On Hamilton-Jacobi partial differential equation and architectures of neural networks

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Context and motivation

- Consider the initial value problem

$$\begin{cases} \dfrac{\partial S}{\partial t}(x,t) + H(\nabla_x S(x,t), x, t) \;=\; \varepsilon \triangle S(x,t), & \text{in } \mathbb{R}^n \times (0,+\infty) \\ S(x,0) \;=\; J(x) & \forall x \in \mathbb{R}^n. \end{cases}$$

- Goals: compute the viscosity solution for a given $(x,t) \in \mathbb{R}^n \times [0,+\infty)$
  - evaluate $S(x,t)$ and $\nabla_x S(x,t)$
  - very high dimension
  - fast to allow applications requiring real-time computations
  - low memory and low energy for embedded system
- Pros and cons for computations with grid-based approaches:
  - many advanced and sophisticated numerical schemes (e.g., ENO, WENO, DG) with excellent theoretical properties
  - the number of grid-points is exponential in n

  $\rightarrow$ using numerical approximations is not doable for $n \geq 4$

Overcoming/mitigating the curse of dimensionality

- Several approaches to mitigate/overcome the curse of differentiability
  - Max-plus methods
    [Akian, Dower, McEneaney, Flening, Gaubert, Qu . . .]
  - Tensor decomposition methods
    [Doglov, Horowitz, Kalise, Kunisch, Todorov, . . .]
  - Sparse grids
    [Bokanovski, Garcke, Grieble, Kang, Klompmaker, Kröner, Wilcox]
  - Model order reduction
    [Alla, Kunisch, Falcone, Wolkwein, . . .]
  - Optimization techniques via representation formulas
    [D., Dower, Osher, Yegerov, . . .]
  - . . .
- More recently, there is a significant trend in using Machine Learning and Neural Network techniques for solving PDEs
  $\rightarrow$ A key idea is to leverage universal approximation theorems

Neural Network: a computational point of view

- Pros and cons of Neural Networks for evaluating solutions
  - It seems to be hard to find Neural Networks that are interpretable, generalizable which yield reproducible results
  - Huge computational advantage
    - dedicated hardware for NN is now available: e.g., Xilinx AI (FPGA + silicon design), Intel AI (FPGA + new CPU assembly instructions), and many other (startup) companies
    - high throughput / low latency (more precise meaning of "fast")
    - low energy requirement (e.g., a few Watts)

    $\rightarrow$ suitable for embedded computing and data centers
- Can we leverage these computational resources for high-dimensional H-J PDEs?
- How can we mathematically certify that Neural Networks (NNs) actually computes a viscosity solution of a H-J PDE?

$\Rightarrow$ Establish new connections between NN architectures and representation formulas of H-J PDE solutions

$\rightarrow$ the physics of some H-J PDEs can be encoded by NN architecture

$\rightarrow$ the parameters of the NN define Hamiltonians and initial data

$\rightarrow$ no approximation: exact evaluation of $S(x,t)$ and $\nabla_x S(x,t)$

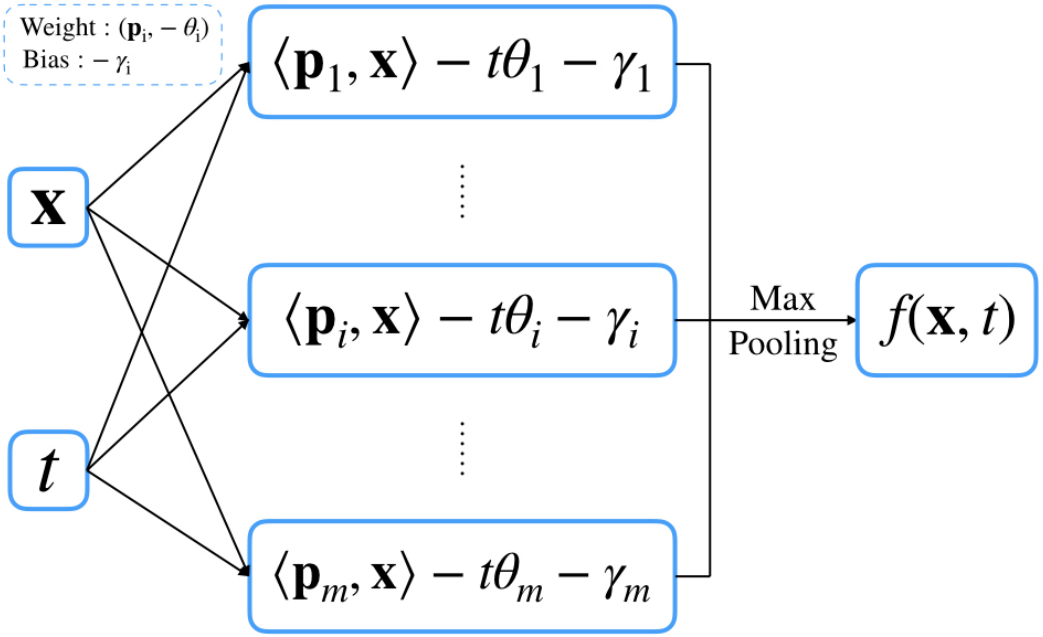
$\rightarrow$ suggests an interpretation of some NN architectures in terms of H-J PDEs

