New deep neural networks solving non-linear inverse problems

or

How to use uniqueness results for inverse problems to design neural networks?

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Inverse problem in a d-dimensional body

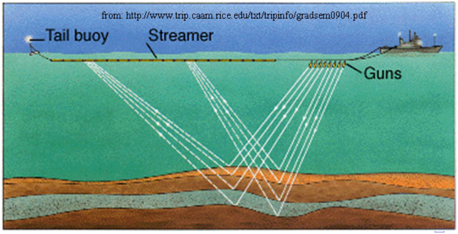
Let $u(x,t) = u^h(x,t)$ solve the wave equation

$$(\partial_t^2 - c(x)^2\Delta)u(x,t) = 0 \quad \text{on } (x,t) \in M \times \mathbb{R}_+,$$
$$\partial_\nu u(x,t)|_{\partial M \times \mathbb{R}_+} = h(x,t), \quad u|_{t=0} = 0, \quad \partial_t u|_{t=0} = 0,$$

where h is boundary source, $M \subset \mathbb{R}^d$. The Neumann-to-Dirichlet map is

$$Y_c h = u^h(x,t)\big|_{(x,t)\in\partial M \times \mathbb{R}_+}.$$

In the inverse problem we aim to find the unknown wave speeds $c(x)$ from boundary measurements Y_c (Traditionally, one denotes $Y_c = \Lambda_c$).
Next we consider this problem in the 1-dimensional case and solve it using neural networks.



Results on the hyperbolic inverse problem:

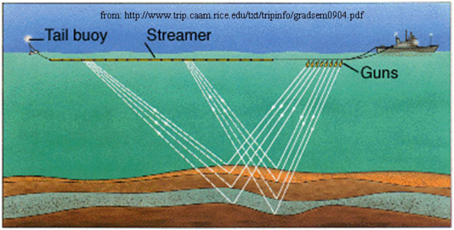
- 1-dimensional problems: Gelfand, Levitan, Marchenko 1950-1960.
- Inverse problem for $\Delta + q$: Nachman-Sylvester-Uhlmann 1988.
- Reconstruction of a Riemannian manifold with time-indepedent metric: Belishev-Kurylev 1992 and Tataru 1995.
- Solution by modified time reversal and focusing of waves: Bingham-Kurylev-L.-Siltanen 2008.
- Combining several measurements for together for the wave equation: Helin-L.-Oksanen 2012.
- Numerical methods for focusing of waves: de Hoop-Kepley-Oksanen 2018.
- Partial data: L.-Oksanen 2014, Mansouri-Milne 2017.
- Inverse problems for the connection Laplacian: Kurylev-Oksanen-Paternain 2018.
- Scattering control: Caday-de Hoop-Katsnelson-Uhlmann 2018.

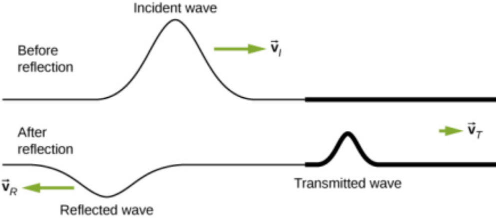
Overview of the talk

1. We consider the solution map $S : Y_c \to c$ that solves the inverse problem in the 1-dimensional case.
   For this, we use the boundary control method (Belishev 1987, Belishev-Kurylev 1992) and its regularized version (Bingham-Kurylev-L.-Siltanen 2008 and Korpela-L.-Oksanen 2018).
2. We propose an architecture of neural networks, where the input is a linear operator Y.
3. We show that the solution map S can be written as a neural network with the proposed architecture.
4. The performance of the trained neural network can be estimated using stability theorems for inverse problems.

