Deep Learning and Numerical PDEs

Finite Neuron Method

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A Model PDE

Given $\Omega \subset \mathbb{R}^d$, consider a $2m$-th order elliptic problems

$$\sum_{|\alpha|=m} (-1)^m \partial^\alpha (a_\alpha(x)\, \partial^\alpha u) + u = f \quad \text{in } \Omega. \tag{1}$$

Special cases:

$$-\Delta u = f \quad (m=1), \quad \Delta^2 u = f \quad (m=2).$$

The Dirichlet boundary condition for the $2m$-th order elliptic problems are

$$B_D^k(u) = 0 \text{ on } \partial\Omega, \quad (0 \le k \le m-1),$$

where B_D^k are given by the following Dirichlet type trace operators

$$B_D^k(u) := \left.\frac{\partial^k u}{\partial \nu^k}\right|_{\partial\Omega} \quad (0 \le k \le m-1). \tag{2}$$

Dirichlet vs Neumann boundary condition

Lemma

For each $k = 0, 1, \ldots, m-1$, there exists a bounded linear differential operator of order $2m-k-1$:

$$B_N^k : H^{2m}(\Omega) \mapsto L^2(\partial\Omega) \tag{3}$$

such that the following identity holds

$$\sum_{|\alpha|=m} (-1)^m \left(\partial^\alpha (a_\alpha\, \partial^\alpha\, u),\, v\right)_{0,\Omega} = \sum_{|\alpha|=m} (a_\alpha \partial^\alpha\, u, \partial^\alpha v)_{0,\Omega} - \sum_{k=0}^{m-1} \langle B_N^k(u), B_D^k(v)\rangle_{0,\partial\Omega} \tag{4}$$

for all $u \in H^{2m}(\Omega), v \in H^m(\Omega)$. Furthermore,

$$\sum_{k=0}^{m-1} \|B_D^k(u)\|_{L^2(\partial\Omega)} + \sum_{k=0}^{m-1} \|B_N^k(u)\|_{L^2(\partial\Omega)} \lesssim \|u\|_{2m,\Omega}. \tag{5}$$

Neumann problem: Consider

$$\begin{cases} \displaystyle\sum_{|\alpha|=m} (-1)^m \partial^\alpha (a_\alpha(x)\, \partial^\alpha\, u) + u = f & \text{in } \Omega, \\ B_N^k(u) = 0 \quad \text{on } \partial\Omega, & 0 \le k \le m-1. \end{cases} \tag{6}$$

Dirichlet and Neumann problems

- Find $u \in V$ such that

$$J(u) = \min_{v \in V} J(v) \tag{7}$$

where

$$J(v) = \frac{1}{2} \int_\Omega \sum_{|\alpha|=m} a_\alpha |\partial^\alpha v|^2 + v^2 dx - \int_\Omega fv dx. \tag{8}$$

Then

$$V = \begin{cases} H^m(\Omega) & \Longleftrightarrow \text{Neumann problem} \\ H_0^m(\Omega) & \Longleftrightarrow \text{Dirichlet problem} \end{cases}$$

Shallow Neural Networks

- A shallow neural network function: with n neurons

$$f(x) = \sum_{i=1}^{n} a_i \sigma(\omega_i \cdot x + b_i) \tag{9}$$

- Common activation functions:
  - Heaviside $\sigma = \begin{cases} 0 & x \leq 0 \\ 1 & x > 0 \end{cases}$
  - Sigmoidal $\sigma = (1 + e^{-x})^{-1}$
  - Rectified Linear with $\sigma = \max(0, x)$
  - Power of a ReLU $\sigma = [\max(0, x)]^k$
  - Cosine $\sigma = \cos(x)$

Approximation properties

General Shallow neural network

$$\Sigma_n^\sigma = \left\{ \sum_{i=1}^n a_i \sigma(\omega_i \cdot x + b_i) : \omega_i \in \mathbb{R}^d, a_i, b_i \in \mathbb{R} \right\}.$$

Preliminary approximation results

$$\inf_{u_n \in \Sigma_n^\sigma} \|u - u_n\|_{L^2(\Omega)} = \mathcal{O}\left(n^{-\frac{1}{2}}\right)$$

(Jones 1992, Barron 1993, Hornik et al 1994, ...)

ReLU^k (Klusowski & Barron 2016, Xu 2020): For $k > m$

$$\inf_{u_n \in \Sigma_n^k} \|u - u_n\|_{H^m(\Omega)} = \mathcal{O}(n^{-\frac{1}{2} - \frac{1}{d}})$$

General activation (Siegel & Xu 2020):

If $\sigma \in W^{m,\infty}(\mathbb{R})$, $|\sigma^{(k)}(s)| \le C(1 + |s|)^{-p}$, $0 \le k \le m + 1$.

$$\inf_{u_n \in \Sigma_n^\sigma} \|u - u_n\|_{H^m(\Omega)} = \mathcal{O}\left(n^{-\frac{1}{2} - \frac{t}{(2+t)(d+1)}}\right) \quad t = \min(p - 1, \epsilon).$$

Application of ReLU^k-DNN for high order PDE in any dimension

Finite neuron method: We take

$$V_n = \Sigma_n^\sigma \subset H^m(\Omega)$$

Neumann Problem: We define DNN-Galerkin approximation $u_n \in V_n$ as follows:

$$J(u_n) = \min_{v \in V_n} J(v). \quad (10)$$

Theorem (Xu, 2020)

Let $u \in V$ and $u_n \in V_n$ be solutions to (7) with $V = H^m(\Omega)$ and (10) respectively. Then

$$\|u - u_n\|_a = \inf_{v_n \in V_n} \|u - v_n\|_a. \quad (11)$$

Error estimates for NN-PDE

For Neumann boundary condition,

$$\|u - u_n\|_{m,\Omega} \lesssim \inf_{v_n \in V_n} \|u - v_n\|_{m,\Omega} = \mathcal{O}(n^{-\frac{1}{2}-\alpha})$$

For Dirichlet problem, similar but less sharp estimates hold.

