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Machine Learning Approximations for Some Parabolic Partial Differential Equations

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Abstract

These lecture notes are devoted to machine learning based algorithms for the approximation of solutions to some second order parabolic partial differential equations (PDE for short). We present a new kind of probabilistic approximation for these PDEs which is based on Neural network approximations. This is referred to as *Machine learning approximation methods*. The paper is divided into three parts. A first part presents approximation results for feedforward neural networks. A second part studies probabilistic representations of solutions to parabolic PDEs in terms of backward stochastic differential equations (BSDEs for short). Finally, a third part deals with the neural network approximations of those BSDEs.

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Contents

1 Introduction

The aim of these notes is to present recent methods for the approximation of some second order parabolic PDEs. More precisely, we focus on PDEs of the form

$$G\Big(t, x, v(t,x), \partial_t v(t,x), \partial_x v(t,x), \partial^2_{xx} v(t,x)\Big) \;\;=\;\; 0\ ,\ \ (t,x)\in[0,T)\times\mathbb{R}^d$$

with terminal condition

$$v(T,x) \;\;=\;\; g(x)\ ,\ \ x\in\mathbb{R}^d\ ,$$

where $\partial_x v$ and $\partial^2_{xx} v$ stand for the gradient and the Hessian matrix of the unknown function v. The PDEs that we consider in these notes have a nonlinearity G that is related to stochastic optimization problems. The approximation of such equations is therefore important for many applications and it has attracted a lot of interest, leading to a huge literature on the subject. This literature can be divided into two parts. The first part concerns the deterministic methods (finite difference, finite volume methods). The second part of the literature focusses on probabilistic methods. Using a so called Feynman-Kac representation of the solution to the PDE, Monte Carlo based methods are derived to estimate the solution v.

In these notes, we present a new kind of probabilistic approximation for these PDEs. This kind of method is based on Neural network approximation and is referred to as Machine learning approximation methods. Machine learning methods were first developed in 90's (see[12, 13, 10], but they have recently attracted a lot of interest due to the development of the computational power of recent machines, which allows to show their strong efficiency in high dimension compared to the existing methods.

These notes are divided into three parts. The first part introduces the structure of neural network functions and the main approximation/density results for this class of functions. The stochastic gradient descent algorithm is also presented for the choice of the approximation parameters and conditions for its convergence are provided.

The second part presents the probabilistic representation of some parabolic semi-linear PDEs. These representations are given in terms of Backward SDEs. A first global presentation of BSDEs is done and existence and uniqueness of solutions are proved for Lipschitz, reflected and constrained BSDEs. We then provide representations for three kind of PDEs. The first kind is the semi-linear PDE that is related to Lipschitz BSDEs. The second kind is the obstacle problem that is represented by reflected BSDEs. Finally, the third kind is the variation inequality with gradient constraints which is linked to constrained BSDEs. Let us mention that those three kind of PDEs are respectively related to optimal control with non-controlled volatility, optimal stopping and stochastic target problems. We refer to [22, 26] for details on those links.

The last part presents approximation algorithms for these three kinds of PDEs using the BSDEs representation and their neural network approximations. We first present three algorithms for semi-linear PDEs. The first algorithm is a forward algorithm from [8, 9] and consists in the approximation of the gradient of the unknown function v. The subsequent algorithms are developed in [11] and consist in a backward approximation of the unknown function and its gradient at the same time. We then consider the approximation of obstacle problems. For that problem, we present two algorithms. The first one is an extension of the previous backward algorithm for semi-linear PDEs and is also studied in [11]. The second algorithm is due to [4]. It uses the link between obstacle problems and optimal stopping problems and approximates an optimal stopping time. We end this part by an algorithm from [14] for the approximation of variational inequalities with gradient constraints based on a constrained Backward SDEs representation.

The paper is organized so that the first two parts can be read independently. Part III needs a good understanding of the results presented in Part I and II.

Let us finally mention that these notes cover only the theoretical side of the subject. In particular, the practical implementation of the presented algorithms and the choice of approximation parameters is not considered here. We therefore would like to encourage the reader to experiment with the presented algorithms and check their efficiency.

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Notations: Given a topological space $\mathcal{X}$, we denote by $\mathcal{B}(\mathcal{X})$ its Borel σ-algebra. For a measured space $(\mathcal{X}, \mathcal{T}, \mu)$ and an integer $p \geq 1$, we denote by $L^p(\mathcal{X}, \mathcal{T}, \mu)$ the space of measurable maps $Y : \mathcal{X} \to \mathbb{R}$ such that

$$\int_{\mathcal{X}} |Y(x)|^p d\mu(x) \quad < \quad +\infty.$$

We endow this space with the semi norm $\|\cdot\|_{L^p(\mathcal{Y},\mathcal{T},\mu)}$ defined by

$$\|Y\|_{L^p(\mathcal{X},\mathcal{T},\mu)} \quad = \quad \Big(\int_{\mathcal{X}} |Y(x)|^p d\mu(x) \Big)^{\frac{1}{p}}, \quad Y \in L^p(\mathcal{X}, \mathcal{T}, \mu) .$$

For simplicity, we still denote by $L^p(\mathcal{Y}, \mathcal{T}, \mu)$ the set of equivalence classes for the μ-a.e. equality so that $\|\cdot\|_{L^p(\mathcal{Y},\mathcal{T},\mu)}$ is a norm on $L^p(\mathcal{Y}, \mathcal{T}, \mu)$.

Throughout these lecture notes, we fix an integer $d \geq 1$ and a complete probability space $(\Omega, \mathcal{A}, \mathbb{P})$ that we suppose rich enough to be endowed with a standard $\mathbb{R}^d$-valued Brownian Motion $W = (W_t)_{t\geq 0}$. We denote by $\mathbb{F} = (\mathcal{F}_t)_{t\geq 0}$ the complete (and right-continuous) filtration generated by W. For $t \geq 0$, we also denote by $\mathbb{F}^t = (\mathcal{F}^t_s)_{s\geq t}$ the complete (and right-continuous) filtration generated by the translated process $W = (W^t_s)_{s\geq t} := (W_{s+t} - W_t)_{s\geq t}$.

Part I: Neural networks approximations

2 What is a Neural Network?

We first give the definition of a (feedforward) neural network. For that sake we fix a function $\rho : \mathbb{R} \to \mathbb{R}$ that we call the **activation function**. We also fix an integer $L \geq 1$ representing the **number of hidden layers** of the neural network. Additionally to the hidden layers, we have input and output layers that we call respectively the **layer** 0 and the **layer** $L + 1$

On each layer $\ell = 0, 1, \ldots, L, L + 1$, we fix an integer $m_\ell \geq 1$ representing the **number of neurons** on the layer ℓ. In particular we call m_0 and m_{L+1} the input and output dimensions respectively. For each $\ell = 1, \ldots, L + 1$ we fix two parameters $\alpha_\ell \in \mathbb{R}^{m_\ell \times m_{\ell-1}}$ and $\beta_\ell \in \mathbb{R}^{m_\ell}$. We then denote by A_ℓ the affine map from $\mathbb{R}^{m_{\ell-1}}$ to $\mathbb{R}^{m_\ell}$ defined by

$$A_\ell(x) \;=\; \alpha_\ell x + \beta_\ell \,, \quad x \in \mathbb{R}^{m_{\ell-1}} \,.$$

We also extend ρ as a function from $\mathbb{R}^d$ into itself for $d \geq 1$ by stating

$$\rho(x_1, \ldots, x_d) \;=\; \Big(\rho(x_1), \ldots, \rho(x_d)\Big) \,,\; (x_1, \ldots, x_d) \in \mathbb{R}^d \,.$$

We are now able to give the definition of a neural network.

