ON SOME NEURAL NETWORK ARCHITECTURES THAT CAN REPRESENT VISCOSITY SOLUTIONS OF CERTAIN HIGH DIMENSIONAL HAMILTON–JACOBI PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. We propose novel connections between several neural network architectures and viscosity solutions of some Hamilton–Jacobi (HJ) partial differential equations (PDEs) whose Hamiltonian is convex and only depends on the spatial gradient of the solution. To be specific, we prove that under certain assumptions, the two neural network architectures we proposed represent viscosity solutions to two sets of HJ PDEs with zero error. We also implement our proposed neural network architectures using Tensorflow and provide several examples and illustrations. Note that these neural network representations can avoid curve of dimensionality for certain HJ PDEs, since they do not involve neither grids nor discretization. Our results suggest that efficient dedicated hardware implementation for neural networks can be leveraged to evaluate viscosity solutions of certain HJ PDEs.

1. Introduction

Hamilton–Jacobi (HJ) partial differential equations (PDEs) arise in areas such as physics [5, 19, 20, 25, 75], optimal control [8, 37, 45, 46, 81], game theory [11, 18, 39, 61], and imaging sciences [27, 29, 30]. In this paper, we consider HJ PDEs with state and time independent Hamiltonian function $H: \mathbb{R}^n \to \mathbb{R}$ and initial data $J: \mathbb{R}^n \to \mathbb{R}$ that read as follows

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

The partial derivative with respect to $t$ and the gradient vector with respect to $x$ of the solution $(x, t) \mapsto S(x, t)$ are denoted by $\frac{\partial S(x, t)}{\partial t}$ and $\nabla_x S(x, t) = \left(\frac{\partial S}{\partial x_1}(x, t), \ldots, \frac{\partial S}{\partial x_n}(x, t)\right)$, respectively. Note that the Hamiltonian $H$ only depends on $\nabla_x S(x, t)$.

Recently, [28] establishes novel connections between some neural network architectures and the viscosity solution of a set of HJ PDEs in the form of (1). (We refer readers to [8, 9, 10, 26] for the definition of the viscosity solution.) In [28], the authors provided the conditions under which their proposed neural network architecture represents the viscosity solution to the corresponding HJ PDEs whose initial data $J$ and Hamiltonian $H$ are related to the parameters in the neural network. Note that in the HJ PDEs they considered, the initial data $J$ is assumed to be a convex piecewise affine function, and the Hamiltonian $H$ also satisfies certain assumptions.

In this paper, we consider the HJ PDEs in the form of (1) satisfying other assumptions. For instance, the Hamiltonian $H$ is convex, while the initial data $J$ is not necessarily convex. Under these assumptions, we prove that the two neural network architectures depicted in Figs. 1 and 2 represent viscosity solutions to the corresponding HJ PDEs in the form of (1), with initial data $J$ and convex Hamiltonian $H$. To be specific, in the first architecture shown in Fig. 1, the convex activation function $L$ in the neural network gives the Lagrangian function, whose Fenchel–Legendre transform gives the Hamiltonian $H$ in the corresponding HJ PDE. The initial data equals the minimum of several functions which are shifted copies of the asymptotic function $L'_\infty$ of $L$. The main result of this connection between the neural network architecture depicted in Fig. 1 and the corresponding HJ PDE is stated in Thm. 3.1. In the second architecture shown in Fig. 2 the activation function gives the initial data $J$ in the HJ PDE. The Hamiltonian $H$ is a piecewise affine convex function determined by the parameters in the neural network. The main result of this connection between the neural network architecture depicted in Fig. 2 and the corresponding HJ PDE is stated in Thm. 3.2.

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To summarize, this paper investigates the connection between several neural network architectures and some specific sets of HJ PDEs. The motivations and advantages of this work are listed as follows:

- Compared with traditional grid based representations, our proposed neural network representations do not involve any discretization of space and time. Hence these neural network representations can avoid the curse of dimensionality for certain HJ PDEs if the correct parameters are provided.
- Our novel connections between certain HJ PDEs and neural networks suggest a possible direction to solve some HJ PDEs by leveraging efficient hardware technologies and silicon-based electric circuits dedicated to neural networks. LeCun mentioned in [76] that the use of neural networks has been greatly influenced by available hardware. There have been many initiatives designing and constructing new hardware for extremely efficient (in terms of speed, latency, throughput or energy) implementations of neural networks. For instance, efficient neural network implementations are developed and optimized using field programmable gate arrays [40, 41, 42], Intel’s architecture [7], Google’s “Tensor Processor Unit” [64], and certain building blocks [70]. To obtain better performance on neural network computation, Xilinx announced a new set of hardware called Versal AI core, while Intel enhances their processors with specific hardware instructions. In addition, there is an evolution of silicon-based electrical circuits for machine learning, for which we refer readers to [28, 55]. LeCun also suggests in [76, Sec. 3] possible new trends for hardware dedicated to neural networks. These trends for efficient neural network implementations motivate our study of the connections between neural network architectures and HJ PDEs.
- This work provides a possible interpretation of specific neural networks from the aspect of HJ PDEs.

Literature review. There is a huge body of literature on overcoming the curse of dimensionality of certain HJ PDEs. These works include, but are not limited to, max-plus algebra methods [81, 4, 35, 44, 49, 52, 83, 84], dynamic programming and reinforcement learning [8, 16], tensor decomposition techniques [34, 57, 104], sparse grids [17, 18, 67], model order reduction [4, 71], polynomial approximation [55, 60], optimization methods [27, 29, 30, 111] and neural networks [28, 6, 32, 51, 59, 60, 74, 89, 97, 99, 101].