Issues:

- Discretization of the integral in $J(v)$, i.e. how do we evaluate

$$\frac{1}{2}\int_\Omega \sum_{|\alpha|=m} a_\alpha |\partial^\alpha v|^2 + v^2 dx - \int_\Omega fv dx? \tag{12}$$

- How to analyze the convergence when numerical quadratures are used?

Convergence analysis when numerical quadratures are used? Existing works:

- M. Hutzenthaler, A. Jentzen, T. Kruse, T. A. Nguyen, and P. Wurstemberger, 2020;
- T. Luo and H. Yang, 2020;
- S. Mishra and T. K. Rusch, 2020; S. Mishra and R. Molinaro, 2020;
- J. Müller and M. Zeinhofer, 2020;
- Y. Shin, Z. Zhang, and G.E. Karniadakis, 2020;
- S. Lanthaler, S. Mishra, G.E. Karniadakis, 2021;
- J. Lu, Y. Lu and M. Wang, 2021;
- H. Son, J. Jang, W. Han, and H. J. Hwang, 2021;

Numerical Quadratures

Given NN:

$$\Sigma_n^k = \left\{ \sum_{i=1}^{n} a_i \sigma_k(\omega_i \cdot x + b_i) : \omega_i \in \mathbb{R}^d, a_i, b_i \in \mathbb{R} \right\}.$$

Numerical Quadrature:

$$\int_\Omega g(x)dx \approx |\Omega| \sum_{i=1}^{N} w_i g(x_i) \tag{13}$$

Consider

$$J(u) = \min J(v), \quad J_N(u_{n,N}) = \min J_N(v_n),$$

where $J_N(v)$ is computed by deterministic numerical quadrature

$$J_N(v) = \sum_{i=1}^{N} w_i \left(\frac{1}{2} \sum_{|\alpha|=m} a_\alpha(x_i)(\partial^\alpha v(x_i))^2 + \frac{1}{2} a_0(x_i)(v(x_i))^2 - f(x_i)v(x_i) \right) \tag{14}$$

or by sampling

$$J_N(v) = \frac{1}{2N} \sum_{i=1}^{N} \sum_{|\alpha|=m} a_\alpha(x_i)(\partial^\alpha v(x_i))^2 + \frac{1}{2N} \sum_{i=1}^{N} a_0(x_i)v(x_i)^2 - \frac{1}{N} \sum_{i=1}^{N} f(x_i)v(x_i). \tag{15}$$

Our objective

Estimate the error $u - u_{n,N}$

Error analysis

Numerical quadrature: for any $g(x)$,

$$\left|\int_\Omega g(x)dx - |\Omega| \sum_{i=1}^{N} w_i g(x_i)\right| \lesssim N^{-\frac{r+1}{d}} \|g\|_{r,1}.$$

Challenges: how to bound

$$\|g\|_{r,1} \leq ?, \quad \text{for} \quad g \in \Sigma_n^\sigma.$$

OK if the following Bernstein or inverse inequality holds for $r > s$

$$\|v_n\|_r \lesssim n^\beta \|v_n\|_s, \quad \forall v_n \in \Sigma_n^k. \tag{16}$$

Bad news: Bernstein inequality does not hold for NN

Given any $\epsilon > 0$, consider an NN function with 3 neurons:

$$u_3(x) = \mathrm{ReLU}(x - \frac{1}{2} + \epsilon) - 2\mathrm{ReLU}(x - \frac{1}{2}) + \mathrm{ReLU}(x - \frac{1}{2} - \epsilon), \quad \forall x \in (0, 1).$$

A direct calculation shows that

$$\int_0^1 |u_3'(x)|^2 dx = 2\epsilon \quad \text{and} \quad \int_0^1 |u_3(x)|^2 dx = \epsilon^2.$$

Therefore

$$|u_3|_{H^1} = \sqrt{\frac{2}{\epsilon}}\|u_3\|_{L^2}, \quad \forall \epsilon > 0$$

As a result, the following Bernstein inequality can not hold for any constant $C(n)$

$$|v_n|_{H^1} \leq C(n)\|v_n\|_{L^2}, \quad \forall v_n \in \Sigma_n^\sigma$$

Our approach: Stable Neural Network

- Consider approximation from the class

$$\Sigma^{\sigma}_{n,M} := \left\{ \sum_{i=1}^{n} a_i \sigma(\omega_i \cdot x + b_i),\ \omega_i \in \mathbb{S}^{d-1},\ |b_i| \le B, \sum_{i=1}^{n} |a_i| \le M \right\} \tag{17}$$

  of neural networks with ℓ^1-bounded outer coefficients.
- More generally for a dictionary $\mathbb{D} \subset H = L^2(\Omega)$, consider

$$\Sigma_{n,M}(\mathbb{D}) = \left\{ \sum_{i=1}^{n} a_i h_i,\ h_i \in \mathbb{D},\ \sum_{i=1}^{n} |a_i| \le M \right\} \tag{18}$$

- Question: What is the "largest" functional class that $\Sigma_{n,M}(\mathbb{D})$ can approximate?

Stable Dictionary Approximation Space

- Define a closed convex hull of $\pm\mathbb{D}$:

$$B_1(\mathbb{D}) = \overline{\left\{ \sum_{j=1}^{n} a_j h_j : \ n \in \mathbb{N}, \ h_j \in \mathbb{D}, \ \sum_{i=1}^{n} |a_i| \le 1 \right\}}, \tag{19}$$

- Define a norm

$$\|f\|_{\mathcal{K}_1(\mathbb{D})} = \inf\{r > 0 : f \in rB_1(\mathbb{D})\}, \tag{20}$$

as the guage of the set $B_1(\mathbb{D})$.