Definition 2.1 (Neural network)**.** *A (feedforward) neural network with activation function ρ, L hidden layers, m_ℓ neurons on layer ℓ and parameters $(\alpha_\ell, \beta_\ell)_{1\leq \ell\leq L}$ is the function*

$$x \in \mathbb{R}^{m_0} \mapsto A_{L+1} \circ \rho \circ A_L \circ \cdots \circ \rho \circ A_1(x) \in \mathbb{R}^{m_{L+1}} \,. \tag{2.1}$$

The coefficients α_ℓ and β_ℓ are respectively called the **weights** and the **biases** of the neural network.

For a sequence $m = (m_0, m_1, \ldots, m_L, m_{L+1}) \in (\mathbb{N} \setminus \{0\})^{L+2}$, we define the set Θ_m of possible parameters:

$$\Theta_m \;=\; \Big\{(\alpha_\ell, \beta_\ell)_{1\leq \ell\leq L+1} \;:\; \alpha_\ell \in \mathbb{R}^{m_\ell\times m_{\ell-1}} \text{ and } \beta_\ell \in \mathbb{R}^{m_\ell} \text{ for } \ell = 1, \ldots, L + 1\Big\} \,.$$

Given $\theta \in \Theta_m$, we denote by NN^θ the function defined by (2.1). For fixed input and output dimensions d_i and d_o, we denote by $\mathfrak{NN}^\rho_{L,d_i,d_o}$ the set of neural networks with activation function ρ, L hidden layers, input and output dimensions d_i and d_o respectively:

$$\mathfrak{NN}^\rho_{L,d_i,d_o} \;=\; \Big\{NN^\theta \;:\; \theta \in \Theta_m, m = (m_0, \ldots, m_{L+1}),\; m_0 = d_i \,, m_{L+1} = d_o\Big\} \,.$$

In the sequel, we restrict to a single output dimension $d_o = 1$, we fix the input dimension $d_i = d$ and we focus on the approximation properties of this set.

3 Approximation results

Artificial neural networks are interesting for their universal approximation properties. Namely, it is possible to construct a neural network that is arbitrarily close to a given function. As far as we know, the earliest papers proving the universal approximation property of neural networks are [12] and [5].

There are several approximation properties. The first one concerns the L^p-type approximation. We fix an integer $p \geq 1$ and a finite measure μ on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$. The universal approximation property in L^p can be stated as follows (see Theorem 1 in [10]).

Theorem 3.1. *Suppose that the activation function ρ is measurable, bounded and nonconstant. Then, for any finite positive measure μ on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$, the set $\mathfrak{NN}^\rho_{L,d,1}$ is dense in $L^p(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mu)$ for any $p \geq 1$.*

The second density property concerns the uniform convergence. We denote by $C(\mathbb{R}^d)$ the set of continuous functions from $\mathbb{R}^d$ to $\mathbb{R}$. We recall that a sequence of function $(f_n)_{n\geq 1}$ of $C(\mathbb{R}^d)$ is said to converge locally uniformly to a function $f \in C(\mathbb{R}^d)$ if for any compact subset Q of $\mathbb{R}^d$

$$\sup_{x\in Q} |f_n(x) - f(x)| \xrightarrow[n\to+\infty]{} 0 .$$

We then have the following density property.

Theorem 3.2. *Suppose that the activation function ρ is continuous, bounded and nonconstant. Then the set $\mathfrak{NN}^\rho_{L,d,1}$ is dense in $C(\mathbb{R}^d)$ for the local uniform convergence.*

The previous result can actually be extended to smooth functions as done in [13]. For $k \geq 1$, we denote by $C^k(\mathbb{R}^d)$ the set of functions from $\mathbb{R}^d$ to $\mathbb{R}$ which are k times differentiable with continuous derivatives up to order k. We say that a sequence $(f_n)_{n\geq 1}$ of $C^k(\mathbb{R}^d)$ converges locally uniformly to a function f in $C^k(\mathbb{R}^d)$ if

$$\sup_Q |f_n - f| + \sum_{i_1+\cdots+i_d\leq k} \sup_Q \left| \frac{\partial^{i_1+\cdots+i_d} f_n}{\partial x_1^{i_1}\cdots\partial x_d^{i_d}} - \frac{\partial^{i_1+\cdots+i_d} f}{\partial x_1^{i_1}\cdots\partial x_d^{i_d}} \right| \xrightarrow[n\to+\infty]{} 0$$

for any compact subset Q of $\mathbb{R}^d$. We have the following extension to $C^k(\mathbb{R}^d)$ of the density result.

Theorem 3.3. *Suppose that the activation function ρ belongs to $C^k(\mathbb{R}^d)$, and that it is bounded and nonconstant. Then the set $\mathfrak{NN}^\rho_{L,d,1}$ is dense in $C^k(\mathbb{R}^d)$ for the local uniform convergence.*

We refer to [10] for a presentation of the previous results and their proofs which are mainly based on functional analysis arguments. Let us mention the paper [1] which proposes a constructive approach to neural networks using the Van der Monde determinant.

Once we get density results, a natural question to ask is how to choose in practice the size of the neural network. Some answers are given by Andrew Barron for the case of a single hidden layer neural network and for an error in $L^2(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mu)$ *i.e.* a mean square error. More precisely, it is proved in [2] that the approximation by single hidden layer neural networks leads to an error of order $O(\frac{1}{\sqrt{m}})$ for an approximated function with enough regularity, where m is the number of neurons on the hidden layer. In [16], the author proved that for a locally integrable activation function ρ, the approximation of a function $f \in W^{k,2}(K)$ by the single hidden layer neural network leads to an L^2 error of order $O(m^{-\frac{k}{d-1}})$, where m is the number of neurons on the hidden layer and $W^{k,2}(K)$ stands for the $(k,2)$-Sobolev space.

For the case of two hidden layers, [17] proved that there exists a strictly increasing sigmoid function ρ such that any continuous function f on $[0,1]^d$ can be arbitrarily approximated by a neural network with $3d$ neurons on the first hidden layer and $6d+3$ neurons on the second hidden layer.

Let us also mention the article [3] which provides an estimation of the mean statistical error as $O(\frac{C}{\sqrt{m}}) + O(\frac{md}{N}\log N)$, for single hidden layer, where m still stands for the number of neurons on the hidden layer and N is the number of samples according to the law μ.

4 Algorithm to choose parameters

We turn to a probabilistic framework. On the complete probability space $(\Omega, \mathcal{A}, \mathbb{P})$, we fix two random variables X and Y valued respectively in $\mathbb{R}^d$ and $\mathbb{R}$. We suppose that there exists a (deterministic) function $f : \mathbb{R}^d \to \mathbb{R}$ such that $Y = f(X)$.