Recently, because of the trends for the efficient hardware implementations, neural networks have been increasingly applied in solving PDEs [6, 32, 51, 59, 60, 74, 89, 97, 99, 101, 13, 12, 14, 15, 22, 24, 31, 33, 36, 43, 47, 50, 52, 55, 63, 68, 69, 72, 73, 77, 80, 85, 86, 104, 106, 107, 108, 109, 110] and inverse problems involving PDEs [101, 79, 78, 87, 88, 90, 92, 93, 94, 105, 112, 113]. Specifically, some high-dimensional HJ PDEs have been numerically solved using neural networks [28, 51, 60, 101]. In [101], the solution to HJ PDEs is approximated by a deep neural network whose loss function is the \( l^2 \) error of the PDE, the initial condition and the boundary condition on randomly sampled points in the domain. In [51], a neural network architecture is proposed to approximate a backward stochastic differential equation which computes the solution to a second order HJ PDE via an associated stochastic representation formula. In [60], Huré et al. approximate the solution and its gradient using two neural networks at each discretized time step. After the neural networks at a larger time \( t_{j+1} \) are trained, the neural networks at \( t_j \) are trained with loss function given by the error of the stochastic representation formula. In [28], a neural network architecture is proposed for representing the viscosity solution to certain high dimensional HJ PDEs without error. In addition, Cárdenas and Gibou [21] use neural networks to compute the mean curvature of the implicit level set function, which is the solution to a specific HJ PDE called level set equation.

Organization of this paper. This paper investigates the connections between two neural network architectures shown in Figs. 1 and 2 and the viscosity solution of some HJ PDEs whose initial data and Hamiltonian satisfy specific assumptions. In Sec. 2 we introduce basic concepts in finite dimensional convex analysis which will be used later in this paper. In Sec. 3 we present the main results. To be specific, we propose two neural network architectures. The first architecture is analyzed in Sec. 3.1, while the second one is analyzed in Sec. 3.2. Thms. 3.1 and 3.2 state that the neural network architectures shown in Figs. 1 and 2 represent viscosity solutions to the HJ PDEs with convex Hamiltonian \( H \) and initial data \( J \) satisfying certain assumptions. We provide several examples and illustrations after each theorem. Finally, a conclusion is drawn in Sec. 4.
2. Background

In this section, we introduce related concepts in convex analysis that will be used in this paper. We refer readers to Hiriart-Urruty and Lemaréchal \cite{53, 54} and Rockafellar \cite{98} for comprehensive references on finite-dimensional convex analysis. For the notation, we use $\mathbb{R}^n$ to denote the $n$-dimensional Euclidean space, on which the Euclidean scalar product is denoted by $\langle \cdot, \cdot \rangle$.

**Definition 1.** (Convex sets and the unit simplex) A set $C \subseteq \mathbb{R}^n$ is called convex if for any $\lambda \in [0, 1]$ and any $x, y \in C$, the element $\lambda x + (1 - \lambda)y$ is in $C$. The unit simplex is a specific convex set in $\mathbb{R}^n$, denoted by $\Lambda_n$, defined by

$$\Lambda_n := \left\{ (\alpha_1, \ldots, \alpha_n) \in [0, 1]^n : \sum_{i=1}^n \alpha_i = 1 \right\}.$$

**Definition 2.** (Domains and proper functions) The domain of a function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is the set $\text{dom } f = \{ x \in \mathbb{R}^n : f(x) < +\infty \}$.

A function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is called proper if its domain is non-empty.

**Definition 3.** (Convex functions, concave functions and lower semicontinuity) A proper function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is called convex if the set $\text{dom } f$ is convex and if for any $x, y \in \text{dom } f$ and all $\lambda \in [0, 1]$, there holds

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y).$$

A function $f : \mathbb{R}^n \to \mathbb{R} \cup \{-\infty\}$ is called concave if $-f$ is a convex function. A proper function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is called lower semicontinuous if for every sequence $(x_k)_{k=1}^{+\infty}$ in $\mathbb{R}^n$ with $\lim_{k \to +\infty} x_k = x \in \mathbb{R}^n$, we have $\lim \inf_{k \to +\infty} f(x_k) \geq f(x)$. The class of proper, lower semicontinuous convex functions is denoted by $\Gamma_0(\mathbb{R}^n)$.

**Definition 4.** (Fenchel–Legendre transform) Let $f \in \Gamma_0(\mathbb{R}^n)$. The Fenchel–Legendre transform $f^* : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ of $f$ is defined as

$$f^*(p) = \sup_{x \in \mathbb{R}^n} \{ \langle p, x \rangle - f(x) \}.$$

For any $f \in \Gamma_0(\mathbb{R}^n)$, the mapping $f \mapsto f^*$ is one-to-one. Moreover, there hold $f^* \in \Gamma_0(\mathbb{R}^n)$ and $(f^*)^* = f$.

**Definition 5.** (Inf-convolution) Let $f, g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be two proper convex functions satisfying

$$f(x) \geq \langle p, x \rangle + a \quad \text{and} \quad g(x) \geq \langle p, x \rangle + a \quad \text{for every } x \in \mathbb{R}^n,$$

for some $p \in \mathbb{R}^n$ and $a \in \mathbb{R}$. The inf-convolution of $f$ and $g$, denoted by $f \boxplus g$, is defined by

$$f \boxplus g(x) = \inf_{u \in \mathbb{R}^n} \{ f(u) + g(x - u) \}.$$

Moreover, the function $f \boxplus g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a proper and convex function \cite[Prop. IV.2.3.2]{53}.