Outline:

- Solution of the inverse problem in 1-dimensional space
- Standard neural networks
- Operator recurrent networks





Inverse problem in 1-dimensional space

Consider the wave equation in one-dimensional space, $x \in \mathbb{R}_+$.
This corresponds to subsurface imaging when the wave speed depends only on the depth.
Let $u(x,t)$ be the solution of the wave equation

$$(\frac{\partial^2}{\partial t^2} - c(x)^2 \frac{\partial^2}{\partial x^2}) u(x,t) = 0, \quad x \in \mathbb{R}_+, \ t \in \mathbb{R}_+$$
$$\frac{\partial}{\partial x} u|_{x=0} = h(t), \quad u|_{t=0} = 0, \quad \frac{\partial}{\partial t} u|_{t=0} = 0,$$

where the wave speed $c(x)$ is unknown. Denote $u(x,t) = u^h(x,t)$.
Let $T > 0$. Suppose we are given the Neumann-to-Dirichlet map, $Y = Y_c$,

$$Y_c h = u^h(x,t)\Big|_{x=0}, \quad t \in (0, 2T).$$

Y_c is a linear operator or "a matrix". Physically,

$$Y_c : \ \text{boundary source } h \ \rightarrow \text{the boundary value of the wave } u|_{x=0}.$$

Travel time function

The travel time for the wave from the boundary point 0 to the point x is

$$\tau(x) = \int_0^x \frac{1}{c(x')}\, dx'.$$

Assume that we can construct the function $\tau^{-1} : \mathbb{R}_+ \to \mathbb{R}_+$. Then we can determine the travel time function $\tau : \mathbb{R}_+ \to \mathbb{R}_+$ and the wave speed by

$$c(x) = \frac{1}{\frac{d}{dx}\tau(x)}.$$

Next, we study the inverse problem of finding the inverse travel time function τ^{-1} when Y_c is given.
We will consider the function $F : Y_c \to \tau^{-1}$ and construct a neural network that approximates F.

Neumann-to-Dirichlet map determines inner products of waves

Denote

$$\begin{aligned}\langle u^f(T), u^h(T)\rangle &= \int_{\mathbb{R}_+} u^f(x,T)u^h(x,T)dV(x), \quad dV = \frac{1}{c(x)^2}dx,\\ \|u^f(T)\|_{L^2(M)} &= \langle u^f(T), u^f(T)\rangle^{\frac{1}{2}}.\end{aligned}$$

By Blagovestchenskii formula,

$$\langle u^f(T), u^h(T)\rangle = \int_0^{2T} (K_Y f)(t)h(t)\,dt, \quad \langle u^f(T), 1\rangle = \int_0^T f(t)(T-t)\,dt$$

where $Y = Y_c$ is the Neumann-to-Dirichlet map,

$$\begin{aligned}&K_Y = JY - RYRJ,\\ &Rf(t) = f(2T-t) \quad \text{"time reversal operator"},\\ &Jf(t) = \tfrac{1}{2}1_{[0,T]}(t)\int_t^{2T-t} f(s)ds \quad \text{"low pass filter"}.\end{aligned}$$

An analytic solution algorithm for the inverse problem

By Bingham-Kurylev-L.-Siltanen 2008 and dH-L-W 2020, the inverse problem is solved as follows: Suppose we are given $Y = Y_c$.

Step 1: For the depth parameter $0 \le s \le T$, let $h_{\beta,s} \in L^2(0,2T)$ solve

$$\min_h \|u^h(T) - 1\|_{L^2}^2 + \beta\|Ah\|_{\ell^1} = \langle K_Y h, h\rangle - 2\langle h, b\rangle + C + \beta\|Ah\|_{\ell^1},$$

where $supp(h) \subset [T-s, T]$.
Here, $A : L^2(0,2T) \to \ell^2$ is an isometry and $K_Y = JY - RYRJ$. Then,

$$\lim_{\beta\to 0} u^{h_{\beta,s}}(x,T) = \begin{cases} 1, & \text{if } \tau(x) \le s \\ 0, & \text{otherwise.} \end{cases} .$$

We call $h_{\beta,s}$ the optimized sources.