We are also given a **loss function** $L : \mathbb{R}\times\mathbb{R} \to \mathbb{R}_+$ which measures the error between the realization Y and an approximate realization $\tilde{Y} = \tilde{f}(X)$ based on an approximation $\tilde{f} \in \mathfrak{NN}^\rho_{L,d,1}$ of f. The aim is to minimize the loss due to the approximation of the function f by a neural network NN^θ

$$V_m \ := \ \min_{\theta\in\Theta_m} \mathbb{E}\Big[L\Big(NN^\theta(X), Y\Big)\Big] . \tag{4.1}$$

We notice that for the case of a quadratic loss function $L(z,y) = |z-y|^2$ for $(z,y) \in \mathbb{R}^2$, and for a measurable and nonconstant activation function, we have from Theorem 3.1

$$\lim_{m\to+\infty} V_m \;=\; 0$$

where $m \to +\infty$ means

$$\min_{1\leq \ell\leq L} m_\ell \to +\infty\;. \tag{4.2}$$

To get a minimizer $\theta^* \in \Theta_m$ for the problem (4.1), we use a **Stochastic Gradient Descent** (SGD for short). More precisely, we look for a solution of the first order condition related to (4.1):

$$\mathbb{E}\Big[\partial_1 L\Big(NN^\theta(X),Y\Big)\nabla_\theta NN^\theta(X)\Big] \;=\; 0\;,$$

where $\partial_1 L$ stands for the partial derivative of L with respect to its first argument and $\nabla_\theta NN^\theta(X)$ stands for the derivative of $NN^\theta(X)$ with respect to the parameters θ. We notice that this equation can be written in the abstract form

$$\mathbb{E}\Big[F(\theta,Z)\Big] \;=\; 0\;,$$

where Z stands for the couple (X,Y). To solve numerically this equation, we introduce the stochastic algorithm $(\theta_n)_{n\geq 0}$ defined by a fixed initial value θ_0 and the recursive equation

$$\theta_{n+1} \;=\; \theta_n - \gamma_{n+1}F(\theta_n, Z_{n+1}) \;\text{ for }\quad n\geq 0\;,$$

where $(Z_n)_{n\geq 1}$ is an IID sequence or random variables following the law of Z and $(\gamma_n)_{n\geq 1}$ is a sequence of positive real numbers. We give below an L^2-convergence result for the sequence $(\theta_n)_{n\geq 1}$ and we refer to Section 2 of Chapter 6 in [19] for more general convergence results.

Theorem 4.1 (Robbins-Monro algorithm)**.** *Suppose that $(\gamma_n)_{n\geq 1}$ satisfies $\gamma_n \geq 0$ for $n\geq 1$, and*

$$\sum_{n=1}^{+\infty}\gamma_n^2 \;<\; +\infty \quad \text{and} \quad \sum_{n=1}^{+\infty}\gamma_n \;=\; +\infty\;.$$

Let $\mathcal{F}_0 := \{\emptyset,\Omega\}$ and $\mathcal{F}_n := \sigma(Z_k,\ 1\leq k\leq n)$ for $n\geq 1$, and suppose that there exists θ^* such that $\mathbb{E}[F(\theta^*,Z)] = 0$ and $(\theta-\theta^*).\mathbb{E}[F(\theta,Z)] > 0$ for all $\theta\neq\theta^*$. Suppose also that $\theta\mapsto \mathbb{E}[F(\theta,Z)]$ is a continuous function and that there exists a constant $C>0$ such that

$$\mathbb{E}[|F(\theta_n,Z_{n+1})|^2|\mathcal{F}_n] \;\leq\; C(1+|\theta_n|^2)\ \mathbb{P}-p.s. \tag{4.3}$$

for all $n\geq 1$. Then $\theta_n \xrightarrow[n\to+\infty]{\mathbb{P}-a.s.} \theta^*$.

To prove this result, we first need the following intermediary result.

Lemma 4.2 (Stochastic Robbins-Siegmund)**.** *Let $(V_n)_n$ and $(\eta_n)_n$ be sequences of $(\mathcal{F}_n)_n$-adapted nonnegative random variables and $(\beta_n)_n$ and $(\chi_n)_n$ be two sequences of nonnegative reals such that $\sum_n\beta_n < +\infty$ and $\sum_n \chi_n < +\infty$ and*

$$\mathbb{E}[V_{n+1}|\mathcal{F}_n] \;\leq\; V_n(1+\beta_n)+\chi_n-\eta_n$$

for all $n\geq 1$. Then $(V_n)_n$ converges $\mathbb{P}$-a.s. to a nonnegative integrable random variable V_∞ and $\sum_n\eta_n < +\infty$ $\mathbb{P}$-a.s.

Proof. Define $\alpha_n = \Big(\prod_{k=1}^n(1+\beta_k)\Big)^{-1}$ (with the convention $\alpha_0 = 1$), $V'_n = \alpha_{n-1}V_n$, $\chi'_n = \alpha_n\chi_n$ and $\eta'_n = \alpha_n\eta_n$. We then have

$$\mathbb{E}[V'_{n+1}|\mathcal{F}_n] \;\leq\; V'_n + \chi'_n - \eta'_n.$$

Hence, the sequence $(Y_n)_{n\geq 1}$ defined by $Y_n = V'_n - \sum_{k=1}^{n-1}\eta'_k - \sum_{k=1}^{n-1}\chi'_k$ is a supermartingale. Since $\beta_n \geq 0$ for all n and $\sum_n \chi_n < +\infty$ we have $\sum_n \chi'_k < +\infty$ and $(Y_n)_{n\geq 1}$ is lower bounded. Hence, it converges $\mathbb{P}$-a.s. to an integrable random variable. Since V'_n and η'_n are non negative, we get that $\sum_n \eta'_n < +\infty$ $\mathbb{P}$-a.s. and V'_n converges $\mathbb{P}$-a.s. to an integrable random variable V'_∞. Finally, since $\sum_n \beta_n < +\infty$, α_n converges. Therefore $\sum_n \eta_n < +\infty$ $\mathbb{P}$-a.s. and V_n converges $\mathbb{P}$-a.s. to an integrable random variable V_∞. □

Proof. (of Theorem 4.1). From Taylor's formula we have

$$\begin{aligned}|\theta_{n+1}-\theta^*|^2 &= |\theta_n-\theta^*|^2 + 2\int_0^1 (t\theta_n + (1-t)\theta_{n+1} - \theta^*).(\theta_{n+1}-\theta_n)dt\\ &\leq |\theta_n-\theta^*|^2 + \gamma_{n+1}^2 F(\theta_n, Z_{n+1})^2 - 2\gamma_{n+1}(\theta_n-\theta^*).F(\theta_n,Z_{n+1})\ .\end{aligned}$$

Taking the conditional expectation given $\mathcal{F}_n$ and using assumption (4.3) we get a constant C such that

$$\begin{aligned}\mathbb{E}[|\theta_{n+1}-\theta^*|^2|\mathcal{F}_n] &\leq |\theta_n-\theta^*|^2 + C\gamma_{n+1}^2(1+|\theta_n|^2)\\ &\quad -2\gamma_{n+1}(\theta_n-\theta^*)\mathbb{E}[F(\theta_n,Z_{n+1})|\mathcal{F}_n]\ .\end{aligned}$$

From Young's inequality, we have $|\theta_n|^2 \leq 2|\theta_n-\theta^*|^2 + 2|\theta^*|^2$. Therefore we get

$$\begin{aligned}\mathbb{E}[|\theta_{n+1}-\theta^*|^2|\mathcal{F}_n] &\leq |\theta_n-\theta^*|^2(1+2C\gamma_{n+1}^2) + C\gamma_{n+1}^2(1+2|\theta^*|^2)\\ &\quad -2\gamma_{n+1}\Big((\theta_n-\theta^*).\mathbb{E}[F(\theta_n,Z_{n+1})|\mathcal{F}_n]\ .\end{aligned}$$