**Definition 6.** (Asymptotic function) Let $f$ be a function in $\Gamma_0(\mathbb{R}^n)$ and $x_0$ be an arbitrary point in $\text{dom } f$. The asymptotic function of $f$, denoted by $f_{\infty}$, is defined by

$$f_{\infty}'(d) = \sup_{s \geq 0} \frac{f(x_0 + sd) - f(x_0)}{s} = \lim_{s \to +\infty} \frac{f(x_0 + sd) - f(x_0)}{s},$$

for every $d \in \mathbb{R}^n$. In fact, this definition does not depend on the point $x_0$. Moreover, the asymptotic function $f_{\infty}'$ is convex and positive 1-homogeneous, i.e., $f_{\infty}'(\alpha d) = \alpha f_{\infty}'(d)$ for every $\alpha > 0$ and $d \in \mathbb{R}^n$. For details, see \cite[Chap. IV.3.2]{53}.

We summarize some notations and definitions in Tab. [1]
Table 1. Notations used in this paper. Here, we use \( f, g \) to denote functions from \( \mathbb{R}^n \) to \( \mathbb{R} \cup \{+\infty\} \) and \( x, y, p, d \) to denote vectors in \( \mathbb{R}^n \). For simplicity, we omit the assumptions in the definitions.

| Notation | Meaning | Definition |
|----------|---------|------------|
| \( \langle \cdot, \cdot \rangle \) | Euclidean scalar product in \( \mathbb{R}^n \) | \( \langle x, y \rangle := \sum_{i=1}^{n} x_i y_i \) |
| \( \Lambda_n \) | The unit simplex in \( \mathbb{R}^n \) | \( \{(\alpha_1, \ldots, \alpha_n) \in [0,1]^n : \sum_{i=1}^{n} \alpha_i = 1\} \) |
| \( \text{dom } f \) | The domain of \( f \) | \( \{x \in \mathbb{R}^n : f(x) < +\infty\} \) |
| \( \Gamma_0(\mathbb{R}^n) \) | A useful and standard class of convex functions | The set containing all proper, convex, lower semi-continuous functions from \( \mathbb{R}^n \) to \( \mathbb{R} \cup \{+\infty\} \) |
| \( f^* \) | Fenchel–Legendre transform of \( f \) | \( f^*(p) := \sup_{x \in \mathbb{R}^n} \{\langle p, x \rangle - f(x)\} \) |
| \( f \Box g \) | Inf-convolution of \( f \) and \( g \) | \( f \Box g(x) = \inf_{u \in \mathbb{R}^n} \{f(u) + g(x - u)\} \) |
| \( f'_\infty \) | The asymptotic function of \( f \) | \( f'_\infty(d) = \sup_{s > 0} \left\{ \frac{1}{s}(f(x_0 + sd) - f(x_0)) \right\} \) |

### 3. Main Results

In this paper, we consider the HJ PDE given by

\[
\begin{align*}
\frac{\partial S}{\partial t}(x, t) + H(\nabla_x S(x, t)) &= 0 \quad \text{in } \mathbb{R}^n \times (0, +\infty), \\
S(x, 0) &= J(x) \quad \text{in } \mathbb{R}^n,
\end{align*}
\]

where \( H: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\} \) is called Hamiltonian, and \( J: \mathbb{R}^n \to \mathbb{R} \) is the initial data. It is well-known that when \( H \) is convex, the viscosity solution is given by the Lax-Oleinik formula \cite{agarwal2005direct, krylov2008second, momen2005algorithms} stated as follows

\[
S_{LO}(x, t) = \inf_{u \in \mathbb{R}^n} \left\{ J(u) + tH^*(\frac{x - u}{t}) \right\} = \inf_{v \in \mathbb{R}^n} \left\{ J(x - tv) + tH^*(v) \right\},
\]

where \( H^* \) is the Fenchel–Legendre transform of \( H \).

In this paper, we represent the Lax-Oleinik formula using two neural network architectures. The first one is given by

\[
f_1(x, t) = \min_{i \in \{1, \ldots, m\}} \left\{ tl \left( \frac{x - u_i}{t} \right) + a_i \right\}.
\]

In this function, \( \{(u_i, a_i)\}_{i=1}^{m} \subset \mathbb{R}^n \times \mathbb{R} \) is the set of parameters, and the function \( L: \mathbb{R}^n \to \mathbb{R} \) is the activation function, which corresponds to the Lagrangian function in the Hamilton–Jacobi theory. An illustration is shown in Fig. 1.

The second neural network architecture is defined by

\[
f_2(x, t) = \min_{i \in \{1, \ldots, m\}} \left\{ \hat{J}(x - tv_i) + tb_i \right\}.
\]

Here, \( \{(v_i, b_i)\}_{i=1}^{m} \subset \mathbb{R}^n \times \mathbb{R} \) is the set of parameters, and \( \hat{J}: \mathbb{R}^n \to \mathbb{R} \) is the activation function, which corresponds to the initial function in the HJ PDE. An illustration is shown in Fig. 2.

#### 3.1. The first architecture

In this subsection, we analyze the first neural network architecture given by Eq. (7). Before introducing the main theorem \ref{mainThm} in this subsection, we prove the following lemma which will be used in the proof of Thm. \ref{mainThm}.

**Lemma 3.1.** Let \( f \) be a function in \( \Gamma_0(\mathbb{R}^n) \) and \( f'_\infty \) be the asymptotic function of \( f \). Then, we have \( f \Box f'_\infty = f \).