- The unit ball is

$$\{f \in H : \|f\|_{\mathcal{K}_1(\mathbb{D})} \le 1\} = B_1(\mathbb{D}). \tag{21}$$

- We have

$$\{f \in H : \|f\|_{\mathcal{K}_1(\mathbb{D})} < \infty\} \tag{22}$$

is a Banach space.

Ref: Siegel, Jonathan W., and Jinchao Xu. "Optimal Approximation Rates and Metric Entropy of ReLU ^{k} and Cosine Networks." arXiv preprint arXiv:2101.12365 (2021).

Stable Dictionary Approximation Space

Theorem (Siegel & Xu 2021)

A function $f \in H = L^2(\Omega)$ can be approximated at all, i.e.

$$\lim_{n\to\infty} \inf_{f_n \in \Sigma^k_{n,M}(\mathbb{D})} \|f - f_n\|_H = 0, \tag{23}$$

for a fixed $M < \infty$ if and only if

$$f \in \mathcal{K}_1(\mathbb{D}) \text{ with } \|f\|_{\mathcal{K}_1(\mathbb{D})} \le M.$$

Furthermore, if

$$\|\mathbb{D}\| \equiv \sup_{h\in\mathbb{D}} \|h\|_H < \infty$$

we have

$$\inf_{f_n \in \Sigma^k_{n,M}(\mathbb{D})} \|f - f_n\|_H \le n^{-\frac{1}{2} - \frac{2(k-m)+1}{2d}} \|\mathbb{D}\| \|f\|_{\mathcal{K}_1(\mathbb{D})}. \tag{24}$$

Error estimates for deterministic numerical quadrature

Consider

$$\Sigma_{n,M}^k = \{\sum_{i=1}^n a_i\sigma_k(\omega_i \cdot x + b_i) : \omega_i \in \mathbb{S}^{d-1}, |b_i| \le B, \sum_{i=1}^n |a_i| \le M\} \subset W^{k,\infty}(\Omega)$$

with

$$M \ge \|u\|_{\mathcal{K}_1(\mathbb{P}_k^d)}.$$

Theorem (Hong, Siegel & Xu 2021)

Let N be the number of quadrature points and

$$J_N(u_{n,N}) = \min_{v \in \Sigma_{n,M}^k} J_N(v). \tag{25}$$

If $N = \mathcal{O}(n^{\frac{d+1+2(k-m)}{k-1}})$*, it holds that*

$$\|u_{n,N} - u\|_a \lesssim n^{-\frac{1}{2}-\frac{2(k-m)+1}{2d}} \|u\|_{\mathcal{K}_1(\mathbb{P}_k^d)}.$$

Sketch of proof

1. For any conforming v,

$$|J_N(v) - J(v)| \le N^{-\frac{k-1}{d}} \|v\|_{k,\infty}. \tag{26}$$

2. Since Ω is bounded, $\omega_i \in \mathbb{S}^{d-1}$, $|b_i| \le B$, $\sum_{i=1}^{n} |a_i| \le M$,

$$\|u_{n,N}\|_{k,\infty} \lesssim M.$$

3. For any n, there exists $v_n \in \Sigma^k_{n,M}$

$$\|u - v_n\|_a \lesssim n^{-\frac{1}{2}-\frac{2(k-m)+1}{2d}} \|u\|_{\mathcal{K}_1(\mathbb{P}^d_k)}. \tag{27}$$

4. Since $J_N(u_{n,N}) \le J_N(v_n)$,

$$\begin{aligned}\frac{1}{2}\|u_{n,N} - u\|_a^2 =& J(u_{n,N}) - J(u) \le J(u_{n,N}) - J_N(u_{n,N}) + J_N(u_{n,N}) - J(v_n) + J(v_n) - J(u)\\ \lesssim& N^{-\frac{k-1}{d}} + \|v_n - u\|_a^2 \lesssim N^{-\frac{k-1}{d}} + n^{-1-\frac{2(k-m)+1}{d}}.\end{aligned}$$

5. Choose $N = \mathcal{O}(n^{\frac{d+1+2(k-m)}{k-1}})$, then

$$\|u_{n,N} - u\|_a \lesssim n^{-\frac{1}{2}-\frac{2(k-m)+1}{2d}}.$$

Error estimate for numerical quadrature by sampling

Quadrature by sampling: Consider

$$J_N(u_{n,N}) = \min_{v \in \Sigma_{n,M}^k} J_N(v),$$

with sampling

$$J_N(v) = \frac{1}{2N} \sum_{i=1}^{N} \sum_{|\alpha|=m} a_\alpha(x_i)(\partial^\alpha v(x_i))^2 + \frac{1}{2N} \sum_{i=1}^{N} a_0(x_i) v(x_i)^2 - \frac{1}{N} \sum_{i=1}^{N} f(x_i) v(x_i). \tag{28}$$

Rademacher complexity: The Rademacher complexity of function class $\mathcal{F}$ on Ω is given by

$$R_N(\mathcal{F}) = \mathbb{E}_{x_1,\ldots,x_N} \mathbb{E}_{\xi_1,\ldots,\xi_N} \left(\sup_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \xi_i f(x_i) \right), \tag{29}$$

where x_i are drawn uniformly at random from Ω and ξ_i are uniformly random signs.

Properties of Rademacher complexity

Lemma

Let $\mathcal{F}, \mathcal{S}$ be classes of functions on Ω. Then the following bounds hold.

