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

Jérôme Darbon

Division of Applied Mathematics, Brown University

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Context and motivation

- Consider the initial value problem

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

- Goals: compute the viscosity solution for a given (x, t)
  - evaluate $S(x, t)$ and $\nabla_x S(x, t)$
  - very high dimension, possibly $n \geq 10^6$
  - fast to allow applications requiring real-time
  - low memory and low energy for embedded system
- Several approaches to mitigate/overcome the curse of differentiability: e.g., Max-plus methods, tensor decomposition methods, sparse grids, optimization techniques via representation formulas, ...
- More recently, there is a significant trend in using Machine Learning and Neural Network techniques for solving PDEs
  $\rightarrow$ 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, generalization that yield reproducible results
  - Huge computational advantage
    - dedicated hardware for NN is now available: e.g., Xilinx AI (FPGA + silicon desing), 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 solution?

$\Rightarrow$ 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

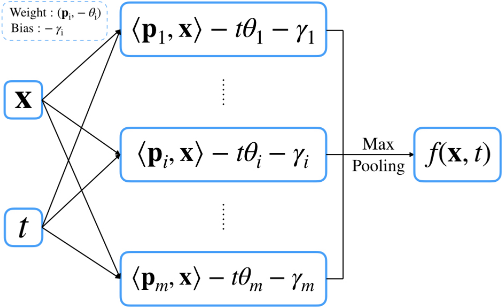
$\rightarrow$ no approximation: exact evaluation of $S(x,t)$ and $\nabla_x S(x,t)$

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

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. (Briefly) “Deep” NN architectures for other H-J PDEs
3. 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

Assumption 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.
  - (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 define 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

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

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

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

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

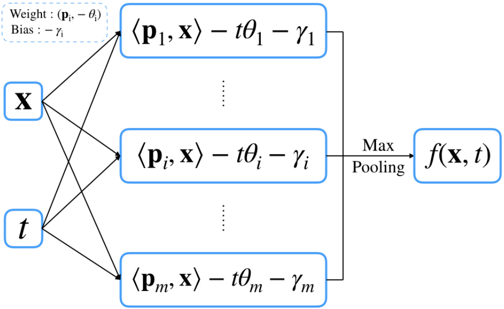
Moreover, f is jointly convex in $(\boldsymbol{x}, t)$.

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

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

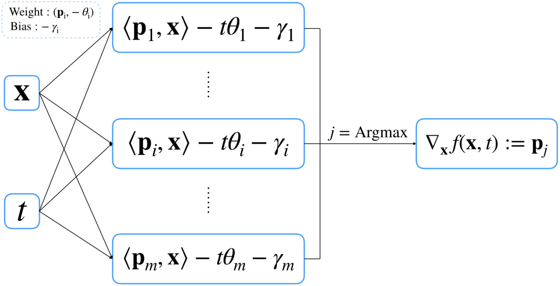
if and only if $\tilde{H}(\boldsymbol{p}_i) = H(\boldsymbol{p}_i)$ for every $i = 1, \ldots, m$ and $\tilde{H}(\boldsymbol{p}) \geqslant H(\boldsymbol{p})$ for every $\boldsymbol{p} \in \mathrm{dom}\, J^*$.

NN computes viscosity solutions



- The network the 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”

Architecture for that gradient map



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

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

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.

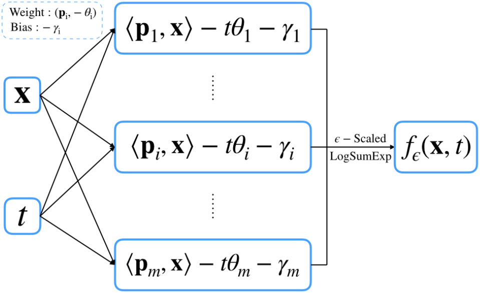
(i) *The neural network u is the entropy solution to the conservation law*

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

(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 $i \in \{1, \ldots, m\}$ and $\tilde{H}(p) \geqslant H(p) + C$ for any $p \in \operatorname{conv} \{p_i\}_{i=1}^m$.

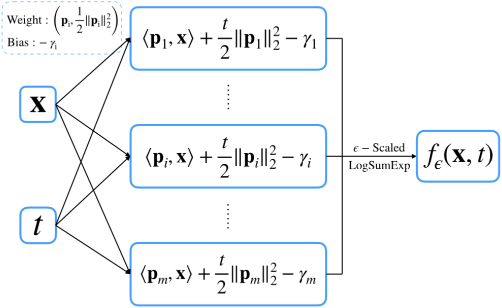


- Replace “max-pooling” by “smooth max pooling”.
- This network defines a function $f : \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}$

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

Specialize this architecture

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



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

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

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 $i \in \{1, \ldots, m\}$. 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 $(\boldsymbol{x}, t)$ the following holds