**Proof.** First we consider the case when \( x \in \text{dom } f \). By definition \ref{def:asymptotic} we have

\[
(f \Box f'_\infty)(x) = \inf_{u \in \mathbb{R}^n} \{f(u) + f'_\infty(x - u)\} \leq f(x) + f'_\infty(0) = f(x),
\]

where the last equality holds because \( f'_\infty(0) = 0 \) by definition \ref{def:asymptotic}. On the other hand, taking \( s = 1, d = x - u \) and \( x_0 = u \) in the second term in Eq. \ref{eq:asymptotic} in definition \ref{def:asymptotic} we obtain

\[
f'_\infty(x - u) \geq f(u + x - u) - f(u) = f(x) - f(u),
\]
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Figure 1. An illustration of the architecture of the neural network (7) that represents the Lax-Oleinik formula with specific initial condition $J = f_1(\cdot, 0)$ defined in (10) and the convex Hamiltonian $H = L^*$. 

For every $u \in \text{dom } f$. As a result, we have 

$$(f \circ f_\infty')(x) = \inf_{u \in \text{dom } f} \{f(u) + f_\infty'(x - u)\} \geq \inf_{u \in \text{dom } f} \{f(u) + f(x) - f(u)\} = f(x).$$

Therefore, we conclude that $(f \circ f_\infty')(x) = f(x)$ for every $x \in \text{dom } f$.

Now, we consider the case when $x \notin \text{dom } f$ and prove $(f \circ f_\infty')(x) = +\infty$. It suffices to prove $f_\infty'(x - u) = +\infty$ for all $u \in \text{dom } f$. Since $u \in \text{dom } f$, Eq. (9) still holds. As a result, we have

$$f_\infty'(x - u) \geq f(x) - f(u) = +\infty,$$

since $x \notin \text{dom } f$ and $u \in \text{dom } f$. Therefore, we conclude that $(f \circ f_\infty')(x) = +\infty = f(x)$ for every $x \notin \text{dom } f$. $\square$

Now, we define the initial data $f_1(\cdot, 0) : \mathbb{R}^n \to \mathbb{R}$ as follows

$$(10) 
\quad f_1(x, 0) = \min_{i \in \{1, \ldots, m\}} \{L_\infty'(x - u_i) + a_i\},$$

where $L_\infty'$ is the asymptotic function of $L$. Then, we present the main theorem stating that the function $f_1$ solves the HJ PDE (5) with the initial condition given by $J = f_1(\cdot, 0)$ defined in (10) and the convex Hamiltonian $H$ which is the Fenchel–Legendre transform of $L$.

**Theorem 3.1.** Let $L : \mathbb{R}^n \to \mathbb{R}$ be a convex uniformly Lipschitz function. Let $f_1$ be the function defined in (7). Then $f_1 = S_{LO}$, where $S_{LO}$ is the Lax–Oleinik formula in (6) with the initial condition $J = f_1(\cdot, 0)$ defined in (10) and the convex Hamiltonian defined by $H = L^*$. Therefore, $f_1$ is a viscosity solution to the corresponding HJ PDE (5).

**Remark 3.1.** In the theorem above, we assume $L$ to be a convex uniform Lipschitz function, which implies that its Fenchel–Legendre transform $H$ has bounded domain, and hence $H$ may take the value $+\infty$ somewhere. As a result, the uniqueness theorem of the viscosity solution in [28, Chap. 10.2] does not hold. To our knowledge, we are not aware of any uniqueness result of the viscosity solution to the HJ PDEs where $\text{dom } H$ is bounded.
Figure 2. An illustration of the architecture of the neural network \[8\] that represents the Lax-Oleinik formula with specific initial condition \( J = \tilde{J} \) and the convex Hamiltonian \( H \) defined in \[12\].

Proof. Since \( L \) is Lipschitz continuous, by [53, Prop. IV.3.2.7] \( L'_\infty \) is finite valued, which implies that \( \mathbb{R}^n \ni x \mapsto f_1(x,0) \) is finite valued and it is a valid initial condition.

Let \( x \in \mathbb{R}^n \) and \( t > 0 \). By definition \[5\] and \[10\], we have

\[
S_{LO}(x,t) = \inf_{u \in \mathbb{R}^n} \left\{ J(u) + th^*(\frac{x-u}{t}) \right\} = \inf_{u \in \mathbb{R}^n} \left\{ \min_{i \in \{1,\ldots,m\}} \{L'_\infty(u-u_i) + a_i\} + th^*\left(\frac{x-u}{t}\right)\right\}
\]

\[
= \min_{i \in \{1,\ldots,m\}} \left\{ a_i + \inf_{u \in \mathbb{R}^n} \left\{ L'_\infty(u-u_i) + th^*\left(\frac{x-u}{t}\right)\right\} \right\}
\]

\[
= \min_{i \in \{1,\ldots,m\}} \left\{ a_i + \left(L'_\infty \triangledown tH^*\left(\frac{\cdot}{t}\right)\right)(x-u_i)\right\}.
\]

