{2} M d^3 n \log(4N(d+1)/\delta)\sqrt{R_S(\boldsymbol{\theta}^0)}}{\lambda_S}, \frac{2^{23} M^3 d^9 n^2 (\log(4N(d+1)/\delta))^4 \sqrt{R_S(\boldsymbol{\theta}^0)}}{\lambda_S^2}\right\},$$

then with probability at least $1 - \delta$ over the random initialization $\boldsymbol{\theta}^0$, we have, for all $t \geq 0$,

$$R_S(\boldsymbol{\theta}(t)) \leq \exp\left(-\frac{N \lambda_S t}{n}\right) R_S(\boldsymbol{\theta}^0).$$

Luo and Y., preprint, 2020

Theorem (A posteriori generalization bound)

For any $\delta \in (0,1)$, with probability at least $1-\delta$ over the choice of random sample locations $S := \{\boldsymbol{x}_i\}_{i=1}^n$, for any two-layer neural network $\phi(\boldsymbol{x};\boldsymbol{\theta})$, we have

$$|R_{\mathcal{D}}(\boldsymbol{\theta}) - R_S(\boldsymbol{\theta})| \le \frac{(\|\boldsymbol{\theta}\|_{\mathcal{P}}+1)^2}{\sqrt{n}} 2M^2 \Big(14d^2\sqrt{2\log(2d)} + \log[\pi(\|\boldsymbol{\theta}\|_{\mathcal{P}}+1)] + \sqrt{2\log(1/3\delta)}\Big)$$

Proof: $|R_{\mathcal{D}}(\boldsymbol{\theta}) - R_S(\boldsymbol{\theta})| \le$ Rademacher complexity + Stat error
$\le O\left(\frac{\|\boldsymbol{\theta}\|_{\mathcal{P}}}{\sqrt{n}}\right) + O\left(\frac{1}{\sqrt{n}}\right)$

Generalization of PDE solvers

Regression: E, Ma, and Wu, CMS, 2019
PDE solvers: Luo and Y., preprint, 2020

Theorem (A priori generalization bound)

Suppose that $f(\boldsymbol{x})$ is in the Barron-type space $\mathcal{B}([0,1]^d)$ and $\lambda \geq 4M^2[2 + 14d^2\sqrt{2\log(2d)} + \sqrt{2\log(2/3\delta)}]$. Let

$$\boldsymbol{\theta}_{S,\lambda} = \arg\min_{\boldsymbol{\theta}} J_{S,\lambda}(\boldsymbol{\theta}) := R_S(\boldsymbol{\theta}) + \frac{\lambda}{\sqrt{n}}\|\boldsymbol{\theta}\|_{\mathcal{P}}^2 \log[\pi(\|\boldsymbol{\theta}\|_{\mathcal{P}} + 1)].$$

Then for any $\delta \in (0,1)$, with probability at least $1-\delta$ over the choice of random samples $S := \{\boldsymbol{x}_i\}_{i=1}^n$, we have

$$\begin{aligned} R_{\mathcal{D}}(\boldsymbol{\theta}_{S,\lambda}) &:= \mathbb{E}_{\boldsymbol{x}\sim\mathcal{D}}\frac{1}{2}(\mathcal{L}\phi(\boldsymbol{x};\boldsymbol{\theta}_{S,\lambda}) - f(\boldsymbol{x}))^2 \\ &\leq \frac{6M^2\|f\|_{\mathcal{B}}^2}{N} + \frac{\|f\|_{\mathcal{B}}^2 + 1}{\sqrt{n}}(4\lambda + 16M^2)\left\{\log[\pi(2\|f\|_{\mathcal{B}} + 1)] \right. \\ &\left. + 14d^2\sqrt{\log(2d)} + \sqrt{\log(2/3\delta)}\right\}. \end{aligned}$$

Proof: $R_{\mathcal{D}}(\boldsymbol{\theta}_{S,\lambda}) \leq$ Approximation error + Rademacher complexity + Stat error $\leq O\left(\frac{\|f\|_{\mathcal{B}}^2}{N}\right) + O\left(\frac{\|\boldsymbol{\theta}\|_{\mathcal{P}}}{\sqrt{n}}\right) + O\left(\frac{1}{\sqrt{n}}\right) \leq O\left(\frac{\|f\|_{\mathcal{B}}^2}{N}\right) + O\left(\frac{\|f\|_{\mathcal{B}}^2}{\sqrt{n}}\right)$

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Collaborators

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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: $f(\boldsymbol{x}) \approx f_p(\boldsymbol{x}) \approx \phi_3 \circ \phi_2 \circ \phi_1(\boldsymbol{x})$
- 2^N pieces per dim and 2^{Nd} pieces with accuracy 2^{-N}
- Floor NN $\phi_1(\boldsymbol{x})$ s.t. $\phi_1(\boldsymbol{x}) = \boldsymbol{\beta}$ for $\boldsymbol{x} \in Q_{\boldsymbol{\beta}}$ and $\boldsymbol{\beta} \in \mathbb{Z}^d$.
- Linear NN ϕ_2 mapping $\boldsymbol{\beta}$ to an integer $k_{\boldsymbol{\beta}} \in \{1, \ldots, 2^{Nd}\}$
- Key difficulty: NN ϕ_3 of width $O(N)$ and depth $O(1)$ fitting 2^{Nd} samples in 1D with accuracy $O(2^{-N})$
- ReLU NN fails

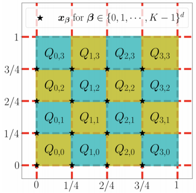

Figure: Uniform domain partitioning.

