A Few Thoughts on Deep Learning-Based Scientific Computing

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Deep Learning for Scientific Computing?

Some pieces of error analysis but 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

Supervised machine learning

- Given data pairs $\{(x_i, y_i = f(x_i))\}$ from an unknown map f;
- Construct a finite family of maps $\{h(x;\theta)\}_\theta$;
- Create an empirical loss to quantify how good $h(x;\theta) \approx f(x)$ is:

$$R_S(\theta) := \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(h(x_i;\theta), y_i) \overset{\text{e.g.}}{=} \frac{1}{N}\sum_{i=1}^{N}(h(x_i;\theta) - y_i)^2;$$

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

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

- Numerical optimization to obtain a numerical solution $h(x;\theta_N)$.

Supervised machine learning

- Data $\{x_i\}_{i=1}^{n}$ are sampled randomly from an unknown distribution $U(x)$;
- Population loss as the ideal averaged prediction error:
$$R_D(\theta) := \mathrm{E}_{x \sim U(\Omega)} \left[\mathcal{L}(h(x;\theta), f(x)) \right],$$
and the ideal prediction $h(x;\theta_D)$ with
$$\theta_D := \mathrm{argmin}\, R_D(\theta).$$
- In practice, $\theta_N \neq \theta_S \neq \theta_D$.
- How good does the actually learned function $h(x;\theta_N)$ predict $f(x)$ when x is unseen?
- $R_D(\theta_N)$ as the expected prediction error over all possible data samples.

Supervised learning

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

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

Supervised learning

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

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

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

Supervised learning

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

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

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

Supervised learning

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

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

- $R_D(\theta_D) = \int_\Omega (h(x;\theta_D) - f(x))^2 d\mu(x) \leq= \int_\Omega (h(x;\tilde{\theta}) - f(x))^2 d\mu(x)$ 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

This talk discusses the case when $h(x;\theta)$ is a deep neural network.

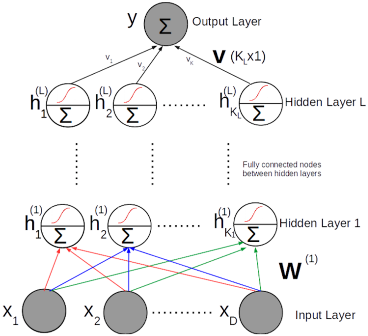
Deep Neural Network

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

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



Deep Learning for Solving PDEs

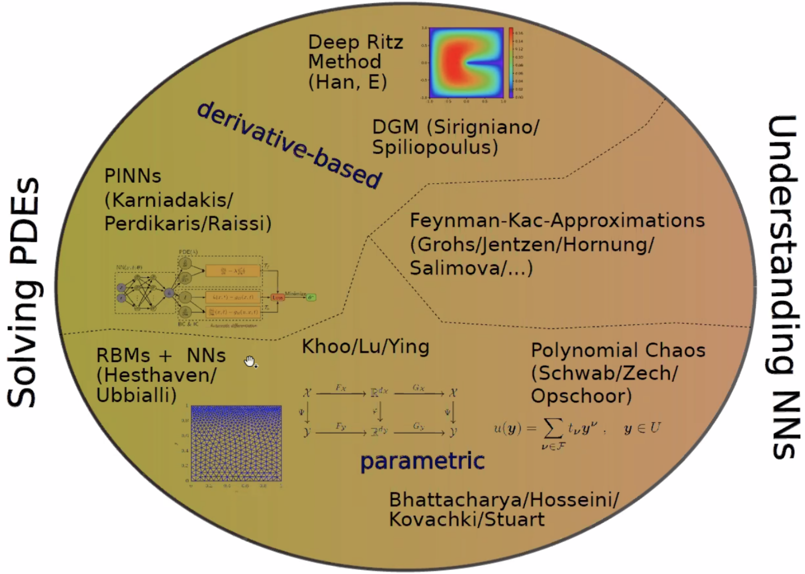


Figure: Figure by Phillip Peterson.