Since \( L \) is convex with dom \( L = \mathbb{R}^n \), then the function \( L \) is continuous [53, Thm. IV.3.1.2]. As a result, \( L \) is a function in \( \Gamma_0(\mathbb{R}^n) \), hence we have \( L = (L^*)^* \), which equals \( H^* \) because we assume \( H = L^* \). Let \( t > 0 \) and \( h : \mathbb{R}^n \to \mathbb{R} \) be defined by \( h(x) = th^*\left(\frac{\cdot}{t}\right) = tL\left(\frac{\cdot}{t}\right) \) for every \( x \in \mathbb{R}^n \). Let \( x_0 \) be an arbitrary point in dom \( h \), which implies \( \frac{\cdot}{t} \in \text{dom } L \). By definition \[6\] the asymptotic function of \( h \) evaluated at \( d \) is given by

\[
h'_\infty(d) = \sup_{s>0} \left\{ \frac{1}{s} \left( sL\left(\frac{x_0+sd}{t}\right) - tL\left(\frac{x_0}{t}\right) \right) \right\} = \sup_{s>0} \left\{ \frac{t}{s} \left( L\left(\frac{x_0}{t} + \frac{s}{t}d\right) - L\left(\frac{x_0}{t}\right) \right) \right\}
\]

\[
= \sup_{\tau>0} \left\{ \frac{1}{\tau} \left( L\left(\frac{x_0}{t} + \tau d\right) - L\left(\frac{x_0}{t}\right) \right) \right\} = L'_\infty(d),
\]

where in the third equality we set \( \tau = \frac{t}{s} \). Hence, using the equality above, the definition of \( h \) and by invoking Lem. \[3.1\] we obtain

\[
\left(L'_\infty \triangledown tH^*\left(\frac{\cdot}{t}\right)\right)(x-u_i) = (h'_\infty \triangledown h)(x-u_i) = h(x-u_i) = tL\left(\frac{x-u_i}{t}\right).
\]
We combine the equality above with (11), to obtain
\[
S_{LO}(x, t) = \min_{i \in \{1, \ldots, m\}} \left\{ a_i + \left( L'_{\infty} \square_{\t} H^* \left( \frac{\cdot}{t} \right) \right)(x - u_i) \right\} = \min_{i \in \{1, \ldots, m\}} \left\{ a_i + tL \left( \frac{x - u_i}{t} \right) \right\} = f_1(x, t).
\]
Therefore, we conclude that \( S_{LO}(x, t) = f_1(x, t) \) for each \( x \in \mathbb{R}^n \) and \( t > 0 \). Then, using the same proof as in [38, Sec. 10.3.4, Thm. 3], we conclude that \( f_1 \) is a viscosity solution to the corresponding HJ PDE (5). □

**Example 3.1.** Let us consider the following one dimensional example that illustrates the function \( f_1: \mathbb{R} \times [0, +\infty) \rightarrow \mathbb{R} \) with three neurons, i.e., we set \( n = 1 \) and \( m = 3 \). The Lagrangian \( L \) is defined as follows
\[
L(x) = \begin{cases} 
-x - \frac{1}{2} & x < -1, \\
\frac{x^2}{2} & -1 \leq x \leq 2, \\
2x - 2 & x > 2,
\end{cases}
\]
for each \( x \in \mathbb{R} \). Then, by Thm. 3.1, the Hamiltonian \( H \) is given by
\[
H(p) = L^*(p) = \begin{cases} 
\frac{p^2}{2} & -1 \leq p \leq 2, \\
+\infty & \text{otherwise.}
\end{cases}
\]
Also, by Thm. 3.1 the initial data \( J \) is given by \( f_1(\cdot, 0) \) defined in (10). In other words, \( J \) is the minimum of three functions, each of which is a shift of the function \( L'_{\infty} \), which by definition 6 reads as follows
\[
L'_{\infty}(x) = \begin{cases} 
-x & x < 0, \\
2x & x \geq 0.
\end{cases}
\]
In this example, we choose the parameters \((u_1, a_1) = (-2, -0.5), (u_2, a_2) = (0, 0)\) and \((u_3, a_3) = (2, -1)\). The corresponding functions \( J, H \) and \( f_1 \) are shown in Fig. 3, where (a) shows the initial value \( J \), (b) shows the convex Hamiltonian \( H \), and (c) and (d) show the solution \( S = f_1 \) evaluated at \( t = 1 \) and \( t = 3 \), respectively.

The corresponding Tensorflow code reads as follows.

```python
import numpy as np
import tensorflow as tf

n_data = 1000
dim = 1

def min_fn(x):
    return tf.math.reduce_min(x, axis=-1)

# L = -x-1/2 if x<-1;
# = x^2/2 if -1<=x<=2;
# = 2x-2 if x>2.

def L_fn(x):
    val1 = -x - 0.5
    val2 = tf.multiply(x, x)/2
    val3 = 2*x - 2
    flag1 = 1 - tf.sign(tf.maximum(x+1, 0))
    flag3 = tf.sign(tf.maximum(x-2, 0))
    flag2 = 1 - flag1 - flag3
    val = tf.multiply(flag1, val1)
    val = tf.add(val, tf.multiply(flag2, val2))
    val = tf.add(val, tf.multiply(flag3, val3))
    return tf.squeeze(val, -1)

tf.reset_default_graph()
Figure 3. The graph of $f_1$ in example 3.1. The figures (a) and (b) show the initial value $J$ and the Hamiltonian $H$, respectively. The figures (c) and (d) show the solution $S = f_1$ evaluated at $t = 1$ and $t = 3$, respectively.