Thus, when β is small,

$$u^{h_{\beta,s}}(x,T) \approx \begin{cases} 1, & \text{if } \tau(x) \le s \\ 0, & \text{otherwise.} \end{cases}$$

An analytic solution algorithm for the inverse problem

Step 2. Using the the optimized sources $h_{\beta,s}$, we compute

$$V(s) = \lim_{\beta\to 0} \int_0^T h_{\beta,s}(t)\,(T-t)dt = \lim_{\beta\to 0} \langle u^{h_{\beta,s}}(T), 1\rangle_{L^2(M)}$$

$$= \mathrm{vol}_c([0,\tau^{-1}(s)]) = \int_0^{\tau^{-1}(s)} \frac{1}{c(x)^2}\,dx,$$

$$w(s) = \frac{\partial}{\partial s} V(s).$$

Then

$$\tau^{-1}(s) = \int_0^s \frac{1}{w(t)}\,dt, \quad \text{and } c(\tau^{-1}(s)) = \frac{1}{w(s)}.$$

An analytic solution algorithm for the inverse problem

The above minimization problem can be solved using an iteration. Writing sources in a finite basis, the inverse problem is solved as follows:

Step 1: For $j = 1, \dots, K$ and $h^{(j)} = h_L^{(j)}$ be computed by doing L steps of the iterated soft thresholding,

$$h_{\ell+1}^{(j)} \quad := \quad \sigma_\beta\Big((I + P_j R Y R J - P_j J Y) h_\ell^{(j)} + P_j b\Big), \quad h_0^{(j)} = 0.$$

Here, $\beta > 0$ is the regularization parameter and

> R is the matrix of the time-reversal operator, P_j is a projector,
> J is the matrix of the low-pass filter, b is a constant vector,

$\sigma_\beta(x) = \text{relu}(x - \beta) - \text{relu}(-x - \beta)$ is soft thresholding, $\text{relu}(x) = \max(x, 0)$.

Step 2. Compute $\tau^{-1}(s_j) \approx G_j(h^{(1)}, \dots, h^{(K)})$, where $s_j = \frac{jT}{K}$ and G_j are explicit functions.

Summary on the analytic solution of the inverse problem

Consider the map $F : Y_c \to \tau^{-1}$ that determines the inverse of the travel time function τ^{-1} (and the wave speed $c(x)$) from the boundary measurements Y_c.

The discretized version of this map, $F : \mathbb{R}^{n\times n} \to \mathbb{R}^{2K}$ can be written as

$$F(Y_c) = G(f^{(1)}(Y_c), f^{(2)}(Y_c), \dots, f^{(K)}(Y_c))$$

where $f^{(j)} : \mathbb{R}^{n\times n} \to \mathbb{R}^{n}$ map Y_c to the optimized sources,

$$f^{(j)}(Y_c) = h^{(j)}.$$

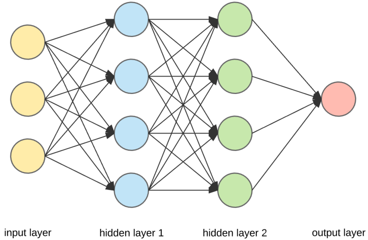
Next we define a family of neural networks (operator recurrent networks) than can approximate functions $f^{(j)} : \mathbb{R}^{n\times n} \to \mathbb{R}^{n}$.

The explicit function G can be approximated by a standard neural network.

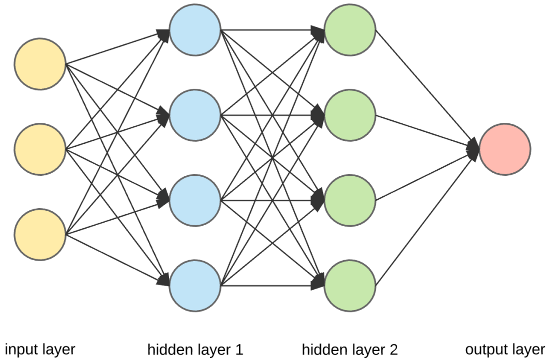
Then, we can approximate F by a neural network.