- $R_N(conv(\mathcal{F})) = R_N(\mathcal{F})$.
- *Define the set* $\mathcal{F} + \mathcal{S} = \{h(x) + g(x) : \ h \in \mathcal{F}, \ g \in \mathcal{S}\}$. *We have*

$$R_N(\mathcal{F} + \mathcal{S}) = R_N(\mathcal{F}) + R_N(\mathcal{S}). \tag{30}$$

- *Suppose that* $\phi : \mathbb{R} \to \mathbb{R}$ *is L-Lipschitz. Let* $\phi \circ \mathcal{F} = \{\phi(h(x)) : \ h \in \mathcal{F}\}$. *Then*

$$R_N(\phi \circ \mathcal{F}) \leq L R_N(\mathcal{F}). \tag{31}$$

- *Suppose that* $f : \Omega \to \mathbb{R}$ *is a fixed function. Let* $f \cdot \mathcal{F} = \{f(x)h(x) : \ h \in \mathcal{F}\}$. *Then*

$$R_N(f \cdot \mathcal{F}) \leq \|f(x)\|_{L^\infty(\Omega)} R_N(\mathcal{F}). \tag{32}$$

Bound by Rademacher complexity

Theorem (Bartlett, 2002)

Let $\mathcal{F}$ be a set of functions. Then

$$\mathbb{E}_{x_1,\ldots,x_N\sim\mu} \sup_{h\in\mathcal{F}} \left| \frac{1}{N}\sum_{i=1}^{N} h(x_i) - \int_{\Omega} h(x)d\mu \right| \leq 2R_N(\mathcal{F}). \tag{33}$$

Bound the error of numerical quadrature by Rademacher complexity

Our function class:

$$\mathcal{F}_{n,M} = \left\{ \frac{1}{2} \sum_{|\alpha|=m} a_\alpha(x)(\partial^\alpha u(x))^2 + \frac{1}{2} u(x)^2 - f(x)u(x) : \ u \in \Sigma_{n,M}(\mathbb{D}) \right\}. \tag{34}$$

Theorem (Hong, Siegel & Xu 2021)

Suppose that $\|a_\alpha\|_{L^\infty(\Omega)}, \|a_0\|_{L^\infty(\Omega)} \leq K$ *and* $\sup_{d\in\mathbb{D}} \|d\|_{W^{m,\infty}} \leq C$. *Then the Rademacher complexity of the set* $\mathcal{F}_{n,M}$ *in* (34) *is bounded by*

$$R_N(\mathcal{F}_{n,M}) \leq CKM \sum_{|\alpha|=m} R_N(\partial^\alpha \mathbb{D}) + CKMR_N(\mathbb{D}) + \|f\|_{L^\infty(\Omega)} MR_N(\mathbb{D}), \tag{35}$$

where $\mathbb{D} = \left\{\sigma_k(\omega \cdot x + b) : \ \omega \in \mathbb{S}^{d-1}, \ |b| \leq B\right\}$ *and* $\partial^\alpha \mathbb{D} = \{\partial^\alpha d : \ d \in \mathbb{D}\}$.

Bound the Rademacher complexity

Theorem (Hong, Siegel & Xu 2021)

Suppose that $\sigma \in W^{m+1,\infty}$. *Then for any* α *with* $|\alpha| \leq m$, *we have*

$$R_N(\mathbb{D}) \lesssim N^{-\frac{1}{2}}, \quad R_N(\partial^\alpha \mathbb{D}) \lesssim N^{-\frac{1}{2}}. \tag{36}$$

where the implied constant is independent of N.

Sketch of Proof

1. Noting that

$$\partial^\alpha \mathbb{D} = \{\omega^\alpha \sigma^{(\alpha)}(\omega \cdot x + b) : \omega \in \mathbb{S}^{d-1}, |b| \le B\}. \tag{37}$$

   hence $|\omega^\alpha|$ is bounded.

2. Since $\sigma \in W^{m+1,\infty}$, we have that $\sigma^{(\alpha)}$ is Lipschitz. We obtained

$$R_N(\partial^\alpha \mathbb{D}) \lesssim R_N(\{\omega \cdot x + b : \omega \in \mathbb{S}^{d-1}, |b| \le B\}. \tag{38}$$

3. It is well-known that the Rademacher complexity of the set of linear functions is bounded by

$$R_N(\{\omega \cdot x + b : \omega \in \mathbb{S}^{d-1}, |b| \le B\} \lesssim N^{-\frac{1}{2}}, \tag{39}$$

   for any distribution on x which is bounded almost surely.

Convergence Analysis Assuming Perfect Optimization

- Suppose we can solve perfectly the optimization problem

$$J_N(u_{n,N}) = \min_{v \in \Sigma^k_{n,M}} J_N(v) \tag{40}$$

- Combining the uniform error bound with optimal approximation rates for ReLU^k networks, we get

Theorem

Suppose that $\|a_\alpha\|_{L^\infty(\Omega)}, \|a_0\|_{L^\infty(\Omega)} \leq K$ *and* $\sup_{d\in\mathbb{D}} \|d\|_{W^{m,\infty}} \leq C$. *Let* $\mathbb{D} = \mathbb{P}^d_k$ *be the dictionary of ReLU*^{k} *ridge functions. Then we have*

$$\mathbb{E}_{x_1,\ldots,x_N}\left[\|u_{n,N} - u\|^2_{H^m(\Omega)}\right] \lesssim MN^{-\frac{1}{2}} + Mn^{-1-\frac{2(k-m)}{d}}. \tag{41}$$

Another Issue

How can we efficiently solve the optimization of the discrete energy, i.e.

$$J_N(u_{n,N}) = \min_{v \in \Sigma_{n,M}^k} J_N(v).$$

Challenge: SGD or Adam

For the ReLU^k shallow neural network, let

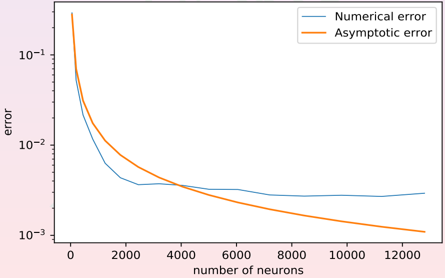
$$u_n = \arg \min_{v_n \in \Sigma_{n,M}(\mathbb{D})} \|v_n - u\| \tag{42}$$

be the solution trained by SGD or Adam, then it is extremely difficult to observe

$$\|u - u_n\| \leq cn^{-\alpha} \tag{43}$$

for any $\alpha > 0$.