$\rightarrow$ does not rely on NN universal approximation theorems

Outline

1. Shallow NN architectures and representation of solution of H-J PDEs
    1. A class of first-order H-J
    2. Associated conservation law (1D)
    3. A class of second order H-J
2. Numerical experiments for solving some inverse problems involving H-J using data and learning/optimization algorithms
3. Suggestions of other NN architectures for other H-J PDEs
4. Some conclusions

A first shallow network architecture



- Architecture: fully connected layer followed by the activation function "max-pooling"
- This network defines a function $f : \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}$

$$f(\boldsymbol{x}, t; \{\boldsymbol{p}_i, \theta_i, \gamma_i\}_{i=1}^m) = \max_{i \in \{1,\dots,m\}} \{\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - t\theta_i - \gamma_i\}.$$

Goal: Find conditions on the parameters such that f satisfies a PDE, and find the PDE

Assumptions on the parameters

- Recall: the network $f(\boldsymbol{x}, t; \{\boldsymbol{p}_i, \theta_i, \gamma_i\}_{i=1}^m) = \max_{i\in\{1,\dots,m\}}\{\langle \boldsymbol{p}_i, \boldsymbol{x}\rangle - t\theta_i - \gamma_i\}$
- We adopt the following assumptions on the parameters:

  (A1) The parameters $\{\boldsymbol{p}_i\}_{i=1}^m$ are pairwise distinct, i.e., $\boldsymbol{p}_i \neq \boldsymbol{p}_j$ if $i \neq j$.
  (A2) There exists a convex function $g\colon\ \mathbb{R}^n \to \mathbb{R}$ such that $g(\boldsymbol{p}_i) = \gamma_i$.
  (A3) For any $j \in \{1, \dots, m\}$ and any $(\alpha_1, \dots, \alpha_m) \in \mathbb{R}^m$ that satisfy

$$\begin{cases} (\alpha_1, \dots, \alpha_m) \in \Delta_m \text{ with } \alpha_j = 0, \\ \sum_{i\neq j} \alpha_i \boldsymbol{p}_i = \boldsymbol{p}_j, \\ \sum_{i\neq j} \alpha_i \gamma_i = \gamma_j, \end{cases}$$

  there holds $\sum_{i\neq j} \alpha_i \theta_i > \theta_j$.

  where Δ_m denotes the unit simplex of dimension m

- ($A1$) and ($A3$) are NOT strong assumptions.
  - ($A1$) simplifies the mathematical analysis - ($A3$) simply states the each "neuron" should contribute to the definition of f.
  - If ($A3$) is not satisfied, then it means that some neurons can be removed and the NN still defines the same function f

Define initial data and Hamiltonians from parameters

- Recall: the network f

$$f(\boldsymbol{x}, t; \{\boldsymbol{p}_i, \theta_i, \gamma_i\}_{i=1}^m) = \max_{i \in \{1,\dots,m\}} \{\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - t\theta_i - \gamma_i\} \tag{1}$$

- Define the initial data J using the NN parameters $\{\boldsymbol{p}_i, \gamma_i\}_{i=1}^m$

$$f(\boldsymbol{x}, 0) = J(\boldsymbol{x}) := \max_{i \in \{1,\dots,m\}} \{\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - \gamma_i\} \tag{2}$$

  Then, $J : \mathbb{R}^n \to \mathbb{R}$ is convex, and its Legendre transform J^* reads

$$J^*(\boldsymbol{p}) = \begin{cases} \min_{\substack{(\alpha_1,\dots,\alpha_m) \in \Delta_m \\ \sum_{i=1}^m \alpha_i \boldsymbol{p}_i = \boldsymbol{p}}} \left\{\sum_{i=1}^m \alpha_i \gamma_i\right\}, & \text{if } \boldsymbol{p} \in \operatorname{conv}\left(\{\boldsymbol{p}_i\}_{i=1}^m\right), \\ +\infty, & \text{otherwise.} \end{cases}$$

  Denote by $\mathcal{A}(\boldsymbol{p})$ the set of minimizers in the above optimization problem.