We apply the Stochastic Robbins-Siegmund Lemma with $V_n = |\theta_n-\theta^*|^2$, $\beta_n = 2C\gamma_{n+1}^2$, $\chi_n = C\gamma_{n+1}^2(1+2|\theta^*|^2)$ and $\eta_n = 2\gamma_{n+1}(\theta_n-\theta^*).\mathbb{E}[F(\theta_n,Z_{n+1})|\mathcal{F}_n]$. We then get the $\mathbb{P}$-a.s. convergence of $|\theta_n-\theta^*|^2$ to some integrable random variable V_∞. Suppose that $\mathbb{P}(V_\infty > 0) > 0$. Then, since V_∞ is integrable, we have $\mathbb{P}(\frac{1}{\varepsilon} > V_\infty > \varepsilon) > 0$ for some $\varepsilon > 0$. From the $\mathbb{P}$-a.s. convergence of $|\theta_n-\theta^*|^2$ to V_∞ we get

$$\frac{2}{\varepsilon} \ \geq\ |\theta_n-\theta^*|^2 \ \geq\ \frac{\varepsilon}{2}$$

for n large enough $\mathbb{P}-a.s.$ on $\{\frac{1}{\varepsilon} > V_\infty > \varepsilon\}$. Since F and θ^* are such that $(\theta-\theta^*).\mathbb{E}[F(\theta,Z)] > 0$ for all $\theta \neq \theta^*$ and $\theta \mapsto \mathbb{E}[F(\theta,Z)]$ is a continuous, there exists $\zeta > 0$ such that

$$(\theta_n-\theta^*).\mathbb{E}[F(\theta_n,Z_{n+1})|\mathcal{F}_n] \ \geq\ \zeta\ ,$$

for n large enough $\mathbb{P}-a.s.$ on $\{\frac{1}{\varepsilon} > V_\infty > \varepsilon\}$. Therefore $\eta_n \geq 2\gamma_{n+1}\zeta$ for n large enough $\mathbb{P}-a.s.$ on $\{\frac{1}{\varepsilon} > V_\infty > \varepsilon\}$. Since $\sum_n \gamma_n = +\infty$, and $\mathbb{P}(\frac{1}{\varepsilon} > V_\infty > \varepsilon) > 0$, this contradicts $\sum_n \eta_n < +\infty$ $\mathbb{P}$-a.s.. Therefore $V_\infty = 0$ $\mathbb{P}$-a.s. and θ_n converges $\mathbb{P}$-a.s. to θ^*. □

Remark 4.3. The choice of the initial value θ_0 and of the sequence $(\gamma_n)_n$ is a central question since a good choice of those parameters can make the algorithm converge very fast, while a poor choice of the parameters can lead to a bad behavior of the algorithm. In practice, the implemented libraries (e.g. PyTorch or TensorFlow) propose specific and optimized ways to choose parameters.

Let us focus on the classical L^2-type error where the loss function L is given by $L(z,y) = \frac{1}{2}|z-y|^2$ for $z, y \in \mathbb{R}$. Then, the SDG algorithm $(\theta_n)_{n\geq 0}$ takes the form

$$\theta_{n+1} \ =\ \theta_n - \gamma_{n+1}\Big(NN^{\theta_n}(X_{n+1}) - Y_{n+1}\Big)\nabla_\theta NN^{\theta_n}(X_{n+1}) \ \text{ for } \quad n \geq 0\ ,$$

where $(X_n, Y_n)_{n\geq 0}$ is an IID sequence following the law of (X, Y). To compute the values θ_n, we need to compute the derivatives of the neural network w.r.t. its parameters. A very efficient algorithm for the computation of the gradient is the **backpropagation algorithm** that we describe below. For the sake of clear presentation, we suppose that all hidden layers have the same number of neurons, that is $m_1 = \cdots = m_L =: m$.

For a given $n \geq 1$, we denote by $\alpha_{\ell,n}$ and $\beta_{\ell,n}$ the weight and bias of the ℓ-th layer at step n *i.e.* $\theta_n = (\alpha_{\ell,n}, \beta_{\ell,n})_{1\leq \ell\leq L+1}$.

Let $x_{\ell-1}(j)$ be the j-th input to the neurons of layer ℓ. Then the i-th element of the ℓ-th layer computes the value $u_\ell(i)$ given by

$$u_\ell(i) = \sum_{j=1}^{m} \alpha_{\ell,n}(i,j) x_{\ell-1}(j) + \beta_{\ell,n}(i)$$

and the value $x_\ell(i)$ of the i-th neuron of layer ℓ is given by $x_\ell(i) = \rho\Big(u_\ell(i)\Big)$, where we recall that ρ is the activation function. The SGD gives the following learning rule

$$\begin{aligned} \alpha_{\ell,n+1}(i,j) &= \alpha_{\ell,n}(i,j) - \gamma_{n+1} e_\ell(i) x_{\ell-1}(j) \\ \beta_{\ell,n+1}(i) &= \beta_{\ell,n}(i) - \gamma_{n+1} e_\ell(i) \end{aligned}$$

for $\ell = 0, \dots, L+1$, where $e_\ell(i)$ is called the error signal of the i-th neuron of the ℓ-th layer. It is given by

$$\begin{aligned} e_{L+1}(i) &= 1 \\ e_L(i) &= \sum_{j=1}^{m} \alpha_{L+1}(j) \rho'(u_{L+1}(j)) \end{aligned}$$

and

$$e_\ell(i) = \rho'(u_\ell(i)) \sum_{i=1}^{m} \alpha_{\ell,n}(i,j) e_{\ell+1}(j)$$

for $\ell = 1, \dots, L-1$. This is called **the backpropagation algorithm** as the variables $e_L(i)$ are computed in a backward way starting with $\ell = L+1$ and ending with $\ell = 1$.

Part II: Probabilistic representations for PDE

5 Backward SDEs

We present in this section the theory of Backward SDEs. For that, we first introduce some notations. We fix a terminal time $T > 0$ and we define for $t \in [0,T]$ the following spaces.

- $S^2_{\mathbb{F}}[t,T]$ (resp. $S^2_{\mathbb{F},c}[t,T]$) is the set of $\mathbb{R}$-valued $\mathbb{F}^t$-adapted *càdlàg*[1] (resp. continuous) processes $Y = (Y_s)_{s\in[t,T]}$ such that $\mathbb{E}\Big[\sup_{s\in[t,T]} |Y_s|^2\Big] < +\infty$. We endow this space with the norm $\|\cdot\|_{S^2[t,T]}$ defined by

$$\|Y\|_{S^2[t,T]} = \sqrt{\mathbb{E}\Big[\sup_{s\in[t,T]} |Y_s|^2\Big]} .$$

- $H^2_{\mathbb{F}}[t,T]$ is the set of $\mathbb{R}^d$-valued $\mathbb{F}^t$-predictable processes $Z = (Z_s)_{s\in[t,T]}$ such that $\mathbb{E}\Big[\int_t^T |Z_s|^2 ds\Big] < +\infty$. We endow this space with the norm $\|\cdot\|_{H^2[t,T]}$ defined by

$$\|Z\|_{H^2[t,T]} = \sqrt{\mathbb{E}\Big[\int_t^T |Z_s|^2 ds\Big]} .$$

We now define the equation to be considered. We first start with the forward part. We are given two mesurable functions $b, \sigma : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d, \mathbb{R}^{d\times d}$ on which we make the following assumption.

(Hb,σ**)**

(i) The functions b and σ are Lipschitz continuous in their space variable uniformly in their time variable: there exists a constant $L_{b,\sigma}$ such that

$$|b(t,x) - b(t,x')| + |\sigma(t,x) - \sigma(t,x')| \leq L_{b,\sigma}|x - x'|$$

for all $t \in [0,T]$ and $x, x' \in \mathbb{R}^d$.

[1] French acronym for 'right-continuous and left-limited'.

(ii) The functions b and σ have linear growth in their space variable uniformly in their time variable: there exists a constant $M_{b,\sigma}$ such that

$$|b(t,x)|+|\sigma(t,x)| \quad \leq \quad M_{b,\sigma}\Big(1+|x|\Big)$$

for all $t\in[0,T]$ and $x\in\mathbb{R}^d$.