Non-convergence for Adam etc for large n



Our approach: Greedy Algorithm

- Orthogonal greedy algorithm (OGA):

$$u_0 = 0,\ g_\ell = \arg\max_{g\in\mathbb{D}} \left|\langle u - u_{\ell-1}, g\rangle_H\right|,\ u_\ell = P_\ell u, \tag{44}$$

  where P_ℓ: orthogonal projection onto span$\{g_1, ..., g_\ell\}$.

- Relaxed greedy algorithm (RGA):

$$\begin{aligned} u_0 &= 0 \\ g_\ell &= \arg\max_{g\in\mathbb{D}} \langle \nabla J_N(u_{\ell-1}), g\rangle \\ u_\ell &= (1 - s_\ell)u_{\ell-1} - M s_\ell g_\ell. \end{aligned} \tag{45}$$

A Property of RGA:

Theorem (Hong, Siegel & Xu 2021)

The $u_\ell, \ell = 1, 2, \cdots$, produced by RGA satisfy $\|u_\ell\|_{\mathcal{K}_1(\mathbb{D})} \le M$ for all ℓ and

$$J_N(u_\ell) - \min_{v\in\Sigma_{n,M}} J_N(v) \lesssim \frac{1}{\ell}. \tag{46}$$

Ref: Ronald A DeVore and Vladimir N Temlyakov. “Some remarks on greedy algorithms". In: Advances in computational Mathematics 5.1 (1996), pp. 173-vvv187.

Main Theorem

Theorem (Hong, Siegel & Xu 2021)

Assume that the true solution $u \in \mathcal{K}_1(\mathbb{D})$ *satisfies* $\|u\|_{\mathcal{K}_1(\mathbb{D})} \leq M$ *and let the numerical solution* $u_{n,M,N} \in \Sigma_{n,M}(\mathbb{D})$ *be obtained by the relaxed greedy algorithm for n steps. Then we have*

$$\mathbb{E}_{x_1,\ldots,x_N}(J(u_{n,M,N}) - J(u)) \leq M\left[C_1(1 + \|f\|_{L^\infty(\Omega)})N^{-\frac{1}{2}} + C_2 M n^{-1}\right]. \quad (47)$$

and

$$\mathbb{E}_{x_1,\ldots,x_N}(\|u_{n,M,N} - u\|^2_{H^m(\Omega)}) \leq M\left[C_1' N^{-\frac{1}{2}} + C_2' M n^{-1}\right], \quad (48)$$

where C_1' *and* C_2' *depend only upon the dictionary and the differential operator.*

Sketch of Proof

1. Recall $J(u_n) = \min_{v \in \Sigma_{n,M}} J(v)$. We write

$$\begin{aligned}\mathbb{E}_{x_1,\ldots,x_N}(J(u_{n,M,N}) - J(u)) \le\ & \mathbb{E}_{x_1,\ldots,x_N}(J_N(u_{n,M,N}) - J_N(u_n)) \\ & + \mathbb{E}_{x_1,\ldots,x_N}(|J_N(u_n) - J(u_n)|) \\ & + \mathbb{E}_{x_1,\ldots,x_N}(|J(u_n) - J(u)|).\end{aligned} \tag{49}$$

2. Since $u_{n,M,N}$ is obtained by the relaxed greedy algorithm for n steps. The first term on the right hand side can be estimated by

$$\begin{aligned}J_N(u_{n,M,N}) - J_N(u_n) &= J_N(u_{n,M,N}) - \min_{v \in \Sigma_{n,M}} J_N(v) + \min_{v \in \Sigma_{n,M}} J_N(v) - J_N(u_n) \\ &\le J_N(u_{n,M,N}) - \min_{v \in \Sigma_{n,M}} J_N(v) \lesssim \frac{1}{n}.\end{aligned} \tag{50}$$

3. The second term on the right is the error of numerical quadrature which is bounded via the Rademacher complexity by

$$CM(K + \|f\|_{L^\infty(\Omega)})N^{-\frac{1}{2}}.$$

4. The third term can be bounded by the approximation error.

PINN (Raissi et al., J. Comput. Phys. 378 (2019), pp. 686–707)

- Loss function for PINN:

$$L(u) = \min_{v \in H^1(\Omega)} L(v) \ \text{ with } \ L(v) = \int_\Omega |\Delta v + f|^2 dx + \int_{\partial\Omega} |\frac{\partial v}{\partial n}|^2 ds. \quad (51)$$

- Discretization of the loss:

$$L_N(u_{n,N}) = \min_{v \in \Sigma^k_{n,M}} L_N(v) \ \text{ with } \ L_N(v) = \frac{1}{N} \sum_{i=1}^{N} |\Delta v(x_i) + f(x_i)|^2 + \frac{1}{N_b} \sum_{i=1}^{N_b} |\frac{\partial v}{\partial n}(x_i)|^2. \quad (52)$$

- Similar results can be obtained for PINN.

Ref: M. Raissi, P. Perdikaris, G. E Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational physics (2019), Volume 378, 686-707

Remarks on the relaxed greedy algorithm

Question: How to solve

$$g_k = \arg\max_{g\in\mathbb{D}} \langle \nabla J_N(u_{k-1}), g\rangle$$

- Feasible for small d ($d = 1, 2, 3$).
- Challenge if d is large, but possible if u has special structure.
- We do not know any other method.