Outline:

- Solution of the inverse problem in 1-dimensional space
- Standard neural networks
- Operator recurrent networks



Standard neural network



- In every node in the hidden layers, one operates with a non-linear activation function ϕ. In this talk, ϕ is the Rectified Linear Unit,

$$\phi(x) = \mathrm{relu}(x) := \max(0, x) = \begin{cases} x, & x > 0, \\ 0, & x \leq 0, \end{cases} \qquad x \in \mathbb{R}.$$

Definition of the standard deep neural network

A standard neural network is a function $f_\theta : \mathbb{R}^{d_0} \to \mathbb{R}^{d_L}$ defined by

$$
\begin{aligned}
h_0 &= x, \\
h_{\ell+1} &= \phi\left(A_\theta^\ell h_\ell + b_\theta^\ell\right), \quad \ell = 0, \dots, L-1, \\
f_\theta(x) &= h_L.
\end{aligned}
$$

Architecture:

- ℓ: the layer index, max depth L.
- h_ℓ: intermediate output at layer ℓ.
- $b_\theta^\ell \in \mathbb{R}^{d_{\ell+1}}$, $A_\theta^\ell \in \mathbb{R}^{d_{\ell+1} \times d_\ell}$ are the biases and weight matrixes that depend on parameters $\theta = (\theta_1, \theta_2, \dots, \theta_m)$.
- ϕ is the activation function, the Rectified Linear Unit (relu)

$$
\phi : \mathbb{R}^d \to \mathbb{R}^d, \quad \phi(x_1, \dots, x_d) = (\max(0, x_1), \dots, \max(0, x_d))
$$

Applications of neural networks in inverse problems

- Modified gradient descent: Adler-Öktem 2017.
- Splines and Neural networks: Unser-Fageot-Ward (SIAM Rev. 2017), Jin-McCann-Froustey-Unser 2017.
- Data driven models: Arridge-Maass-Öktem-Schönlieb (Acta Numerica 2019)
- Generative adversarial networks: Bora-Jalal-Price-Dimakis 2017, Lunz-Öktem-Schönlieb 2018.
- Neumann Networks: Gilton-Ongie-Willett 2019.
- Diffusion problems: Arridge-Hauptmann 2019, Antholzer-Haltmeier-Schwab 2019, Agnelli-Col-L.-Murthy-Santacesaria-Siltanen 2020.
- Limited angle tomograpy: Bubba-Kutyniok-L.-Marz-Samek-Siltanen-Srinivasan 2019.
- Scattering problems: Uhlmann-Wang 2018, Khoo-Ying 2019, Li-Wang-Teixeira-Liu-Nehorai-Cui 2019, Wei-Chen 2019.

A modification of a neural network

Recall: A standard deep neural network is a function $f_\theta : \mathbb{R}^{d_0} \to \mathbb{R}^{d_L}$ that takes in a vector $x \in \mathbb{R}^{d_0}$ and computes following operations

$$\begin{aligned} h_0 &= x, \\ h_{\ell+1} &= \phi\left(A_\theta^\ell h_\ell + b_\theta^\ell\right), \quad \ell = 0, \dots, L-1, \\ f_\theta(x) &= h_L. \end{aligned}$$

We will modify this: We define a function $f_\theta : \mathbb{R}^{n\times n} \to \mathbb{R}^n$ that takes in a linear operator $Y \in \mathbb{R}^{n\times n}$ and computes following operations

$$\begin{aligned} h_0 &= b^0, \\ h_{\ell+1} &= \phi\left(A_\theta^\ell Y h_\ell + b_\theta^\ell\right), \quad \ell = 0, \dots, L-1, \\ f_\theta(Y) &= h_L. \end{aligned}$$

Outline:

- Solution of the inverse problem in 1-dimensional space
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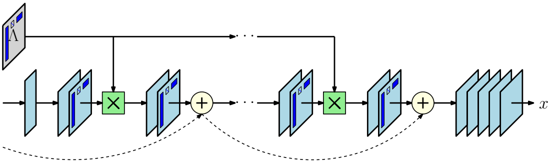
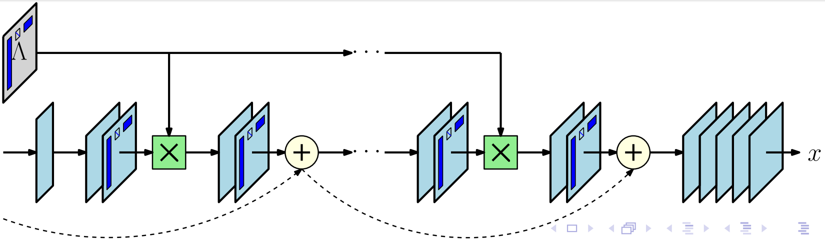