```python
u_true = np.array([[-2], [0], [2]])
a_true = np.array([-0.5, 0, -1])
u_param = tf.Variable(u_true, name = "u0", dtype = tf.float64) 
a_param = tf.Variable(a_true, name = "a0", dtype = tf.float64) 
x_placeholder = tf.placeholder(tf.float64, shape=(n_data, 1, dim)) 
t_placeholder = tf.placeholder(tf.float64, shape=(n_data, 1))

x_grid0 = np.arange(n_data) * (10.0 / n_data) - 5
x_grid0 = np.expand_dims(x_grid0, axis = -1)
t_grid0 = np.arange(n_data) * 0 + 3
x_grid0 = np.expand_dims(x_grid0, axis = -1)
t_grid = np.expand_dims(t_grid0, axis = -1)
t_grid = np.expand_dims(t_grid0, axis = -1)

def construct_nn(x_in, t_in):
    val0 = tf.subtract(x_in, u_param)
    val1 = tf.div(val0, tf.expand_dims(t_in, -1))
    val2 = L_fn(val1)
```
val3 = tf.add(tf.multiply(val2, t_in), a_param)
y_ = min_fn(val3)
return y_
y_nn = construct_nn(x_placeholder, t_placeholder)
sess = tf.Session()
sess.run(tf.global_variables_initializer())
y_val = sess.run(y_nn, {x_placeholder: x_grid, t_placeholder: t_grid})

Example 3.2. We now present a high dimensional example. To be specific, the dimension is set to be \( n = 10 \), and the solution \( f_1 : \mathbb{R}^{10} \times [0, +\infty) \rightarrow \mathbb{R} \) is represented by a neural network with three neurons, i.e., \( m = 3 \). The activation function \( L \) is given by

\[
L(x) = \max\{\|x\|_2 - 1, 0\} = \begin{cases} \|x\|_2 - 1 & \text{if } \|x\|_2 > 1, \\ 0 & \text{if } \|x\|_2 \leq 1. \end{cases}
\]

The corresponding Hamiltonian is given by

\[
H(p) = L^*(p) = \begin{cases} \|p\|_2 & \text{if } \|p\|_2 \leq 1, \\ +\infty & \text{if } \|p\|_2 > 1. \end{cases}
\]

The parameters are chosen to be \( u_1 = (-2, 0, 0, 0, \ldots, 0) \), \( u_2 = (2, -2, -1, 0, \ldots, 0) \), \( u_3 = (0, 2, 0, 0, \ldots, 0) \), \( a_1 = -0.5 \), \( a_2 = 0 \) and \( a_3 = -1 \).

By definition \( 6 \) and straightforward computation, we obtain \( L_\infty(d) = \|d\|_2 \). Hence, the initial condition for the corresponding HJ PDE is given by Eq. \( \[10\] \), which in this example reads

\[
J(x) = \min_{i \in \{1, 2, 3\}} \{\|x - u_i\|_2 + a_i\}.
\]

The accompanying figure \[4\] shows the graph of \( f_1 \) for a 2-dimensional slice. To be specific, we fix \( x = (x_1, x_2, 0, \ldots, 0) \), and compute \( f_1(x, t) \) at \( t = 10^{-6}, 1, 3 \) and \( 5 \). Note that the formula \( \[7\] \) is not well-defined for \( t = 0 \), hence we use a small number \( 10^{-6} \) instead. In each figure, the color is given by the function value \( f_1(x, t) \) and the \( x \) and \( y \) axes represent the variables \( x_1 \) and \( x_2 \), respectively. The solutions evaluated at \( t = 10^{-6}, t = 1, t = 3 \) and \( t = 5 \) are shown in \( (a), (b), (c) \) and \( (d) \), respectively.

3.2. The second architecture. In this part, we analyze the second neural network architecture given by Eq. \( \[8\] \). Here, we assume the parameters \( \{(v_i, b_i)\}_{i=1}^m \) satisfy the following assumption

(H) There exists a convex function \( \ell : \mathbb{R}^n \rightarrow \mathbb{R} \) satisfying \( \ell(v_i) = b_i \) for all \( i \in \{1, \ldots, m\} \).

Under this assumption, we present the following main theorem which states that the second architecture gives a viscosity solution to the corresponding HJ PDE, where the initial data is given by the activation function \( J \) in the neural network, and the Hamiltonian is a convex piecewise affine function determined by the parameters \( \{(v_i, b_i)\}_{i=1}^m \).

Theorem 3.2. Assume the function \( J : \mathbb{R}^n \rightarrow \mathbb{R} \) is a concave function and the assumption (H) is satisfied. Let \( f_2 \) be the function defined in \( \[8\] \). Then \( f_2 = S_{LO} \), where \( S_{LO} \) is the Lax–Oleinik formula defined by \( \[6\] \) with initial condition \( J = \bar{J} \) and the Hamiltonian \( H \) defined by

\[
(12) \quad H(p) = \max_{i \in \{1, \ldots, m\}} \{\langle p, v_i \rangle - b_i\},
\]

for every \( p \in \mathbb{R}^n \). Hence \( f_2 \) is a concave viscosity solution to the corresponding HJ PDE \( \[11\] \).

Proof. By assumption (H) and simply changing the notations in \( \[28\] \), Lem. 3.1], we have

\[
(13) \quad H^*(v) = \min_{m} \left\{ \sum_{i=1}^m \alpha_i b_i : (\alpha_1, \ldots, \alpha_m) \in \Lambda_m, \sum_{i=1}^m \alpha_i v_i = v \right\},
\]

for each \( v \in \text{co} \{v_1, \ldots, v_m\} = \text{dom} \ H^* \), where \( \Lambda_m \) is the unit simplex defined in \( \[2\] \). Also, we have \( H^*(v_k) = b_k \) for each \( k \in \{1, \ldots, m\} \).
Figure 4. A two dimensional slice of the graph of \( f_1 \) in example 3.2. In each figure, the x and y axes correspond to the variables \( x_1 \) and \( x_2 \), which are the first and second coordinates of the variable \( x = (x_1, x_2, 0, \ldots, 0) \). The color is given by the function value \( f_1(x, t) \). The figures (a), (b), (c) and (d) show contour lines of the solution \( f_1(x, t) \) at \( t = 10^{-6}, t = 1, t = 3 \) and \( t = 5 \), respectively.

For each \( x \in \mathbb{R}^n, t > 0 \) and \( v \in \text{co} \{v_1, \ldots, v_m\} \), let \( \alpha = (\alpha_1, \ldots, \alpha_m) \in \Lambda_m \) be the minimizer in the minimization problem in (13) evaluated at \( v \). In other words, we have

\[
\begin{aligned}
\sum_{i=1}^m \alpha_i &= 1, \\
\sum_{i=1}^m \alpha_i v_i &= v, \\
\sum_{i=1}^m \alpha_i b_i &= H^*(v), \quad \text{and} \quad \alpha_j \in [0, 1] \quad \text{for each} \quad j \in \{1, \ldots, m\}.
\end{aligned}
\]

Then, by (14) and the assumption that \( J = \tilde{J} \) is concave, we have

\[
\begin{aligned}
J(x - tv) + tH^*(v) &= J\left( \sum_{i=1}^m \alpha_i (x - tv_i) \right) + t \sum_{i=1}^m \alpha_i b_i \\
&\geq \sum_{i=1}^m \alpha_i J(x - tv_i) + \sum_{i=1}^m \alpha_i t b_i \\
&= \sum_{i=1}^m \alpha_i (J(x - tv_i) + t b_i) \\
&\geq \min_{i \in \{1, \ldots, m\}} \{ J(x - tv_i) + t b_i \} = f_2(x, t).
\end{aligned}
\]

As a result, we conclude that

\[
S_{LO}(x, t) = \inf_{v \in \text{dom} H^*} \{ J(x - tv) + tH^*(v) \} \geq f_2(x, t).
\]
On the other hand, recall that \( b_k = H^*(v_k) \) for each \( k \in \{1, \ldots, m\} \), hence we obtain

\[
f_2(x, t) = \min_{i \in \{1, \ldots, m\}} \{ J(x - tv_i) + tH^*(v_i) \} \geq \inf_{v \in \mathbb{R}^n} \{ J(x - tv) + tH^*(v) \} = S_{LO}(x, t).
\]

Therefore, we conclude that \( f_2(x, t) = S_{LO}(x, t) \) for each \( x \in \mathbb{R}^n \) and \( t > 0 \).

Note that \( H \) is a convex function, since it is the maximum of affine functions. Then, by the same proof as in [38, Sec. 10.3.4, Thm. 3], we conclude that \( f_2 \) is a viscosity solution to the corresponding HJ PDE. Moreover, since \( J \) is concave, \( f_2 \) is the minimum of concave functions, which implies the concavity of \( f_2 \). □

**Remark 3.2.** In the second architecture, if we furthermore assume that the initial condition \( J = \tilde{J} \) is uniformly Lipschitz, then \( f_2 \) is the unique uniformly continuous viscosity solution to the corresponding HJ PDE. This conclusion directly follows from [4, Thm. 2.1].

**Example 3.3.** Here, we provide a one dimensional example of the function \( f_2 \). To be specific, we consider \( f_2 : \mathbb{R} \times [0, +\infty) \rightarrow \mathbb{R} \) represented by the neural network in Fig. 2 with three neurons, i.e., we set \( n = 1 \) and \( m = 3 \). The initial value is given by \( J(x) = -\frac{x^2}{2} \) for each \( x \in \mathbb{R} \), and the Hamiltonian \( H \) is given by the piecewise affine function in Eq. (12) with \( (v_1, b_1) = (-2, 0.5) \), \( (v_2, b_2) = (0, -5) \) and \( (v_3, b_3) = (2, 1) \). The functions \( J, H \) and \( f_2 \) are shown in Fig. 5 where (a) shows the initial value \( J \), (b) shows the convex Hamiltonian \( H \), and (c) and (d) show the solution \( S = f_2 \) evaluated at \( t = 1 \) and \( t = 3 \), respectively.

![Figure 5](image)

Figure 5. The graph of \( f_2 \) in example 3.3. The figures (a) and (b) show the initial value \( J \) and the Hamiltonian \( H \), respectively. The figures (c) and (d) show the solution \( S = f_2 \) evaluated at \( t = 1 \) and \( t = 3 \), respectively.
The corresponding Tensorflow code is given as follows.