Orthogonal greedy algorithm

- Orthogonal greedy algorithm (OGA) for function approximation in a Hilbert space H:

$$u_0 = 0,\ g_n = \arg\max_{g \in \mathbb{D}} \left|\langle u - u_{n-1}, g\rangle_H\right|,\ u_n = P_n u, \tag{53}$$

where P_n: orthogonal projection onto V_n =span$\{g_1, ..., g_n\}$.

Theorem

Assume that the true solution $u \in \mathcal{K}_1(\mathbb{D})$ and let the numerical solution u_n be obtained by the orthogonal greedy algorithm for n steps. If $\|\mathbb{D}\|_H := \sup_{d\in\mathbb{D}} \|d\|_H < \infty$, then we have

$$\|u - u_n\|_H \leq \|\mathbb{D}\|_H \|u\|_{\mathcal{K}_1(\mathbb{D})} n^{-\frac{1}{2}}. \tag{54}$$

Ref: Andrew R. Barron, Albert Cohen, Wolfgang Dahmen, Ronald A. DeVore "Approximation and learning by greedy algorithms," The Annals of Statistics, Ann. Statist. 36(1), 64-94, (February 2008).

Proof

1. Using the orthogonality
$$u_n = \arg\min_{v_n \in V_n} \|u - v_n\|_H. \tag{55}$$

2. Since $u_{n-1} + \alpha g_n \in V_n$ for $\forall \alpha \in \mathbb{R}$, taking $\alpha = c\langle u - u_{n-1}, g_n\rangle_H$ where $c = (\|\mathbb{D}\|_H)^{-2}$, we have
$$\begin{aligned} \|u - u_n\|_H^2 &\le \|u - u_{n-1} - \alpha g_n\|_H^2 \\ &= \|u - u_{n-1}\|_H^2 - 2c\langle u - u_{n-1}, g_n\rangle\langle u - u_{n-1}, g_n\rangle + \alpha^2\|g_n\|_H^2 \\ &= \|u - u_{n-1}\|_H^2 - c(2 - c\|g_n\|_H^2)|\langle u - u_{n-1}, g_n\rangle_H|^2 \\ &\le \|u - u_{n-1}\|_H^2 - c|\langle u - u_{n-1}, g_n\rangle_H|^2 \end{aligned} \tag{56}$$

3. The second term on the right can be estimated as follows: let $u \in \mathcal{K}_1(\mathbb{D})$ be expanded by $u = \sum_{k\ge 0} \beta_k h_k$ for $h_k \in \mathbb{D}$,
$$\begin{aligned} \|u - u_{n-1}\|_H^2 = \langle u - u_{n-1}, u - u_{n-1}\rangle_H &= \langle u - u_{n-1}, u\rangle_H \\ &= \langle u - u_{n-1}, \sum_{k\ge 0} \beta_k h_k\rangle \\ &\le \|u\|_{\mathcal{K}_1(\mathbb{D})} \max_{g\in\mathbb{D}} |\langle u - u_{n-1}, g\rangle_H| \\ &= \|u\|_{\mathcal{K}_1(\mathbb{D})} |\langle u - u_{n-1}, g_n\rangle_H|. \end{aligned} \tag{57}$$

Proof

1. This give

$$|\langle u - u_{n-1}, g_n\rangle_H| \geq \|u\|^{-1}_{\mathcal{K}_1(\mathbb{D})}\|u - u_{n-1}\|^2_H. \tag{58}$$

2. By (56) and (58), we have

$$\begin{aligned}\|u - u_n\|^2_H &\leq \|u - u_{n-1}\|^2_H \left(1 - \frac{c}{\|u\|^2_{\mathcal{K}_1(\mathbb{D})}}\|u - u_{n-1}\|^2_H\right) \\ &= \|u - u_{n-1}\|^2_H \left(1 - \frac{1}{\|\mathbb{D}\|^2_H\|u\|^2_{\mathcal{K}_1(\mathbb{D})}}\|u - u_{n-1}\|^2_H\right).\end{aligned} \tag{59}$$

3. The result follows from a mathematical induction, since $\|u - u_0\|_H = \|u\|_H \leq \|\mathbb{D}\|_H\|u\|_{\mathcal{K}_1(\mathbb{D})}$, and

$$\text{for nonnegative series } a_0 \leq M, \quad a_n \leq a_{n-1}\left(1 - \frac{a_{n-1}}{M}\right) \Longrightarrow a_n \leq \frac{M}{n+1}, \quad n \in \mathbb{N}. \tag{60}$$

NN with OGA for Data fitting

Example (2D approximation)

Consider approximating the following 2D function

$$u(x,y) = \cos(2\pi x)\cos(2\pi y), \quad (x,y) \in (0,1)^2.$$

By fixing $\|\omega\| = 1$ and $b \in [-2,2]$, the convergence order of OGA is shown in Table below for ReLU^k neural networks. Theoretical order is shown in parenthesis.

n	$k=1(n^{-1.25})$		$k=2(n^{-1.75})$		$k=3(n^{-2.25})$	
	$\|u-u_n\|_{L^2}$	order	$\|u-u_n\|_{L^2}$	order	$\|u-u_n\|_{L^2}$	order
2	4.969e-01	-	4.998e-01	-	4.976e-01	-
4	4.883e-01	0.025	4.992e-01	0.002	4.957e-01	0.006
8	2.423e-01	1.011	3.233e-01	0.627	4.193e-01	0.242
16	6.632e-02	1.869	4.911e-02	2.719	1.099e-01	1.932
32	2.206e-02	1.588	1.688e-02	1.541	8.075e-03	3.767
64	1.060e-02	1.058	4.156e-03	2.022	1.149e-03	2.813
128	4.284e-03	1.306	9.773e-04	2.088	2.185e-04	2.395
256	1.703e-03	1.331	2.622e-04	1.898	4.718e-05	2.211