- Define the Hamiltonian H: $\mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ by

$$H(\boldsymbol{p}) := \begin{cases} \inf_{\alpha \in \mathcal{A}(\boldsymbol{p})} \left\{\sum_{i=1}^m \alpha_i \theta_i\right\}, & \text{if } \boldsymbol{p} \in \operatorname{dom} J^*, \\ +\infty, & \text{otherwise.} \end{cases} \tag{3}$$

NN computes viscosity solutions

Theorem

Assume (A1)-(A3) hold. Let f be the neural network defined by Eq. (1) with parameters $\{(\boldsymbol{p}_i, \theta_i, \gamma_i)\}_{i=1}^m$. Let J and H be the functions defined in Eqs. (2) and (3), respectively, and let $\tilde{H}\colon\ \mathbb{R}^n \to \mathbb{R}$ be a continuous function. Then the following two statements hold.

(i) *The neural network f is the unique uniformly continuous viscosity solution to the Hamilton–Jacobi equation*

$$\begin{cases} \frac{\partial f}{\partial t}(\boldsymbol{x}, t) + H(\nabla_{\boldsymbol{x}} f(\boldsymbol{x}, t)) = 0, & \boldsymbol{x} \in \mathbb{R}^n, t > 0, \\ f(\boldsymbol{x}, 0) = J(\boldsymbol{x}), & \boldsymbol{x} \in \mathbb{R}^n. \end{cases} \tag{4}$$

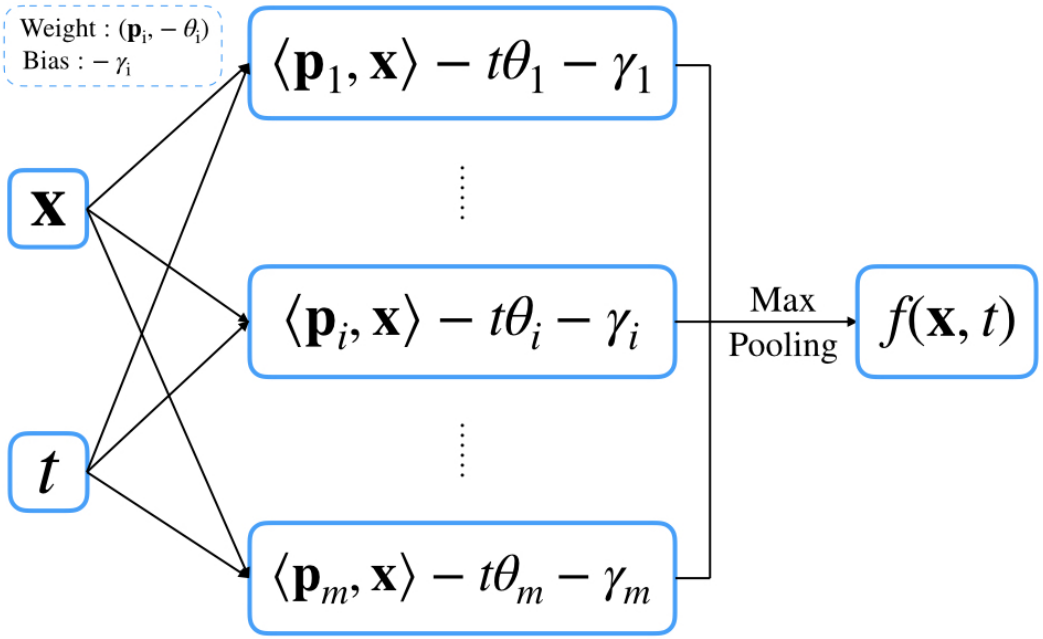
Moreover, f is jointly convex in ($\boldsymbol{x}$,t).

(ii) *The neural network f is the unique uniformly continuous viscosity solution to the Hamilton–Jacobi equation*

$$\begin{cases} \frac{\partial f}{\partial t}(\boldsymbol{x}, t) + \tilde{H}(\nabla_{\boldsymbol{x}} f(\boldsymbol{x}, t)) = 0, & \boldsymbol{x} \in \mathbb{R}^n, t > 0, \\ f(\boldsymbol{x}, 0) = J(\boldsymbol{x}), & \boldsymbol{x} \in \mathbb{R}^n. \end{cases} \tag{5}$$

if and only if $\tilde{H}(\boldsymbol{p}_i) = H(\boldsymbol{p}_i)$ for every $i = 1, \ldots, m$ and $\tilde{H}(\boldsymbol{p}) \geqslant H(\boldsymbol{p})$ for every $\boldsymbol{p} \in \operatorname{dom} J^*$.