Using [18, Theorem 5.2.1], we can define, under **(H**b,σ**)**, the process $X^{t,x}$ as the unique solution in $\Big(S^2_{\mathbb{F},c}[t,T]\Big)^d$ to the SDE

$$X^{t,x}_s \quad = \quad x+\int_t^s b(r,X^{t,x}_r)dr+\int_t^s \sigma(r,X^{t,x}_r)dW_r, \quad s\in[t,T]\ ,$$

for $t\in[0,T]$ and $x\in\mathbb{R}^d$.

We now define the backward equation. To this end, we consider two functions $f:[0,T]\times\mathbb{R}^d\times\mathbb{R}\times\mathbb{R}^d\to\mathbb{R}$ and $g:\mathbb{R}^d\to\mathbb{R}$ on which we make the following assumption.

(Hf,g**)**

(i) The functions f and g are continuous and satisfy the following growth property: there exist two constants M_f and M_g such that

$$\begin{aligned}|f(t,x,y,z))| \quad &\leq \quad M_f\Big(1+|x|+|y|+|z|\Big)\\ |g(x)| \quad &\leq \quad M_g(1+|x|)\end{aligned}$$

for all $t\in[0,T]$, $x\in\mathbb{R}^d$, $y\in\mathbb{R}$ and $z\in\mathbb{R}^d$.

(ii) The function f is Lipschitz continuous in the backward space variables uniformly in the time and forward variables: there exists a constant L_f such that

$$|f(t,x,y,z)-f(t,x,y',z')| \quad \leq \quad L_f\Big(|y-y'|+|z-z'|\Big)$$

for all $t\in[0,T]$, $x\in\mathbb{R}^d$, $y,y'\in\mathbb{R}$ and $z,z'\in\mathbb{R}^d$.

A solution to the backward SDE with coefficients (t,x,f,g) is a couple $(Y^{t,x},Z^{t,x})\in S^2_{\mathbb{F},c}[t,T]\times H^2_{\mathbb{F}}[t,T]$ such that

$$Y^{t,x}_s \quad = \quad g(X^{t,x}_T)+\int_s^T f(r,X^{t,x}_r,Y^{t,x}_r,Z^{t,x}_r)dr-\int_s^T Z^{t,x}_r.dW_r \tag{5.1}$$

for all $s\in[t,T]$. We first state the well-posedness of this equation.

Theorem 5.1. *Under **(H**b,σ**)** and **(H**f,g**)**, the BSDE* (5.1) *admits a unique solution* $(Y^{t,x},Z^{t,x})\in S^2_{\mathbb{F},c}[t,T]\times H^2_{\mathbb{F}}[t,T]$ *for any* $(t,x)\in[0,T]$.

Proof. The proof consists in a Picard iteration procedure. We introduce the map $\Phi:\ S^2_{\mathbb{F},c}[t,T]\times H^2_{\mathbb{F}}[t,T]\to S^2_{\mathbb{F},c}[t,T]\times H^2_{\mathbb{F}}[t,T]$ defined by $\Phi(U,V)=(Y,Z)$, where (Y,Z) is the solution to the BSDE

$$Y_s \quad = \quad g(X^{t,x}_T)+\int_s^T f(r,X^{t,x}_r,U_r,V_r)dr-\int_s^T Z_r.dW_r \tag{5.2}$$

for all $s\in[t,T]$. We need to show that the map Φ is well defined, that is, for any $(U,V)\in S^2_{\mathbb{F},c}[t,T]\times H^2_{\mathbb{F}}[t,T]$, equation (5.2) admits a unique solution. We first notice that the component Y is given by

$$Y_s \quad = \quad \mathbb{E}\Big[g(X^{t,x}_T)+\int_s^T f(r,X^{t,x}_r,U_r,V_r)ds|\mathcal{F}^t_s\Big]\ .$$

Then by Itô's martingale representation Theorem, there exists a unique $Z \in H^2_{\mathbb{F}}[t,T]$ such that

$$g(X_T^{t,x}) + \int_t^T f(r, X_r^{t,x}, U_r, V_r)dr = \mathbb{E}\Big[g(X_T^{t,x}) + \int_t^T f(r, X_r^{t,x}, U_r, V_r)dr\Big] + \int_t^T Z_r.dW_r\ .$$

Taking the conditional expectation given $\mathcal{F}_s^t$ we get

$$Y_s + \int_t^s f(r, X_r^{t,x}, U_r, V_r)dr \quad = \quad Y_0 + \int_t^s Z_r.dW_r$$

from which we deduce that (Y,Z) is a solution to (5.2). Finaly, The BDG Inequality ensures that $Y \in S^2_{\mathbb{F},c}[t,T]$.

To show that (5.1) admits a unique solution, we prove that Φ is a strict contraction on $S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T]$. To this end we introduce the modified norm $\|.\|_\gamma$ defined by

$$\|(Y,Z)\|_\gamma \quad = \quad \sqrt{\mathbb{E}\Big[\int_t^T e^{\gamma s}\Big(|Y_s|^2 + |Z_s|^2\Big)ds\Big]}$$

for $(Y,Z) \in S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T]$. Fix $(U,V),(U',V') \in S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T]$ and define $(Y,Z) = \Phi(U,V)$, $(Y',Z') = \Phi(U',V')$, $(\delta U, \Delta V) = (U-U', V-V')$ and $(\delta Y, \Delta Z) = (Y-Y', Z-Z')$. Using $(\mathbf{H}b,\sigma)$, we get from Itô's formula the existence of a constant K such that

$$\begin{aligned} e^{\gamma s}\mathbb{E}|\delta Y_s|^2 + \mathbb{E}\int_s^T e^{\gamma r}\Big(\gamma|\delta Y_r|^2 + |\delta Z_r|^2\Big)dr \quad &\leq \\ KE\int_s^T e^{\gamma r}|\delta Y_r|(|\delta U_r| + |\delta V_r|)dr \quad &\leq \\ 4K^2\mathbb{E}\int_s^T e^{\gamma r}|\delta Y_r|^2 dr + \frac{1}{2}\mathbb{E}\int_s^T e^{\gamma r}(|\delta U_r|^2 + |\delta V_r|^2)dr & \end{aligned}$$

for all $s \in [t,T]$. We take $\gamma = 1 + 4K^2$, and we get

$$\|(\delta Y, \delta Z)\|_\gamma \quad \leq \quad \frac{1}{\sqrt{2}}\|(\delta U, \delta V)\|_\gamma$$

which shows that Φ is a strict contraction. $\square$

We now turn to the case where we impose a constraint on the solution (Y,Z) of the BSDE.

We first consider the reflected case where we ask the component Y of the solution to stay above an obstacle. More precisely, we fix a function $h : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ and we look for a solution (Y,Z) to (5.1) such that

$$Y_s \quad \geq \quad h(s, X_s^{t,x})$$

for all $s \in [t,T]$. Unfortunately, this problem is ill-posed as we cannot find such a solution in many cases. We therefore relax the equation (5.1) by adding a nondecreasing process K that helps the component Y to satisfy the obstacle constraint. We introduce the subset $A^2_{\mathbb{F}}[t,T]$ of $S^2_{\mathbb{F}}[t,T]$ (resp. $A^2_{\mathbb{F},c}[t,T]$ of of $S^2_{\mathbb{F},c}[t,T]$) consisting of nondecreasing processes $K = (K_s)_{s\in[t,T]} \in S^2_{\mathbb{F}}[t,T]$ (resp. $S^2_{\mathbb{F},c}[t,T]$) such that $K_t = 0$. We then look for a triplet $(Y,Z,K) \in S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T] \times A^2_{\mathbb{F},c}[t,T]$ satisfying the reflected BSDE

$$Y_s^{t,x} \quad = \quad g(X_T^{t,x}) + \int_s^T f(r, X_r^{t,x}, Y_r^{t,x}, Z_r^{t,x})dr - \int_s^T Z_r^{t,x}.dW_r + K_T^{t,x} - K_s^{t,x}\ , \qquad s \in [t,T] \tag{5.3}$$

and the obstacle constraint

$$Y_s^{t,x} \quad \geq \quad h(s, X_s^{t,x})\ , \qquad s \in [t,T]\ . \tag{5.4}$$

The introduction of the component K in the solution gives more freedom than needed. The consequence is that the equation (5.3)-(5.4) might have several solutions. As the process K is needed to help the component Y to satisfy (5.4), we can ask in addition that it "pushes" Y the less possible to satisfy (5.4). This leads to the following minimality constraint

$$\int_t^T \Big((Y_s^{t,x} - h(s, X_s^{t,x})\Big)dK_s^{t,x} \quad = \quad 0\ . \tag{5.5}$$

To ensure the well posedness of the reflected BSDE, we also introduce the following assumption on the function h.