```python
import numpy as np
import tensorflow as tf

n_data = 1000
dim = 1

def min_fn(x):
    return tf.math.reduce_min(x, axis=-1)

# J = -x^2/2.
def J_fn(x):
    val = -tf.multiply(x, x)/2
    return tf.squeeze(val, -1)

tf.reset_default_graph()

v_true = np.array([[-2], [0], [2]])
b_true = np.array([0.5, -5, 1])
v_param = tf.Variable(v_true, name = "v0", dtype = tf.float64)
b_param = tf.Variable(b_true, name = "b0", dtype = tf.float64)
x_placeholder = tf.placeholder(tf.float64, shape=(n_data, 1, dim))
t_placeholder = tf.placeholder(tf.float64, shape=(n_data, 1))

x_grid0 = np.arange(n_data) * (10.0 / n_data) - 5
t_grid0 = np.arange(n_data) * 0 + 3
x_grid = np.expand_dims(x_grid0, axis = -1)
x_grid = np.expand_dims(x_grid, axis = -1)
t_grid = np.expand_dims(t_grid0, axis = -1)

def construct_nn(x_in, t_in):
    t = tf.expand_dims(t_in, -1)
    val0 = tf.subtract(x_in, tf.multiply(t, v_param))
    val1 = J_fn(val0)
    val2 = tf.add(val1, tf.multiply(t_in, b_param))
    y_ = min_fn(val2)
    return y_