Definition

An *operator recurrent network* with depth L, width n and parameters $\theta \in [-1,1]^D \subset \mathbb{R}^D$ is a function $f_\theta : \mathbb{R}^{n\times n} \to \mathbb{R}^n$ given by

$$
\begin{aligned}
h_0 &= b_\theta^{0,1},\\
h_\ell &= b_\theta^{\ell,1} + A_\theta^{\ell,1} h_{\ell-1} + A_\theta^{\ell,2} Y h_{\ell-1} + \phi\left[b_\theta^{\ell,2} + A_\theta^{\ell,3} h_{\ell-1} + A_\theta^{\ell,4} Y h_{\ell-1}\right],\\
f_\theta(Y) &= h_L,
\end{aligned}
$$

where the initial vector $h_0 = b_\theta^{0,1} \in \mathbb{R}^n$ is independent of the input $Y \in \mathbb{R}^{n\times n}$ and $A_\theta^{\ell,i} \in \mathbb{R}^{n\times n}$, $b_\theta^{\ell,i} \in \mathbb{R}^n$.
Activation functions ϕ are *relu* functions.



Iteration in the analytic algorithm is a neural network

Recall the earlier: The optimized sources were computed by doing L steps of the iterated soft thresholding,

$$h_{\ell+1}^{(j)} \;:=\; \sigma_\beta\Big((I + P_j R Y R J - P_j J Y) h_\ell^{(j)} + P_j b\Big), \quad h_0^{(j)} = 0.$$

Here, $\beta > 0$ and

R is the matrix of the time-reversal operator, P_j is a projector,
J is the matrix of the low-pass filter, b is a constant vector,

This iteration can be written as an operator recurrent network by using matrixes of operators.

Parametrization of the weight matrixes in the network

The weight matrixes $A_\theta^{\ell,i} \in \mathbb{R}^{n\times n}$ have the form

$$A_\theta^{\ell,i} = A^{\ell,i,(0)} + A_\theta^{\ell,i,(1)}, \quad A_\theta^{\ell,k,i,(1)} = \sum_{p=1}^{n} \theta_{2p-1}^{\ell,i}(\theta_{2p}^{\ell,i})^T,$$

where $A^{\ell,i,(0)}$ are fixed matrixes that do not depend on θ,
$A_\theta^{\ell,i,(1)}$ are sparse matrixes that are determined by parameters $\theta_p^{\ell,i} \in \mathbb{R}^n$.

The above iterated soft thresholding can be written as an operator recurrent network as follows:

- The compact operators in the analytic method (e.g. the low pass filter J) are replaced by sparse matrixes $A_\theta^{\ell,i,(1)}$. These matrixes are learned from the training data.
- Non-compact operators in the analytic method (e.g. the identity operator I or the time reversal R) determine the fixed matrixes $A^{\ell,i,(0)}$. The matrixes $A^{\ell,i,(0)}$ are not learned but determined by the analytic method.

Loss function and regularization

Next, we consider a general target function $f : \mathbb{R}^{n\times n} \to \mathbb{R}^n$.
We want to learn the parameters θ such that the neural network $f_\theta : \mathbb{R}^{n\times n} \to \mathbb{R}^n$ approximate the function $f : \mathbb{R}^{n\times n} \to \mathbb{R}^n$.

Definition

The regularized loss function $\mathcal{L}$ with regularization parameter $\alpha > 0$ is given by

$$\mathcal{L}(\theta, Y) = \|f_\theta(Y) - f(Y)\|^2_{\mathbb{R}^n} + \alpha\mathcal{R}(\theta)$$

To make the weight matrixes $A_\theta^{\ell,i,(1)}$ sparse, we use the ℓ^1-norm

$$\mathcal{R}(\theta) = \|\theta\|_1 = \sum_{\ell,k,p} \|\theta_p^{\ell,i}\|_{\mathbb{R}^n}.$$

Training a neural network with sampled data

Assume that Y is random and has a priori distribution μ, that is, $Y \sim \mu$.