Table: Convergence order of OGA with $ReLU^k$ activation function

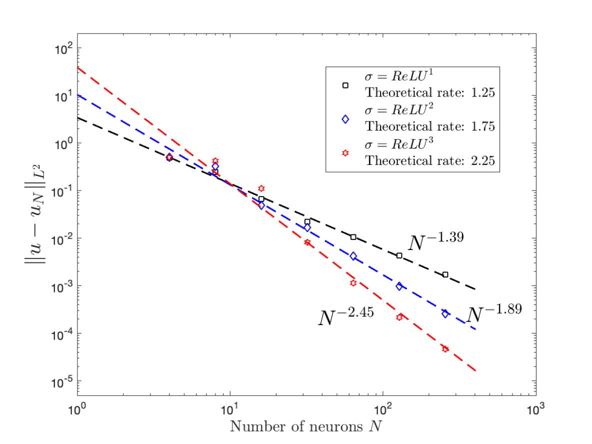


Figure: Convergence order of OGA with $ReLU^k$ activation function

NN with OGA for Numerical PDE

Example (1D elliptic equation)

Let us consider the 1D second order elliptic equation on $\Omega = (-1, 1)$:

$$-u'' + u = f, \text{ in } \Omega \tag{61}$$

$$\frac{\partial u}{\partial n} = 0, \text{ on } \partial\Omega. \tag{62}$$

with the source term $f = (1 + \pi^2)\cos(\pi x)$, then the analytical solution is $u(x) = \cos(\pi x)$. Let $\sigma = \mathrm{ReLU}^2$ and the convergence rates are predicted theoretically.

n	$\|u - u_n\|_{L^2}$	order(n^{-3})	$\|u - u_n\|_{H^1}$	order(n^{-2})
16	7.86e-04	-	2.79e-02	-
32	7.70e-05	3.35	5.89e-03	2.24
64	8.45e-06	3.19	1.36e-03	2.11
128	9.68e-07	3.13	3.22e-04	2.08
256	1.18e-07	3.04	7.81e-05	2.04
512	1.44e-08	3.03	1.94e-05	2.01
1024	1.83e-09	2.97	4.86e-06	1.99
2048	2.50e-10	2.88	1.28e-06	1.93

Table: L^2 and H^1 numerical error of the OGA solution

OGA v.s. SGD and Adam

We take the learning rate $\eta = 1e-3$ for SGD and Adam. It is difficult to observe any convergence order from the solutions of SGD or Adam:

	Adam				SGD			
n	$\|u-u_n\|_{L^2}$	order	$\|u-u_n\|_{H^1}$	order	$\|u-u_n\|_{L^2}$	order	$\|u-u_n\|_{H^1}$	order
16	1.61e-02	-	1.45e-01	-	1.30e-02	-	1.52e-01	-
32	3.71e-03	2.12	5.84e-02	1.32	9.35e-03	0.47	1.13e-01	0.43
64	1.80e-03	1.04	3.46e-02	0.76	7.11e-03	0.39	8.64e-02	0.38
128	5.52e-04	1.70	1.43e-02	1.27	5.91e-03	0.27	7.22e-02	0.26
256	2.26e-04	1.29	6.99e-03	1.04	5.75e-03	0.04	7.03e-02	0.04
512	1.88e-04	0.27	3.90e-03	0.84	4.41e-03	0.38	5.40e-02	0.38
1024	2.09e-04	-0.16	2.56e-03	0.61	1.52e-03	1.54	1.99e-02	1.43
2048	4.11e-04	-0.97	2.51e-03	0.03	3.22e-03	-1.09	3.56e-02	-0.84

Table: Numerical results from different training methods.

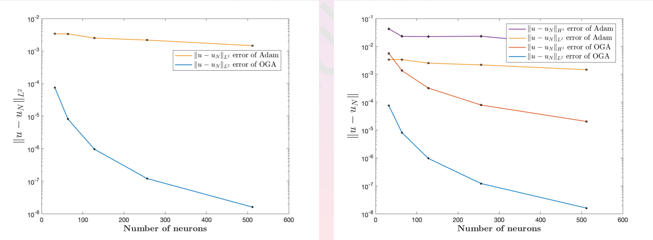


Figure: OGA vs Adam

NN with OGA for 4th order PDE

Example (1D 4th-order equation)

We consider the 4th-order equation $(-\Delta)^2 u + u = f$ on $(-1, 1)$ with

$$u(x) = (1 - x)^4 (1 + x)^4.$$

Take $\sigma = \mathrm{ReLU}^3$. The convergence orders with $\|\cdot\|_0$ and $\|\cdot\|_a$ errors are listed in the following table to confirm 4th order and 2nd order convergence, respectively.

n	$\|u - u_n\|_{L^2}$	order	$\|u - u_n\|_a$	order
2	8.762e-01	-	6.063e+00	-
4	9.892e-01	-0.17	4.122e+00	0.56
8	1.493e-02	6.05	1.069e+00	1.95
16	2.608e-04	5.84	1.431e-01	2.90
32	1.089e-05	4.58	3.120e-02	2.20
64	5.530e-07	4.30	6.639e-03	2.23
128	2.989e-08	4.21	1.679e-03	1.98
256	1.746e-09	4.10	4.092e-04	2.04

Table: The $\|\cdot\|_0$ and $\|\cdot\|_a$ errors of the OGA solution.