NN computes viscosity solutions



- The network computes viscosity solution for H and J given by parameters
- Hamiltonians are not unique. However, among all possible Hamiltonians, H is the smallest one.
- In addition, $\nabla_x S(x, t)$ (when it exists) is given by the element that realizes the maximum is the "max-pooling"

NN computes viscosity solutions: An example

- Consider $J_{orig}(\boldsymbol{x}) = \|\boldsymbol{x}\|_\infty$ and $H_{orig}(\boldsymbol{p}) = -\frac{\|\boldsymbol{p}\|_2^2}{2}$ for every $\boldsymbol{x}, \boldsymbol{p} \in \mathbb{R}^n$.
- Denote by e_i the i^{th} standard unit vector in $\mathbb{R}^n$. Let $m = 2n$, $\{\boldsymbol{p}_i\}_{i=1}^m = \{\pm e_i\}_{i=1}^n$, $\theta_i = -\frac{n}{2}$, and $\gamma_i = 0$ for every $i \in \{1, \dots, m\}$.
- The viscosity solution S is given by

$$S(\boldsymbol{x}, t) = \|\boldsymbol{x}\|_\infty + \frac{nt}{2} = \max_{i \in \{1,\dots,m\}} \{\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - t\theta_i - \gamma_i\}, \text{ for every } \boldsymbol{x} \in \mathbb{R}^n \text{ and } t \geqslant 0.$$

- Hence, S can be represented using the proposed neural network with parameters $\{(\boldsymbol{p}_i, -\frac{n}{2}, 0)\}_{i=1}^m$.
- The parameters $\{(\boldsymbol{p}_i, -\frac{n}{2}, 0)\}_{i=1}^m$ define the following initial data and smallest Hamiltonian

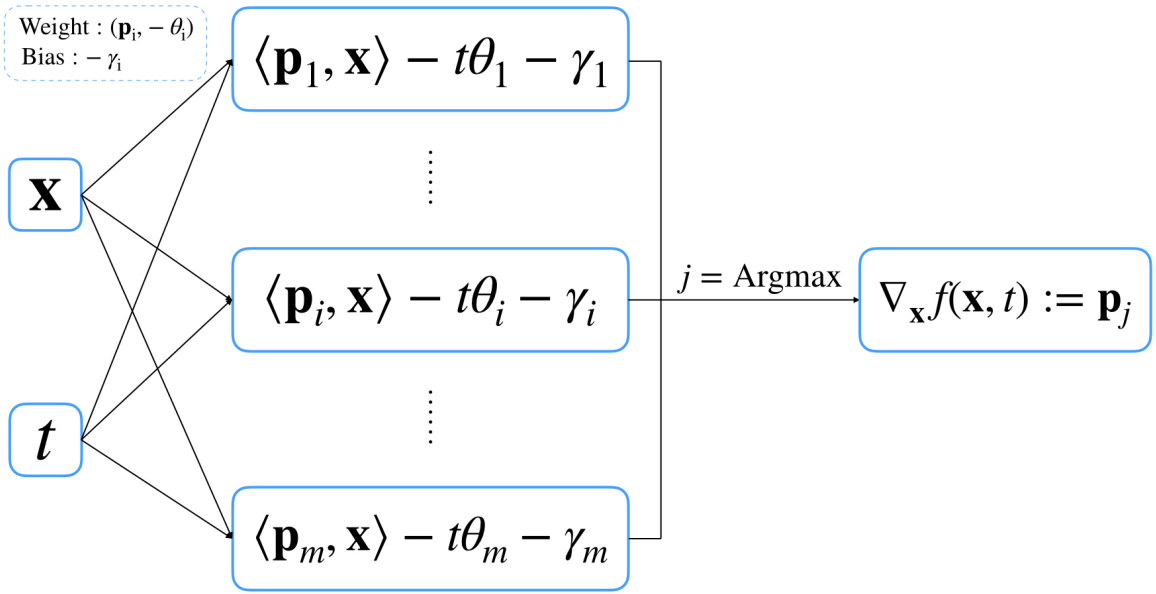
$$J(\boldsymbol{x}) = \|\boldsymbol{x}\|_\infty, \text{ for every } \boldsymbol{x} \in \mathbb{R}^n;$$

$$H(\boldsymbol{p}) = \begin{cases} -\frac{n}{2}, & \boldsymbol{p} \in B_n; \\ +\infty, & \text{otherwise}, \end{cases}$$

where B_n is the unit ball with respect to the l^1 norm in $\mathbb{R}^n$, i.e.,
$B_n = \operatorname{conv}\{\pm e_i : \ i \in \{1, \dots, n\}\}$

- By Thm. 1, S is a viscosity solution to the HJ PDE (5) if and only if $\tilde{H}(\boldsymbol{p}_i) = -\frac{n}{2}$ for every $i \in \{1, \dots, m\}$ and $\tilde{H}(\boldsymbol{p}) \geq -\frac{n}{2}$ for every $\boldsymbol{p} \in B_n \setminus \{\boldsymbol{p}_i\}_{i=1}^m$.
- Therefore, the Hamiltonian H_{orig} is one candidate satisfying these constraints.