y_nn = construct_nn(x_placeholder, t_placeholder)
sess = tf.Session()
sess.run(tf.global_variables_initializer())
y_val = sess.run(y_nn, {x_placeholder: x_grid, t_placeholder: t_grid})
sess.close()
```

Example 3.4. Here, we present a high dimensional example. We choose the dimension to be \( n = 10 \). We consider the solution \( f_2 : \mathbb{R}^{10} \times [0, +\infty) \to \mathbb{R} \) represented by the neural network in Fig. 2 with three neurons, i.e., we set \( m = 3 \). Similar to the one dimensional case, the activation function \( \tilde{J} \) is chosen to be \( \tilde{J}(x) = -\frac{\|x\|^2}{2} \) for every \( x \in \mathbb{R}^{10} \). Hence, by Thm. 3.2, the initial data in the corresponding HJ PDE is given by \( J(x) = \tilde{J}(x) = -\frac{\|x\|^2}{2} \). The parameters are chosen to be \( v_1 = (-2,0,0,0,\ldots,0) \), \( v_2 = (2,-2,-1,0,\ldots,0) \), \( v_3 = (0,2,0,0,\ldots,0) \), \( b_1 = 0.5 \), \( b_2 = -5 \) and \( b_3 = 1 \). Then the Hamiltonian is the corresponding convex piecewise affine function defined in (12).
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Figure 6. A two-dimensional slice of the graph of $f_2$ in example 3.4. In each figure, the $x$ and $y$ axes correspond to the variables $x_1$ and $x_2$, which are the first and second coordinates of the variable $x = (x_1, x_2, 0, \ldots, 0)$. The color is given by the function value $f_2(x, t)$. The figures (a), (b), (c) and (d) show contour lines of the solution $f_2(x, t)$ at $t = 0$, $t = 1$, $t = 3$ and $t = 5$, respectively.

The solution $f_2$ is shown in Fig. 6. We fix $x = (x_1, x_2, 0, \ldots, 0)$ and compute $f_2(x, t)$ for $t = 0$, $1$, $3$ and $5$. In each figure, the color is given by the function value $f_2(x, t)$ and the $x$ and $y$ axes represent the variables $x_1$ and $x_2$, respectively. The solutions at $t = 0$, $t = 1$, $t = 3$ and $t = 5$ are shown in (a), (b), (c) and (d), respectively.

When $H$ is the $l_1$-norm, i.e., $H(p) = |p|_1$ for each $p \in \mathbb{R}^5$, the Hamiltonian $H$ can be written in the form of Eq. (12) with $m = 2^n$, $b_i = 0$ for each $i \in \{1, \ldots, m\}$ and

$$\{v_i\}_{i=1}^m = \{(w_1, w_2, \ldots, w_n) \in \mathbb{R}^n : w_j \in \{\pm 1\} \forall j \in \{1, \ldots, n\}\}.$$

The corresponding function $f_2$ is shown in Fig. 7.
When $H$ is the $l^\infty$-norm, i.e., $H(p) = \|p\|_\infty$ for each $p \in \mathbb{R}^5$, the Hamiltonian $H$ can be written in the form of Eq. (12) with $m = 2n$, $b_i = 0$ for each $i \in \{1, \ldots, m\}$ and

$$\{v_i\}_{i=1}^m = \{\pm e_j\}_{j=1}^n,$$

where $e_j$ is the $j$-th coordinate basis vector in $\mathbb{R}^n$. The corresponding function $f_2$ is shown in Fig. 8.

**Figure 7.** A two dimensional slice of the graph of $f_2$ in example 3.5. The initial data $J$ is given by $J(x) = -\frac{\|x\|_2^2}{2}$ and the Hamiltonian $H$ is the $l^1$ norm. In each figure, the x and y axes correspond to the variables $x_1$ and $x_2$, which are the first and second coordinates of the variable $x = (x_1, x_2, 0, \ldots, 0)$. The color is given by the function value $f_2(x, t)$. The figures (a), (b), (c) and (d) show contour lines of the solution $f_2(x, t)$ at $t = 0$, $t = 1$, $t = 3$ and $t = 5$, respectively.

4. Conclusion

In this paper, we investigated two neural network architectures shown in Figs. 1 and 2 and proved that these two architectures represent viscosity solutions to two sets of HJ PDEs whose convex Hamiltonian $H$ and initial data $J$ satisfy certain assumptions in Thms. 3.1 and 3.2, respectively. This connection provides a possible interpretation for some neural network architectures. Our results suggest that efficient dedicated hardware implementation for neural networks can be leveraged to evaluate viscosity solutions of certain HJ PDEs.
Figure 8. A two dimensional slice of the graph of $f_2$ in example 3.5. The initial data $J$ is given by $J(x) = -\frac{\|x\|^2}{2}$ and the Hamiltonian $H$ is the $\ell^\infty$ norm. In each figure, the x and y axes correspond to the variables $x_1$ and $x_2$, which are the first and second coordinates of the variable $x = (x_1, x_2, 0, \ldots, 0)$. The color is given by the function value $f_2(x, t)$. The figures (a), (b), (c) and (d) show contour lines of the solution $f_2(x, t)$ at $t = 0$, $t = 1$, $t = 3$ and $t = 5$, respectively.

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ON SOME NEURAL NETWORK ARCHITECTURES THAT CAN REPRESENT VISCOSITY SOLUTIONS OF CERTAIN HIGH DIMENSIONAL HAMILTON–JACOBI PARTIAL DIFFERENTIAL EQUATIONS

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