Let $Y_1, Y_2, \dots, Y_N$ be independent samples from a priori distribution μ. Suppose we are given the training set

$$S = \{(Y_1, f(Y_1)), \dots, (Y_N, f(Y_N))\}.$$

Training of the neural network means minimizing the the empirical loss function,

$$\theta(S) = \operatorname*{argmin}_{\theta} \mathcal{L}(\theta, S),$$

$$\mathcal{L}(\theta, S) = \frac{1}{N} \sum_{i=1}^{N} \|f_\theta(Y_i) - f(Y_i)\|^2_{\mathbb{R}^n} + \alpha \|\theta\|_1.$$

Definition of the optimal neural network

For a network f_θ with parameters θ, the expected loss is

$$\mathcal{L}(\theta, \mu) := \mathbb{E}_{Y \sim \mu} \left[\mathcal{L}(\theta, Y) \right].$$

The parameters θ^* of the optimal neural network $f_{\theta^*} : \mathbb{R}^{n \times n} \to \mathbb{R}^n$ are

$$\theta^* = \underset{\theta}{\text{argmin}}\ \mathcal{L}(\theta, \mu).$$

Neural network vs. analytic solution algorithm

Let $f_{\theta_0}(Y)$ be a deterministic approximation of an analytic solution algorithm (e.g. the analytic solution method for the inverse problem).

A trivial, but important result is that

$$\mathbb{E}_{Y\sim\mu}\left[\mathcal{L}(\theta^*, Y)\right] \leq \mathbb{E}_{Y\sim\mu}\left[\mathcal{L}(\theta_0, Y)\right].$$

This means that the optimal neural network $f_{\theta^*}(Y)$ has at least as good expected performance as $f_{\theta_0}(Y)$.

Approximation of the target function by a neural network

Definition

We say that the target function $f : \mathbb{R}^{n \times n} \to \mathbb{R}^n$ can be approximated with accuracy ε_0 by a neural network with a depth L and a sparsity bound R_0, if there is θ_0 such that

$$\|\theta_0\|_1 \leq R_0, \tag{1}$$

and the network f_{θ_0} satisfies

$$\sup_{\|Y\| \leq 1} \|f(Y) - f_{\theta_0}(Y)\|_{\mathbb{R}^n} \leq \varepsilon_0. \tag{2}$$

Stability results for the inverse problem for the 1-dimensional wave equation [Korpela-L.-Oksanen 2018], show that (1)-(2) are valid with $\varepsilon_0 > 0$, $L = C \log(1/\varepsilon_0)$, $n = C\varepsilon_0^{-175}$, and $R_0 = C\varepsilon_0^{-16}$.

How well a trained network works?

Next we estimate the expected performance gap between the trained neural network $f_{\theta(S)}$ and the optimal neural network f_{θ^*}, that is,

$$\mathcal{G}_{per}(S) = \left| \mathbb{E}_{Y \sim \mu} \mathcal{L}(\theta(S), Y) - \mathbb{E}_{Y \sim \mu} \mathcal{L}(\theta^*, Y) \right|$$

$\mathcal{G}_{per}(S)$ is the difference of the expected loss of $f_{\theta(S)}$ and f_{θ^*}.

Also, we estimate the expected generalization error that is the difference of the empirical loss function and the true loss function for the neural network $f_{\theta(S)}$,

$$\mathcal{G}_{gen}(S) = \left| \mathcal{L}(\theta(S), S) - \mathbb{E}_{Y \sim \mu} \mathcal{L}(\theta(S), Y) \right|.$$

$\mathcal{G}_{gen}(S)$ measures how well we can estimate the performance of $f_{\theta(S)}$ with a general input Y by using only the training data.