Architecture for the gradient map



- This NN architecture computes the spatial gradient of the solution (i.e., the momentum)
- Consider $u : \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}^n$ defined by

$$u(x,t) = \nabla_x f(x,t) = p_j, \text{ where } j \in \underset{i \in \{1,\ldots,m\}}{\arg\max} \{\langle p_i, x \rangle - t\theta_i - \gamma_i\}. \quad (6)$$

NN architecture and 1D conservation laws

Theorem

Consider the one-dimensional case, i.e., $n = 1$. Suppose assumptions (A1)-(A3) hold. Let $u := \nabla_x f$ be the function from $\mathbb{R} \times [0, +\infty)$ to $\mathbb{R}$ defined in Eq. (6). Let J and H be the functions defined in Eqs. (2) and (3), respectively, and let $\tilde{H} \colon \mathbb{R} \to \mathbb{R}$ be a locally Lipschitz continuous function. Then the following two statements hold.

(i) *The neural network u is the entropy solution to the conservation law*

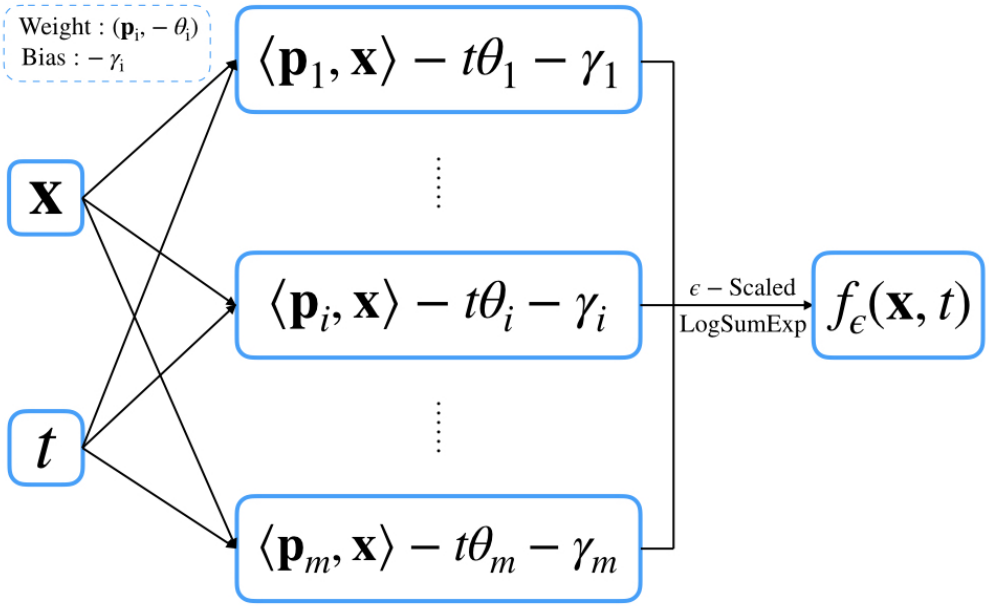
$$\begin{cases} \frac{\partial u}{\partial t}(x,t) + \nabla_x H(u(x,t)) = 0, & x \in \mathbb{R}, t > 0, \\ u(x,0) = \nabla J(x), & x \in \mathbb{R}. \end{cases} \tag{7}$$

(ii) *The neural network u is the entropy solution to the conservation law*

$$\begin{cases} \frac{\partial u}{\partial t}(x,t) + \nabla_x \tilde{H}(u(x,t)) = 0, & x \in \mathbb{R}, t > 0, \\ u(x,0) = \nabla J(x), & x \in \mathbb{R}, \end{cases} \tag{8}$$

if and only if there exists a constant $C \in \mathbb{R}$ such that $\tilde{H}(p_i) = H(p_i) + C$ for every $i \in \{1, \dots, m\}$ and $\tilde{H}(p) \geqslant H(p) + C$ for any $p \in \operatorname{conv} \{p_i\}_{i=1}^m$.