(Hh) The function h is continuous and satisfies the following growth property: there exists a constant M_h such that

$$|h(t,x)| \quad \leq \quad M_h\Big(1+|x|\Big)$$

for all $t \in [0,T]$ and $x \in \mathbb{R}^d$.

We are now able to state the well posedness of this triplet of equations.

Theorem 5.2. *Suppose that $g(x) \geq h(T,x)$, for all $x \in \mathbb{R}^d$. Under **(H**b,σ**)**, **(H**f,g**)** and **(H**h**)**, the BSDE* (5.3)-(5.4)-(5.5) *admits a unique solution $(Y^{t,x}, Z^{t,x}, K^{t,x}) \in S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T] \times A^2_{\mathbb{F},c}[t,T]$ for any $(t,x) \in [0,T]$.*

Proof. (Sketch) As for the non-reflected case, the proof consists in defining a map $\Phi: S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T] \to S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T]$ defined by $\Phi(U,V) = (Y,Z)$ where (Y,Z) is the solution to the reflected BSDE

$$\begin{aligned} Y_s \quad = \quad & g(X_T^{t,x}) + \int_s^T f(r, X_r^{t,x}, U_r, V_r)dr - \int_t^T Z_r.dW_r \\ & + K_T^{t,x} - K_s^{t,x}\;, \qquad s \in [t,T]\;, \end{aligned} \tag{5.6}$$

for all $s \in [0,T]$, and satisfies (5.4)-(5.5). Then this map Φ is shown to be a strict contraction for the modified norm $\|\cdot\|_\gamma$ used in the proof of Theorem 5.1. $\square$

Remark 5.3. Let us mention that the solution of the BSDE admits the following optimal stopping representation:

$$Y_s^{t,x} \quad = \quad \operatorname*{ess\,sup}_{\tau \in \mathcal{T}_{[s,T]}} \mathbb{E}\Big[g(X_T^{t,x})\mathbb{1}_{\tau=T} + h(\tau, X_\tau^{t,x})\mathbb{1}_{\tau<T} + \int_s^\tau f(r, X_r^{t,x}, Y_r^{t,x}, Z_r^{t,x})dr \Big| \mathcal{F}_s^t\Big]$$

where $\mathcal{T}_{[s,T]}$ stands for the set of $\mathbb{F}^t$ stopping times valued in $[s,T]$ for all $s \in [t,T]$. In particular, to show that the map Φ is well defined, the process

$$Y_s^{t,x} \quad = \quad \operatorname*{ess\,sup}_{\tau \in \mathcal{T}_{[s,T]}} \mathbb{E}\Big[g(X_T^{t,x})\mathbb{1}_{\tau=T} + h(\tau, X_\tau^{t,x})\mathbb{1}_{\tau<T} + \int_s^\tau f(r, X_r^{t,x}, U_r^{t,x}, V_r^{t,x})dr \Big| \mathcal{F}_s^t\Big]$$

is proved to be solution of (5.6). We refer to Proposition 5.1 and Theorem 5.2 in [6] for the details of the proof.

We now turn to the second case of constraint on the BSDE. To this end, we introduce a closed, convex and bounded set

$$\mathcal{C} \quad \subset \quad \mathbb{R}^d \quad , \quad \text{such that } 0 \in \mathcal{C} \tag{5.7}$$

As for the reflected case, we look for a triplet $(Y^{t,x}, Z^{t,x}, K^{t,x}) \in S^2_{\mathbb{F},c}[t,T] \times H^2_{\mathbb{F}}[t,T] \times A^2_{\mathbb{F},c}[t,T]$ satisfying the dynamics (5.3), but we impose the following constraint on the component Z

$$Z_s^{t,x} \quad \in \quad \sigma(s, X_s^{t,x})^\top \mathcal{C}\;, \qquad d\mathbb{P} \otimes ds - a.e. \tag{5.8}$$

Unfortunately, we are not able to provide a minimality condition as (5.5) for the reflected case. Moreover, the components Y and K might not be continuous as in the previous cases. We therefore look for a minimal solution, that is, a triplet $(Y^{t,x}, Z^{t,x}, K^{t,x}) \in S^2_{\mathbb{F}}[t,T] \times H^2_{\mathbb{F}}[t,T] \times A^2_{\mathbb{F}}[t,T]$ satisfying (5.3)-(5.8) such that for any other triplet $(\tilde{Y}^{t,x}, \tilde{Z}^{t,x}, \tilde{K}^{t,x}) \in S^2_{\mathbb{F}}[t,T] \times H^2_{\mathbb{F}}[t,T] \times A^2_{\mathbb{F}}[t,T]$ solution to (5.3)-(5.8) we have

$$Y_s^{t,x} \quad \leq \quad \tilde{Y}_s^{t,x}\;, \quad s \in [t,T]\;.$$

This kind of BSDEs is related to the super-replication problem in finance (see e.g. [7]). To get existence and uniqueness of such a minimal solution, we need to strengthen the assumptions on the forward coefficients b and σ

(Hb,σ)'

(i) The values of the matrix-valued function σ are invertible.

(ii) The functions b, σ and σ^{-1} are bounded: there exists a constant $M_{b,\sigma}$ such that

$$|b(t,x)|+|\sigma(t,x)|+|\sigma^{-1}(t,x)| \quad \leq \quad M_{b,\sigma}$$

for all $t\in[0,T]$ and $x\in\mathbb{R}^d$.

We impose additional assumptions on the backward coefficients f and g.

(Hf,g)'

(i) The function g is bounded: there exists a constant M_g such that $|g(x)|\leq M_g$ for all $x\in\mathbb{R}^d$.

(ii) The function f is continuous and satisfies the following growth property: there exists a constant M_f such that

$$|f(t,x,y,z)| \quad \leq \quad M_f\Big(1+|y|+|z|\Big)$$

for all $t\in[0,T]$, $x\in\mathbb{R}^d$, $y\in\mathbb{R}$ and $z\in\mathbb{R}^d$.

We also introduce the support function $\delta_{\mathcal{C}}$ of the convex set $\mathcal{C}$ defined by

$$\delta_{\mathcal{C}}(u) \quad = \quad \sup_{p\in\mathcal{C}} u\cdot p$$

for all $u\in\mathbb{R}^d$. We recall the following characterization of the convex set $\mathcal{C}$ (see Theorem 13.1 in [25])

$$p\in\mathcal{C} \quad \Leftrightarrow \quad \inf_{|u|=1}\Big\{\delta_{\mathcal{C}}(u)-p.u\Big\}\geq 0 \tag{5.9}$$

The general existence and uniqueness result is stated as follows.