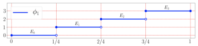

Figure: Floor function.

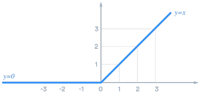

Figure: ReLU function.

Key ideas of our approximation

Binary representation and approximation

$\theta = \sum_{\ell=1}^{\infty} \theta_\ell 2^{-\ell}$ with $\theta_\ell \in \{0, 1\}$ is approximated by $\sum_{\ell=1}^{N} \theta_\ell 2^{-\ell}$ with an error 2^{-N}.

Bit extraction via a floor NN of width 2 and depth 1

$$\phi_k(\theta) := \lfloor 2^k \theta \rfloor - 2\lfloor 2^{k-1}\theta \rfloor = \theta_k$$

Bit extraction via a floor NN of width 2N and depth 1

Given $\theta = \sum_{\ell=1}^{\infty} \theta_\ell 2^{-\ell}$

$$\phi(\theta) := \begin{pmatrix} \phi_1(\theta) \\ \vdots \\ \phi_N(\theta) \end{pmatrix} = \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_N \end{pmatrix} \in \mathbb{Z}^N$$

Key ideas of our approximation

Encoding K numbers to one number

- Extract bits $\{\theta_1^{(k)}, \ldots, \theta_N^{(k)}\}$ from $\theta^{(k)} = \sum_{\ell=1}^{\infty} \theta_\ell^{(k)} 2^{-\ell}$ for $k = 1, \ldots, K$
- sum up to get $a = \sum_{\ell=1}^{N} \theta_\ell^{(1)} 2^{-\ell} + \sum_{\ell=N+1}^{2N} \theta_\ell^{(2)} 2^{-\ell} + \cdots + \sum_{\ell=(K-1)N+1}^{KN} \theta_\ell^{(K)} 2^{-\ell}$

Decoding one number to get the k-th numbers

- Extract bits $\{\theta_1^{(k)}, \ldots, \theta_N^{(k)}\}$ from a via

$$\psi(k) := \phi(2^{(k-1)N} a - \lfloor 2^{(k-1)N} a \rfloor)$$

  of width $O(N)$ and depth $O(1)$.
- sum up to get $\theta^{(k)} \approx \sum_{\ell=1}^{N} \theta_\ell^{(k)} 2^{-\ell} = [2^{-1}, \ldots, 2^{-N}]\psi(k) := \gamma(k)$,
- $\gamma(k)$ is an NN of width $O(N)$ and depth $O(1)$.

Key Lemma

There exists an NN γ of width $O(N)$ and depth $O(1)$ that can memorize arbitrary samples $\{(k, \theta^{(k)}\}_{k=1}^{K}$ with a precision 2^{-N}.

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: $f(\boldsymbol{x}) \approx f_p(\boldsymbol{x}) \approx \phi_3 \circ \phi_2 \circ \phi_1(\boldsymbol{x})$
- 2^N pieces per dim and 2^{Nd} pieces with accuracy 2^{-N}
- Floor NN $\phi_1(\boldsymbol{x})$ s.t. $\phi_1(\boldsymbol{x}) = \boldsymbol{\beta}$ for $\boldsymbol{x} \in Q_{\boldsymbol{\beta}}$ and $\boldsymbol{\beta} \in \mathbb{Z}^d$.
- Linear NN ϕ_2 mapping $\boldsymbol{\beta}$ to an integer $k_{\boldsymbol{\beta}} \in \{1, \ldots, 2^{Nd}\}$
- Key difficulty: NN ϕ_3 of width $O(N)$ and depth $O(1)$ fitting 2^{Nd} samples in 1D with accuracy $O(2^{-N})$
- Key Lemma: There exists an NN γ of width $O(N)$ and depth $O(1)$ that can memorize arbitrary samples $\{(k, \theta^{(k)})\}_{k=1}^{K}$ with a precision 2^{-N}.

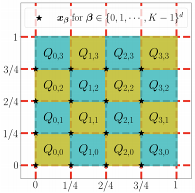

Figure: Uniform domain partitioning.

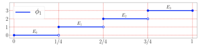

Figure: Floor function.

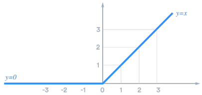

Figure: ReLU function.

DNNs with advanced activation function

EUAF is more powerful than bit extraction.

Lemma (Curve filling in K-dimensions (Shen, Y., and Zhang (arXiv:2107.02397))

For any $K \in \mathbb{N}^+$, the following point set

$$\left\{ \left[\sigma_1\left(\tfrac{w}{\pi+1}\right),\ \sigma_1\left(\tfrac{w}{\pi+2}\right),\ \cdots,\ \sigma_1\left(\tfrac{w}{\pi+K}\right)\right]^T : w \in \mathbb{R} \right\} \subseteq [0,1]^K$$

is dense in $[0,1]^K$, where π is the ratio of the circumference of a circle to its diameter.

Proof.

Ideas:

- Transcendental number $+$ distinct rational numbers $\rightarrow$ rationally independent numbers
- Rationally independent numbers $+$ periodic functions $\rightarrow$ dense set in $[0,1]^K$

□

For arbitrary K, NN with width 1 and depth 2 constructed with EAUF can fit K points up to arbitrary accuracy.