Another shallow architecture

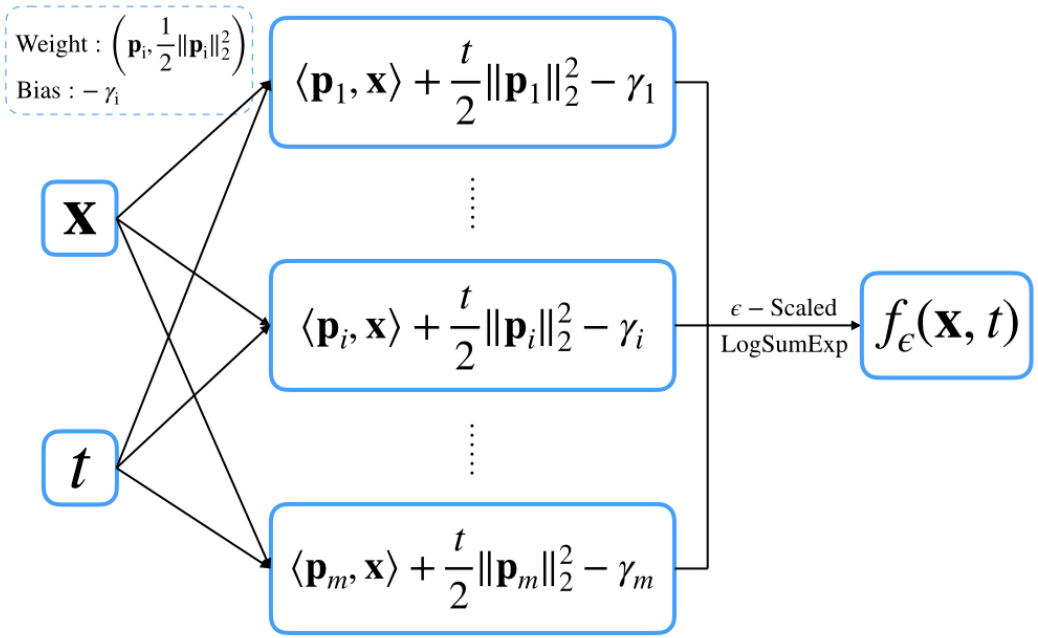


- Replace “max-pooling” by “smooth max pooling”.
- This network defines a function $f : \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}$

$$f_\epsilon(\boldsymbol{x}, t) := \epsilon \log \left(\sum_{i=1}^{m} e^{(\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - t\theta_i - \gamma_i)/\epsilon} \right).$$

Specialize this architecture

Specialize the parameters: $\theta_i = -\frac{1}{2}\|p_i\|_2^2 \quad$ for $i = 1, \ldots, m$



- This network defines the function $f : \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}$

$$f_\epsilon(\boldsymbol{x}, t) := \epsilon \log \left(\sum_{i=1}^{m} e^{\left(\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle + \frac{t}{2}\|\boldsymbol{p}_i\|_2^2 - \gamma_i \right)/\epsilon} \right). \tag{9}$$

NN computes viscosity solutions of some second order H-J PDEs

Theorem

Let f_ϵ defined by (9) with parameters $\{\boldsymbol{p}_i, \theta_i, \gamma_i\}_{i=1}^m$ and let $\theta_i = -\frac{1}{2}\|\boldsymbol{p}_i\|_2^2$ for $i \in \{1, \dots, m\}$. For every $\epsilon > 0$, the neural network $f_\epsilon \equiv \epsilon \log(w_\epsilon)$ is the unique smooth solution to the second-order Hamilton–Jacobi equation

$$\begin{cases} \frac{\partial f_\epsilon(\boldsymbol{x},t)}{\partial t} - \frac{1}{2}\|\nabla_{\boldsymbol{x}} f_\epsilon(\boldsymbol{x},t)\|_2^2 = \frac{\epsilon}{2}\triangle_{\boldsymbol{x}} f_\epsilon(\boldsymbol{x},t) & \text{in } \mathbb{R}^n \times (0,+\infty), \\ f_\epsilon(\boldsymbol{x},0) = \epsilon \log\left(\sum_{i=1}^m e^{(\langle \boldsymbol{p}_i, \boldsymbol{x}\rangle - \gamma_i)/\epsilon}\right) & \forall \boldsymbol{x} \in \mathbb{R}^n. \end{cases} \tag{10}$$

Moreover, f_ϵ is jointly convex in $(\boldsymbol{x}, t)$ and the following holds

$$\lim_{\substack{\epsilon \to 0 \\ \epsilon > 0}} f_\epsilon(\boldsymbol{x},t) = \max_{i \in \{1,\dots,m\}} \{\langle \boldsymbol{p}_i, \boldsymbol{x}\rangle + \frac{t}{2}\|\boldsymbol{p}_i\|_2^2 - \gamma_i\} \tag{11}$$

for every $\boldsymbol{x} \in \mathbb{R}^n$ and $t \geqslant 0$. Finally, if assumptions (A1)-(A3) hold, then the right hand side of (11) solves the first-order Hamilton–Jacobi equation (5) with $\tilde{H} := -\frac{1}{2}\|\cdot\|_2^2$.

Partial summary

- We have exhibited classes of network architecture that represent viscosity solution of some H-J PDEs
- Initial data and Hamiltonians are induced by the parameters of the network
  - Initial datum is completely determined by the parameters of the NN
  - Hamiltonians are not unique, but there exists a smallest Hamiltonian that is completely determined by the parameters of the NN.