Theorem 5.4. *Under* **(Hb,σ)***,* **(Hb,σ)'***,* **(Hf,g)** *and* **(Hf,g)'***, there exists a unique minimal solution to* (5.3)-(5.8)*.*

Proof. (Sketch) We first construct a solution to (5.3)-(5.8). Under **(Hf,g)** and **(Hf,g)'** and since $0\in\mathcal{C}$, a straightforward computation shows that the processes

$$\tilde{Y}_s^{t,x} \quad = \quad (M_g+1)e^{M_f(T-s)}-1, \quad s\in[t,T)\ , \quad U_T \quad = \quad g(X_T^{t,x})$$

and $\tilde{Z}_s^{t,x}=0, \quad s\in[t,T)$, give a solution to (5.3)-(5.8). We can then apply Theorem 4.2 in [21] and we get existence an uniqueness of the minimal solution to (5.3)-(5.8). Moreover, this minimal solution is the limit of the following penalized BSDEs:

$$Y_s^{t,x,n} \quad = \quad g(X_T^{t,x})+\int_s^T f_n(r,X_r^{t,x},Y_r^{t,x,n},Z_r^{t,x,n})dr-\int_s^T Z_r^{t,x,n}.dW_r \tag{5.10}$$

for all $s\in[t,T]$ where the functions f_n are defined by

$$f_n(t,x,y,z) \quad = \quad f(t,x,y,z)+n\Big(\inf_{|u|=1}\Big\{\delta_{\mathcal{C}}(u)-\sigma^\top(t,x)^{-1}z.u\Big\}\Big)$$

for all $(t,x,y,z)\in[0,T]\times\mathbb{R}^d\times\mathbb{R}\times\mathbb{R}^d$. The sequence $(Y^{t,x,n})_{n\geq 0}$ is non-decreasing and converges pointwisely to $Y^{t,x}$ and we also have

$$\mathbb{E}\Big[\int_t^T|Z_s^{t,x,n}-Z_s^{t,x}|^p ds\Big] \quad \to \quad 0$$

$$\mathbb{E}\Big[|K_T^{t,x}-n\int_t^T\inf_{|u|=1}\Big(\delta_{\mathcal{C}}(u)-\sigma^\top(s,X_s^{t,x})^{-1}Z_s^{t,x,n}.u\Big)ds|^p\Big] \quad \to \quad 0$$

as $n\to+\infty$ for all $p\in[1,2)$. From those convergences we deduce that

$$\int_t^T\inf_{|u|=1}\Big(\delta_{\mathcal{C}}(u)-\sigma^\top(s,X_s^{t,x})^{-1}Z_s^{t,x}.u\Big)ds \quad = \quad 0\ ,$$

which, combined with (5.9), shows that the constraint is satisfied at the limit. □

6 Semi-linear PDEs

We now show that solutions to BSDEs provide probabilistic representations for solution to semi-linear partial differential equations. We denote by $C^{1,2}([0,T]\times\mathbb{R}^d)$ the set of functions φ from $[0,T]\times\mathbb{R}^d$ which are one time differentiable w.r.t. the $t\in[0,T]$ and twice differentiable w.r.t. $x\in\mathbb{R}^d$ with continuous derivatives $\partial_t\varphi$, $\partial_x\varphi$ and $\partial^2_{xx}\varphi$.

We consider the parabolic PDE defined on $\mathbb{R}^d\times[0,T]$ by

$$\begin{cases} -\partial_t v(t,x)-\mathcal{L}v(t,x)-f\Big(t,x,v(t,x),\sigma^\top(t,x)\partial_x v(t,x)\Big)=0 \\ \text{ for } (t,x)\in[0,T)\times\mathbb{R}^d\ , \\ v(T,x)=g(x) \qquad \text{for } x\in\mathbb{R}^d\ . \end{cases} \tag{6.1}$$

Here $\mathcal{L}$ stands for the second order partial differential operator related to the diffusion X and defined by

$$\mathcal{L}\varphi(t,x) \;=\; b(t,x).\partial_x\varphi(t,x)+\frac{1}{2}\mathrm{Tr}\Big(\sigma\sigma^\top(t,x)\partial^2_{xx}\varphi(t,x)\Big)$$

for $\varphi\in C^{1,2}([0,T]\times\mathbb{R}^d)$ and $(t,x)\in[0,T]\times\mathbb{R}^d$. We first provide a link between BSDE (5.1) and PDE (6.1) in the regular case.

Theorem 6.1. *Let $v\in C^0([0,T]\times\mathbb{R}^d)\cap C^{1,2}([0,T)\times\mathbb{R}^d)$ be a classical solution of* (6.1)*, such that for some constants $C,q>0$ we have*

$$|\partial_x v(t,x)| \;\le\; C(1+|x|^q), \tag{6.2}$$

for all $(t,x)\in[0,T)\times\mathbb{R}^d$. Then, for each (t,x), $(v(s,X^{t,x}_s),\sigma^\top\partial_x v(s,X^{t,x}_s))_{s\in[t,T]}$[2] *is the solution of the BSDE* (5.1)*. In particular, we have $v(t,x)=Y^{t,x}_t$ for all $(t,x)\in[0,T]\times\mathbb{R}^d$.*

Proof. The proof consists in applying Itô's formula to $(v(s,X^{t,x}_s))_{s\in[t,T]}$ and using condition (6.2) to ensure that $(v(s,X^{t,x}_s),\sigma^\top\partial_x v(s,X^{t,x}_s))_{s\in[t,T]}\in S^2_{\mathbb{F},c}[t,T]\times H^2_{\mathbb{F}}[t,T]$. □

We aim to extend this link, in particular we would like to produce a solution to PDE (6.1) from the solution of the BSDE (5.1) using the formula $v(t,x)=Y^{t,x}_t$. Unfortunately, this function v might not be regular and we need to define a weak notion of solutions to (6.1).

Definition 6.2. *(i) $v\in C([0,T]\times\mathbb{R}^d)$ is called a viscosity subsolution of* (6.1) *if $v(T,x)\le g(x)$, $x\in\mathbb{R}^d$, and moreover for any $\varphi\in C^{1,2}([0,T]\times\mathbb{R}^d)$ and $(t,x)\in[0,T)\times\mathbb{R}^d$ which is a local maximum of $v-\varphi$ we have*

$$-\partial_t\varphi(t,x)-\mathcal{L}\varphi(t,x)-f(t,x,\varphi(t,x),\sigma^\top(t,x)\partial_x\varphi(t,x)) \;\le\; 0\ .$$

(ii) $v\in C([0,T]\times\mathbb{R}^d)$ is called a viscosity supersolution of (6.1) *if $v(T,x)\ge g(x)$, $x\in\mathbb{R}^d$, and for any $\varphi\in C^{1,2}([0,T]\times\mathbb{R}^d)$ and $(t,x)\in[0,T)\times\mathbb{R}^d$ which is a local minimum of $v-\varphi$ we have*

$$-\partial_t\varphi(t,x)-\mathcal{L}\varphi(t,x)-f(t,x,\varphi(t,x),\sigma^\top(t,x)\partial_x\varphi(t,x)) \;\ge\; 0\ .$$

(iii) $v\in C([0,T]\times\mathbb{R}^d)$ is called a viscosity solution of (6.1) *if it is both a sub and supersolution.*

In the sequel, we say that a function $\varphi:\ [0,T]\times\mathbb{R}^d\to\mathbb{R}$ has polynomial growth if there exist an integer $p\ge1$ and a constant $C>0$ such that

$$|\varphi(t,x)| \;\le\; C\Big(1+|x|^p\Big) \tag{6.3}$$

for all $(t,x)\in[0,T]\times\mathbb{R}^d$.