Theorem

Let $\alpha > 0$.
Let $S = \{(Y_1, f(Y_1)), \dots, (Y_N, f(Y_N))\}$ *be the training set that consists of* N *independent samples from the distribution* μ. *Then,*

$$\mathbb{P}_{S\sim\mu^N}\left[\mathcal{G}_{gen}(S) \leq \delta\right] \geq 1 - C_1 \left(\frac{1}{\delta}\right)^{C_2} \exp\left(-\frac{1}{50n^2\|f\|_\infty^4}\delta^2 \cdot N\right)$$

where

$$C_1 = \exp\left(8^{L+4} n^{\frac{3}{2}} (1 + \|f\|_\infty) \exp(5\|f\|_\infty^2 \alpha^{-1})\right),$$
$$C_2 = 8^{L+1} n \exp(4\|f\|_\infty^2 \alpha^{-1}),$$

Theorem

Suppose the target function f can be approximated with accuracy ε_0 by a neural network with the depth L and the sparsity bound R_0.
Let $\alpha \geq \varepsilon_0^2/R_0$.
Let $S = \{(Y_1, f(Y_1)), \dots, (Y_N, f(Y_N))\}$ be the training set that consists of N independent samples from the distribution μ. Then,

$$\mathbb{P}_{S\sim\mu^N}\left[\mathcal{G}_{gen}(S) \leq \delta\right] \geq 1 - C_1\left(\frac{1}{\delta}\right)^{C_2} \exp\left(-\frac{1}{50n^2\|f\|_\infty^4}\delta^2 \cdot N\right)$$

where

$$C_1 = \exp\left(8^{L+3} n^{\frac{3}{2}} (R_0 + L + \|f\|_\infty)\, e^{6R_0}\alpha^{-1/2}\right),$$
$$C_2 = 8^{L+1} n\, e^{6R_0}\alpha^{-1/2}.$$

Theorem

Suppose the target function f can be approximated with accuracy ε_0 by a neural network with the depth L and the sparsity bound R_0.
Let $\alpha \geq \varepsilon_0^2/R_0$.
Let $S = \{(Y_1, f(Y_1)), \dots, (Y_N, f(Y_N))\}$ be the training set that consists of N independent samples from the distribution μ. Then,

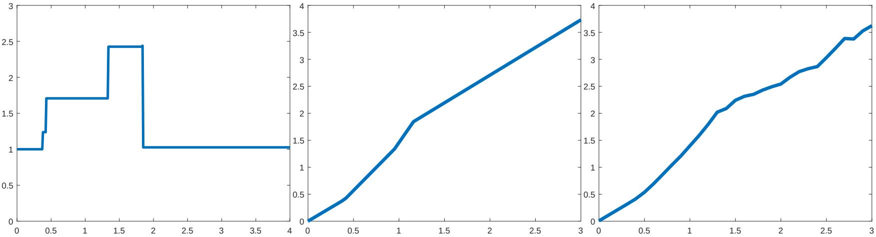
$$\mathbb{P}_{S\sim\mu^N}\left[\mathcal{G}_{per}(S) \leq 2\delta\right] \geq 1 - 2C_1\left(\frac{1}{\delta}\right)^{C_2} \exp\left(-\frac{1}{50n^2\|f\|_\infty^4}\delta^2 \cdot N\right)$$

where

$$C_1 = \exp\left(8^{L+3} n^{\frac{3}{2}} (R_0 + L + \|f\|_\infty)\, e^{6R_0}\alpha^{-1/2}\right),$$
$$C_2 = 8^{L+1} n\, e^{6R_0}\alpha^{-1/2}.$$

Learning travel depth in inverse problem for wave equation

Preliminary numerical tests on solving the inverse problem for a wave equation with a recurrent operator neural network (without sparsity):



(a) $c(x)$ (b) True depth (c) Predicted depth

Sample piecewise-constant wavespeed $c(x)$; True depth $\tau^{-1}(t)$ on how deep the waves propagate as a function of time t; Predicted depth as a function of time.

Numerical details: Training with piecewise-constant medium; 5000 data pairs, 20% withheld as testing data; Testing error: 6.3e-5; Networks with 16.5M parameters, sparsity regularization is not yet implemented.

Thank you for your attention!

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