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3. Suggestions of other NN architectures for other PDEs
4. Some conclusions

Trying to solve some simple inverse problems

- We are given data samples $\{(\boldsymbol{x}_j, t_j, S(\boldsymbol{x}_j, t_j))\}_{j=1}^N$, where $\{(\boldsymbol{x}_j, t_j)\}_{j=1}^N \subset \mathbb{R}^n \times [0, +\infty)$, we train the neural network f with structure linear + max-pooling using the mean square loss function defined by

$$I(\{(\boldsymbol{p}_i, \theta_i, \gamma_i)\}_{i=1}^m) = \frac{1}{N} \sum_{j=1}^{N} |f(\boldsymbol{x}_j, t_j; \{(\boldsymbol{p}_i, \theta_i, \gamma_i)\}_{i=1}^m) - S(\boldsymbol{x}_j, t_j)|^2.$$

- The training problem is formulated as

$$\underset{\{(\boldsymbol{p}_i, \theta_i, \gamma_i)\}_{i=1}^m \subset \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}}{\arg\min} I(\{(\boldsymbol{p}_i, \theta_i, \gamma_i)\}_{i=1}^m).$$

- After training, we approximate the initial condition in the HJ equation, denoted by $\tilde{J}$, by evaluating the trained neural network at $t = 0$, i.e., we approximate the initial condition by

$$\tilde{J} := f(\cdot, 0).$$

- We obtain partial information of the Hamiltonian H using the parameters in the trained neural network via the following procedure: (i) detect the effective neurons of the network, which we define to be the affine functions $\{\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - t\theta_i - \gamma_i\}$ that contribute to the pointwise maximum in the neural network f. Denote by L the set of indices that correspond to the parameters of the effective neurons, i.e.,

$$L := \bigcup_{\boldsymbol{x} \in \mathbb{R}^n,\, t \geq 0} \underset{i \in \{1, \ldots, m\}}{\arg\max} \{\langle \boldsymbol{p}_i, \boldsymbol{x} \rangle - t\theta_i - \gamma_i\},$$

  and we finally use each effective parameter $(\boldsymbol{p}_l, \theta_l)$ for $l \in L$ to approximate the point $(\boldsymbol{p}_l, H(\boldsymbol{p}_l))$ on the graph of the Hamiltonian.

Randomly piecewise affine Hamiltonian and Initial data

- We randomly select m parameters $\boldsymbol{p}_i^{true}$ in $[-1,1)^n$ for $i \in \{1,\dots,m\}$, and define θ_i^{true} and γ_i^{true} as follows

Case 1. $\theta_i^{true} = -\|\boldsymbol{p}_i^{true}\|_2$ and $\gamma_i^{true} = 0$, for $i \in \{1,\dots,m\}$.
Case 2. $\theta_i^{true} = -\|\boldsymbol{p}_i^{true}\|_2$ and $\gamma_i^{true} = \frac{1}{2}\|\boldsymbol{p}_i^{true}\|_2^2$, for $i \in \{1,\dots,m\}$.
Case 3. $\theta_i^{true} = -\frac{1}{2}\|\boldsymbol{p}_i^{true}\|_2^2$ and $\gamma_i^{true} = 0$, for $i \in \{1,\dots,m\}$.
Case 4. $\theta_i^{true} = -\frac{1}{2}\|\boldsymbol{p}_i^{true}\|_2^2$ and $\gamma_i^{true} = \frac{1}{2}\|\boldsymbol{p}_i^{true}\|_2^2$, for $i \in \{1,\dots,m\}$.

- Define the function S as

$$S(\boldsymbol{x},t) := \max_{i\in\{1,\dots,m\}} \{\langle \boldsymbol{p}_i^{true}, \boldsymbol{x}\rangle - t\theta_i^{true} - \gamma_i^{true}\}.$$

  By our Thm. this function S is a viscosity solution to the HJ equations whose Hamiltonian and initial function are the piecewise affine functions.

- We train the neural network f with training data $\{(\boldsymbol{x}_j, t_j, S(\boldsymbol{x}_j,t_j))\}_{j=1}^N$, where the points $\{(\boldsymbol{x}_j,t_j)\}_{j=1}^N$ are randomly sampled in $\mathbb{R}^n \times [0,+\infty)$ with respect to the standard normal distribution for each $j \in \{1,\dots,N\}$
  - The number of training data points is $N = 20{,}000$. We run 60,000 descent steps using the Adam optimizer to train the neural network f.
  - The parameters for the Adam algorithm are chosen to be $\beta_1 = 0.5$, $\beta_2 = 0.9$, the learning rate is 10^{-4} and the batch size is 500.

Measure of performance

- We compute the relative mean square errors of the sorted parameters in the trained neural network, denoted by $\{(\boldsymbol{p}_i, \theta_i, \gamma_i)\}_{i=1}^m$, and the sorted underlying true parameters $\{(\boldsymbol{p}_i^{true}, \theta_i^{true}, \gamma_i^{true})\}_{i=1}^m$. To be specific, the errors are computed as follows

$$\text{relative mean square error of } \{\boldsymbol{p}_i\} = \frac{\sum_{i=1}^m \|\boldsymbol{p}_i - \boldsymbol{p}_i^{true}\|_2^2}{\sum_{i=1}^m \|\boldsymbol{p}_i^{true}\|_2^2},$$

$$\text{relative mean square error of } \{\theta_i\} = \frac{\sum_{i=1}^m |\theta_i - \theta_i^{true}|^2}{\sum_{i=1}^m |\theta_i^{true}|^2},$$

$$\text{relative mean square error of } \{\gamma_i\} = \frac{\sum_{i=1}^m |\gamma_i - \gamma_i^{true}|^2}{\sum_{i=1}^m |\gamma_i^{true}|^2}.$$

- We test Cases 1–4 on the neural networks with 2 and 4 neurons, and repeat the experiments 100 times. We then compute the relative mean square errors in each experiments and take the average.
- Note that all relative errors should be 0 provided the optimizer is able to find a global minimizer.