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

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

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

Literature Review

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

Analysis tools

- Polynomial approximations
- The law of large number
- Kolmogorov-Arnold representation theory
- Bit extraction technology (Bartlett et al., 1998; Harvey et al., 2017)

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

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

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

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 (Preprint, 2021)

Curse of dimensionality exists!

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

Does smoothness help?

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

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

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 (preprint, 2020)

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
- 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

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 (preprint, 2020)

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 (preprint, 2020)

Further interpretation of our result

Does the domain $[0, 1]^d$ matter? No

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

- Error rate $3\lambda(3R\sqrt{d})^\alpha 2^{-\alpha N}$ in the L^∞-norm and $E = [-R, R]^d$.

Further interpretation of our result

Does ω_f matter? Yes

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

- $\omega_f(r) = \frac{1}{\ln(1/r)}$

$$3(N\ln 2 - \tfrac{1}{2}\ln d - \ln 2)^{-1}$$

- $\omega_f(r) = \frac{1}{\ln^{1/d}(1/r)}$

$$3(N\ln 2 - \tfrac{1}{2}\ln d - \ln 2)^{-1/d}$$

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

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

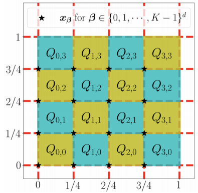


Figure: Uniform domain partitioning.

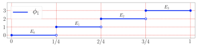


Figure: Floor function.

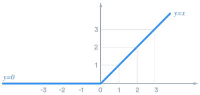


Figure: ReLU function.

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 $\boldsymbol{\beta} \in \mathbb{Z}^d$.
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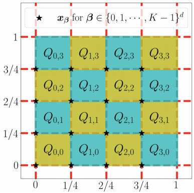
- Key difficulty: NN ϕ_3 of width $O(N)$ and depth $O(1)$ fitting 2^{Nd} samples in 1D with accuracy $O(2^{-N})$
- Key Lemma: There exists an NN γ of width $O(N)$ and depth $O(1)$ that can memorize arbitrary samples $\{(k, \theta^{(k)})\}_{k=1}^{K}$ with a precision 2^{-N}.



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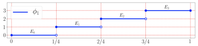

Figure: Floor function.

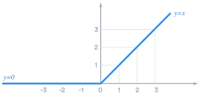

Figure: ReLU function.

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:

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, 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

Key Analysis of Neural Tangent Kernel

Simplifying the residual dynamic via approximation:

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

- Training samples $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]^T$;
- Learning rate η;
- Width N;
- Gram matrix $\boldsymbol{H}_t := (\frac{1}{N}\langle \nabla\phi(\boldsymbol{x}_i;\boldsymbol{\theta}_t), \nabla\phi(\boldsymbol{x}_j;\boldsymbol{\theta}_t)\rangle)_{n\times n}$;
- NTK $\boldsymbol{H} = \lim_{N\to\infty} \boldsymbol{H}_0$;
- $\approx$ valid when $\boldsymbol{\theta}_{t+1} \approx \boldsymbol{\theta}_t \leftarrow \eta \approx 0$;
- $\approx$ valid when $\boldsymbol{\theta}_t \approx \boldsymbol{\theta}_0 \leftarrow \eta \approx 0$ and $N \to \infty$;
- $\approx$ valid when $N \to \infty$ 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: $\phi(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{k=1}^{N} a_k \sigma(\boldsymbol{w}_k^T \boldsymbol{x})$ 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 $t \geq 0$,

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

Generalization of PDE solvers

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

$$
\begin{aligned}
|R_{\mathcal{D}}(\boldsymbol{\theta}) - R_S(\boldsymbol{\theta})| \quad \leq \quad & \frac{(\|\boldsymbol{\theta}\|_{\mathcal{P}}+1)^2}{\sqrt{n}} 2M^2 \left(14d^2\sqrt{2\log(2d)}\right. \\
& \left. + \log[\pi(\|\boldsymbol{\theta}\|_{\mathcal{P}}+1)] + \sqrt{2\log(1/3\delta)}\right)
\end{aligned}
$$

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

Generalization of PDE solvers

Regression: E, Ma, and Wu, 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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