Numerical experiments of OGA

Example (2D 4th-order equation)

Next consider the $\|\cdot\|_0$ and $\|\cdot\|_a$ errors of OGA for 2D 4th-order equations on $\Omega = (-1, 1)^2$. Let the exact solution to be $u(x, y) = (x^2 - 1)^4(y^2 - 1)^4$ to satisfy the Neumann boundary conditions. We have

n	$\|u - u_n\|_{L^2}$	order	$\|u - u_n\|_a$	order
2	6.528e-01	-	7.927e+00	-
4	7.859e-01	-0.27	7.593e+00	0.06
8	9.906e-01	-0.33	6.295e+00	0.27
16	8.215e-01	0.27	4.003e+00	0.65
32	1.513e-01	2.44	1.446e+00	1.47
64	7.206e-02	1.07	4.747e-01	1.61
128	2.259e-02	1.67	1.809e-01	1.39
256	4.696e-03	2.27	6.970e-02	1.38

Table: The convergence order with $\|\cdot\|_0$ and $\|\cdot\|_a$ errors by OGA.

Nonlinear problem: 2D

Example (A nonlinear 2D example)

Consider the following nonlinear 2D equation $-\Delta u + u^3 + u = f$ on $(0,1)^2$ with $\partial u/\partial n = 0$. The analytical solution is $u = \cos(2\pi x)\cos(2\pi y)$ and the dictionary for RGA is taken as

$$\mathbb{D} = \{\sigma(w_1 x + w_2 y + b) | (w_1, w_2, b) \in [-20, 20]^3\}$$

where $\sigma(x)$ is the sigmoid function. The convergence is considered on the approximating space where $\|u\|_{\mathcal{K}_1(\mathbb{D})} \leq M = 15$.

n	$\|u - u_n\|_2$	order	$\|Du - Du_n\|_2$	order	$J(u_n) - J(u)$	order(n^{-1})
16	7.847e-01	-	4.645e+00	-	1.805e+04	-
32	6.679e-01	0.23	2.955e+00	0.65	7.563e+03	1.25
64	2.370e-01	1.49	1.675e+00	0.82	2.328e+03	1.70
128	1.216e-01	0.96	1.087e+00	0.62	9.680e+02	1.27
256	6.184e-02	0.98	5.205e-01	1.06	2.222e+02	2.12
512	3.797e-02	0.70	3.611e-01	0.53	1.067e+02	1.06
1024	2.687e-02	0.50	2.110e-01	0.77	3.662e+01	1.54
2048	1.072e-02	1.33	1.432e-01	0.56	1.663e+01	1.14

Table: Convergence order of RGA.

Nonlinear problem: 2D

Example (2D Poisson-Boltzmann equation)

Consider the PB equation $-\Delta u + \kappa \sinh(u) = f$ on the sphere $\{(x, y) | x^2 + y^2 \leq 4\}$ with $\partial u/\partial n = 0$. The energy functional for this problem is

$$\mathcal{J}(u) = \int_\Omega \left(\frac{1}{2} |\nabla u|^2 + \kappa \cosh(u) - fu \right) dx,$$

which is a strictly convex and coercive energy as long as $\kappa > 0$. We set $\kappa = 1$ and consider the radially symmetric solution

$$u(x, y) = \cos\left(\frac{\pi}{2} \sqrt{x^2 + y^2}\right).$$

n	$\|u - u_n\|_2$	order	$\|Du - Du_n\|_2$	order	$J(u_n) - J(u)$	order(n^{-1})
16	1.103e+00	-	2.470e+00	-	1.512e+05	-
32	6.499e-01	0.76	1.845e+00	0.42	7.750e+04	0.96
64	5.440e-01	0.26	1.536e+00	0.26	5.480e+04	0.50
128	2.435e-01	1.16	7.509e-01	1.03	1.285e+04	2.09
256	1.507e-01	0.69	4.532e-01	0.73	4.690e+03	1.45
512	7.373e-02	1.03	2.659e-01	0.77	1.423e+03	1.72
1024	2.949e-02	1.32	1.647e-01	0.69	5.363e+02	1.41
2048	2.401e-02	0.30	1.156e-01	0.51	2.571e+02	1.06

Table: Convergence order of RGA for the 2D Poisson-Boltzmann equation.

10D example

Example (10D Poisson equation)

Consider a 10d elliptic equation in the following form

$$-\nabla \cdot (\alpha \nabla u) + u = f,\ x \in (0,1)^{10}, \quad \frac{\partial u}{\partial n} = 0,\ x \in \partial(0,1)^{10}. \tag{63}$$

We take

$$u = \sum_{i=1}^{10} \cos(\pi x_i), \quad \alpha = \sqrt{1 + \sum_{i=1}^{10} (x_i - \frac{1}{2})^2}. \tag{64}$$

We discretize the energy using 100 million quasi-Monte-Carlo samples in $[0,1]^{10}$ and optimize the energy using the OGA with dictionary

$$\mathbb{P}_2^{10,r} = \{\sigma(\omega \cdot x + b),\ \omega = \pm e_i,\ i = 1, .., 10,\ b \in [-2,2]\}, \tag{65}$$

and we obtained

n	$\|u - u_n\|_{L^2}$	order(n^{-3})	$\|u - u_n\|_{H^1}$	order(n^{-2})
2	2.058e+00	0.00	6.778e+00	0.00
4	1.850e+00	0.15	6.139e+00	0.14
8	1.307e+00	0.50	4.604e+00	0.42
16	5.019e-01	1.38	3.184e+00	0.53
32	4.702e-02	3.42	5.988e-01	2.41
64	4.629e-03	3.34	1.104e-01	2.44
128	4.437e-04	3.38	2.272e-02	2.28
256	5.411e-05	3.04	5.194e-03	2.13

Summary

1. Using neural network to solve $2m$-th order PDEs.
2. Inverse inequality does not hold for the neural network function class
3. Using the good property of stable neural network
4. Convergence analysis for sampling
5. Greedy algorithm to solve the optimization problem.

References

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Thank you very much!