Numerical results: 2 neurons

# Case		Case 1	Case 2	Case 3	Case 4
Averaged Relative Errors of $\{p_i\}$	2D	4.10E-03	2.10E-03	3.84E-03	2.82E-03
	4D	1.41E-09	1.20E-09	1.38E-09	1.29E-09
	8D	1.14E-09	1.03E-09	1.09E-09	1.20E-09
	16D	1.14E-09	6.68E-03	1.23E-09	7.74E-03
	32D	1.49E-09	3.73E-01	1.46E-03	4.00E-01
Averaged Relative Errors of $\{\theta_i\}$	2D	4.82E-02	7.31E-02	1.17E-01	1.79E-01
	4D	3.47E-10	2.82E-10	1.15E-09	1.15E-09
	8D	1.47E-10	1.08E-10	2.10E-10	2.25E-10
	16D	5.44E-11	1.69E-03	4.75E-11	4.12E-03
	32D	3.61E-11	3.27E-01	6.42E-03	2.39E-01
Averaged Relative Errors of $\{\gamma_i\}$	2D	1.35E-02	1.01E-01	1.33E-02	9.24E-02
	4D	3.71E-10	1.24E-09	3.67E-10	1.10E-09
	8D	2.91E-10	1.74E-10	2.82E-10	2.01E-10
	16D	2.80E-10	2.08E-04	3.10E-10	3.20E-04
	32D	3.56E-10	1.88E-02	1.56E-01	3.62E-02

Numerical results: 4 neurons

# Case		Case 1	Case 2	Case 3	Case 4
Averaged Relative Errors of $\{p_i\}$	2D	3.12E-01	2.21E-01	2.85E-01	2.14E-01
	4D	7.82E-02	6.12E-02	7.92E-02	4.30E-02
	8D	2.62E-02	4.31E-03	4.02E-02	7.82E-03
	16D	2.88E-02	3.64E-02	4.35E-02	1.73E-02
	32D	1.42E-02	3.72E-01	1.42E-01	5.04E-01
Averaged Relative Errors of $\{\theta_i\}$	2D	2.59E-01	3.68E-01	4.82E-01	1.34E+00
	4D	6.07E-02	8.37E-02	9.47E-02	1.23E-01
	8D	1.04E-02	8.48E-03	1.41E-02	1.31E-02
	16D	2.66E-03	2.53E-02	7.80E-03	1.90E-02
	32D	8.09E-04	4.41E-01	1.81E-02	3.66E-01
Averaged Relative Errors of $\{\gamma_i\}$	2D	1.01E-02	3.19E-01	1.51E-02	2.65E-01
	4D	6.72E-03	1.79E-02	1.03E-02	1.30E-02
	8D	3.22E-03	2.34E-03	3.93E-03	2.65E-03
	16D	9.48E-03	3.70E-03	1.92E-02	1.94E-03
	32D	1.33E-02	5.35E-02	4.73E-01	1.17E-01

Partial summary

- Off the shelf standard stochastic optimization optimizer used in machine learning may not yield “good minimizer” for these non-convex optimization problems
- Other numerical experiments have been conducted and yield the same mixed results.

Outline

1. Shallow NN architectures and representation of solution of H-J PDEs
    1. A class of first-order H-J
    2. Associated conservation law (1D)
    3. A class of second order H-J
2. Numerical experiments for solving some inverse problems involving H-J using data and learning/optimization algorithms
3. Suggestions of other NN architectures for other PDEs
4. Some conclusions

Possible extensions

Draw architectures based on Lax-Oleinik formulas on balckboard

Conclusion + ongoing work

- Some NN architectures represent viscosity solutions of certain H-J PDEs in very high-dimensions
- Hamiltonian and initial data are given by the parameters. Specifically,
  - Initial data completely determined by the NN parameters
  - Hamiltonians may not be unique, however, the smallest Hamiltonian is well defined and determined by the parameters.
- Preliminary results on solving some simple inverse problems involving these NN architecture do not yield satisfactory results.
  - Standard stochastic gradient algorithm may not be able to find a "good" minimizer

  $\rightarrow$ Use properties of HJ solutions to design taylored numerical optimization algorithms.
- We have obtained similar theorems for Lax-Oleinik-based formulas NN architecture

  $\rightarrow$ it paves the way to combine the NN architectures with Max-Plus methods
- Extension to optimal control of linear ODEs using a generalized Hopf-based formula
- FPGA implementation is underway