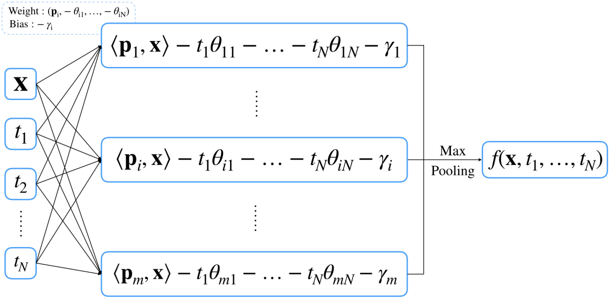
$$\lim_{\substack{\epsilon \to 0 \\ \epsilon > 0}} f_\epsilon(\boldsymbol{x}, t) = \max_{i \in \{1,\ldots,m\}} \{\langle \boldsymbol{p}_i, \boldsymbol{x}\rangle + \frac{t}{2}\|\boldsymbol{p}_i\|_2^2 - \gamma_i\} \tag{11}$$

holds 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 $\tilde{H} := -\frac{1}{2}\|\cdot\|_2^2$.

Summary and extension to other PDEss

- We have exhibited classes of network architecture that represents viscosity solution of some H-J PDEs
- Initial data and Hamiltonians are induced by the parameters of the network
- These architectures can be extended to cope with other PDEs
  We briefly present architectures and ideas for other PDEs
  - (similar) architectures to multi-time H-J PDEs
  - "Deep" ResNet-based architecture and method of characteristics

Extension to Multi-time H-J PDE

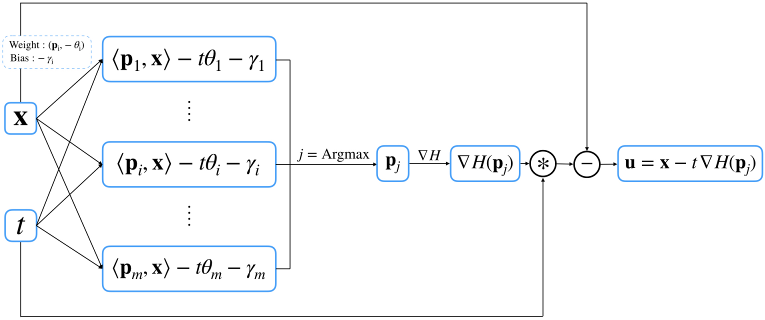


- The network defines a function $f : \mathbb{R}^n \times [0, +\infty)^N \to \mathbb{R}$ which satisfies the following multi-time H-J PDE

$$\begin{cases} \dfrac{\partial f}{\partial t_i}(x,t) + H_i(\nabla_x f(x,t)) = 0 & \text{for } i = 1, \ldots, N \\ f(x, 0, \ldots, 0) = J(x) & \text{for every } x \in \mathbb{R}^n \end{cases}$$

- Not necessarily a viscosity solution. It depends if the semi-groups associated to each time commute.

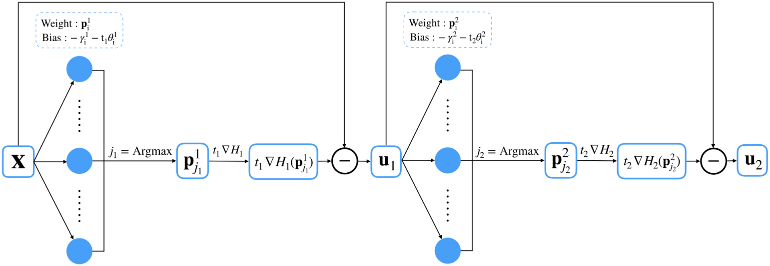
ResNet Variants, Generalized Moreau-Yosida identities and Lax-Oleinik formula



- Generalized Moreau identity (convex case): $x = u(x,t) + t\nabla H(p(x,t))$
  $\to$ p is a maximizer of the Hopf formula
  $\to$ u is a miminizer of the Lax-Oleinik formula
- The network defines the map $u : \mathbb{R}^n \times (0, +\infty) \to \mathbb{R}^n$
- Therefore all information for the characteristics

A Deep NN architecture

- We can fixed a sequence of time t_i and Hamiltonian H_i and iterates the previous map. This gives the following “deep” ResNet-based NN (2 layers)



- So we have $x - t_1\nabla H(p_1) - t_2\nabla H(p_2) = u_2(x,t)$
- Under appropriate assumptions these architectures compute the characteristics and can be used for solving some H-J PDE with certain Hamiltonian with state and time dependence.

Conclusion

- Some NN architectures represent viscosity solutions of certain H-J PDEs in very high-dimensions
- Hamiltonian and initial data are given by the parameters
- "Chaining" these architectures + ResNet pave the way to cope with more general Hamiltonians
- We also used these NN architectures for "solving" some inverse problems involving H-J PDEs (not presented here)
  $\rightarrow$ "learning" corresponds to solving non-convex optimization problem
  $\rightarrow$ Implementation using TensorFlow
  $\rightarrow$ Numerical results show that "standard" optimization methods (e.g., ADAM) can provide excellent or terrible results