[2] Here and in the sequel, we take the convention $\partial_x v(T,X^{t,x}_T)=0$ if $\partial_x v(T,.)$ does not exist.

Theorem 6.3. *Under assumptions* ***(H****b*, σ***)*** *and* ***(H****f*, g***)***, *the function* v *defined by*

$$v(t,x) \quad = \quad Y_t^{t,x} \;, \quad (t,x) \in [0,T] \times \mathbb{R}^d \;, \tag{6.4}$$

where $(Y^{t,x}, Z^{t,x})$ *is the unique solution to* (5.1)*, is a continuous function which has polynomial growth, and is a viscosity solution of* (6.1)*.*

We refer to [20, Theorem 2.4] for the viscosity solution property and [23, Theorem 5.9] for the uniqueness. Let us mention that in the framework of viscosity solutions, the uniqueness is shown by proving a comparison result between subsolutions and supersolutions.

7 Obstacle problems

We turn to another class of parabolic PDEs called obstacle problem. This kind of equation take the following form:

$$\begin{cases} \min\Big\{ -\partial_t v(t,x) - \mathcal{L}v(t,x) - f\Big(t,x,v(t,x),\sigma^\top \partial_x v(t,x)\Big) \;, \\ \qquad v(t,x) - h(t,x)\Big\} = 0 \text{ for } (t,x) \in [0,T) \times \mathbb{R}^d \;, \\ v(T,x) = g(x) \qquad \text{for } x \in \mathbb{R}^d \;. \end{cases} \tag{7.1}$$

We aim at relating this equation to reflected BSDEs. For that we first give the definition of viscosity solutions for this kind of PDE.

Definition 7.1. *(i)* $v \in C([0,T] \times \mathbb{R}^d)$ *is called a viscosity subsolution of* (7.1) *if* $v(T,x) \leq g(x)$*,* $x \in \mathbb{R}^d$*, and moreover for any* $\varphi \in C^{1,2}([0,T] \times \mathbb{R}^d)$ *and* $(t,x) \in [0,T) \times \mathbb{R}^d$ *which is a local maximum of* $v - \varphi$ *we have*

$$\min\Big\{ -\partial_t\varphi(t,x) - \mathcal{L}\varphi(t,x) - f(t,x,\varphi(t,x),\sigma^\top(t,x)\partial_x\varphi(t,x)) \;,\; \varphi(t,x) - h(t,x)\Big\} \leq 0 \;.$$

(ii) $v \in C([0,T] \times \mathbb{R}^d)$ *is called a viscosity supersolution of* (7.1) *if* $v(T,x) \geq g(x)$*,* $x \in \mathbb{R}^d$*, and for any* $\varphi \in C^{1,2}([0,T] \times \mathbb{R}^d)$ *and* $(t,x) \in [0,T) \times \mathbb{R}^d$ *which is a local minimum of* $v - \varphi$ *we have*

$$\min\Big\{ -\partial_t\varphi(t,x) - \mathcal{L}\varphi(t,x) - f(t,x,\varphi(t,x),\sigma^\top(t,x)\partial_x\partial_x\varphi(t,x)) \;,\; \varphi(t,x) - h(t,x)\Big\} \geq 0 \;.$$

(iii) $v \in C([0,T] \times \mathbb{R}^d)$ *is called a viscosity solution of* (7.1) *if it both is a sub and supersolution.*

Theorem 7.2. *Under assumptions* ***(H****b*, σ***)***, ***(H****f*, g***)*** *and* ***(H****h***)***, *the function* v *defined by*

$$v(t,x) \quad = \quad Y_t^{t,x} \;, \quad (t,x) \in [0,T] \times \mathbb{R}^d \;, \tag{7.2}$$

where $(Y^{t,x}, Z^{t,x}, K^{t,x})$ *is the unique solution to* (5.3)-(5.4)-(5.5)*, is a continuous function which grows at most polynomially at infinity, and is the unique viscosity solution of* (7.1)*.*

We refer to [6, Theorems 8.5 and 8.6] for the proof. Let us mention that the proof of the viscosity solution property is done by a penalization argument which allows to use the viscosity property in the non-reflected case and pass to the limit by a stability property for viscosity solutions.

8 Variational inequalities

We turn to another class of PDEs called variational inequalities. Those PDEs take the following form.

$$\begin{cases} \min\Big\{ -\partial_t v(t,x) - \mathcal{L}v(t,x) - f\Big(t,x,v(t,x),\sigma^\top(t,x) v(t,x)\Big) \;, \\ \qquad H\Big(\partial_x v(t,x)\Big)\Big\} = 0 \text{ for } (t,x) \in [0,T) \times \mathbb{R}^d \;, \\ v(T,x) = g(x) \qquad \text{for } x \in \mathbb{R}^d \;. \end{cases} \tag{8.1}$$

Here H is defined by

$$H(p) \quad = \quad \inf_{|u|=1} \Big(\delta_{\mathcal{C}}(u) - p.u\Big)$$

for all $p \in \mathbb{R}^d$ and $\mathcal{C}$ is the closed, convex and bounded set defined in (5.7). For this kind of PDE, the solutions may be discontinuous. We therefore need to extend the definition of viscosity solutions to include discontinuous functions. We say that a function $\varphi : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ is lower-semicontinuous (resp. upper-semicontinuous) if

$$\begin{array}{rcl} \liminf_{(t',x')\to(t,x)} \varphi(t',x') & \geq & \varphi(t,x) \\ (\text{resp. } \liminf_{(t',x')\to(t,x)} \varphi(t',x') & \leq & \varphi(t,x) \ ) \end{array}$$

for all $(t,x) \in [0,T] \times \mathbb{R}^d$. We denote by $LSC([0,T] \times \mathbb{R}^d)$ (resp. $USC([0,T] \times \mathbb{R}^d)$) the set of lower-semicontinuous (resp. upper-semicontinuous) function from $[0,T] \times \mathbb{R}^d$ to $\mathbb{R}$.

For a locally bounded function $u : [0,T] \times \mathbb{R}^d \to \mathbb{R}$, we denote by u_* and u^* its lower and upper-semicontinuous envelope respectively, *i.e.* u_* (resp. u^*) is the greatest (resp. smallest) element of $LSC([0,T] \times \mathbb{R}^d)$ (resp. $USC([0,T] \times \mathbb{R}^d)$) smaller (resp. greater) than u on $[0,T) \times \mathbb{R}^d$. u_* and u^* are given by

$$\begin{array}{rcl} u_*(t,x) & = & \liminf_{(t',x')\to(t,x)\ ,\ t'<T} u(t',x') \\ u^*(t,x) & = & \limsup_{(t',x')\to(t,x)\ ,\ t'<T} u(t',x') \end{array}$$

We are now able to give the definition of discontinuous viscosity solutions.

Definition 8.1. *(i) $v \in USC([0,T]\times\mathbb{R}^d)$ is called a viscosity subsolution of* (8.1) *if for any $\varphi \in C^{1,2}([0,T]\times\mathbb{R}^d)$ and $(t,x) \in [0,T] \times \mathbb{R}^d$ which is a local maximum of $v - \varphi$ we have*

$$\min\Big\{ -\partial_t\varphi(t,x) - \mathcal{L}\varphi(t,x) - f(t,x,\varphi(t,x),\sigma^\top(t,x)\partial_x\varphi(t,x))\ ,\ H\Big(\partial_x\varphi(t,x)\Big)\Big\} \leq 0\ ,$$

for $t \in [0,T)$, and $\min\Big\{v(T,x) - g(x)\ ,\ H\Big(\partial_x\varphi(T,x)\Big)\Big\} \leq 0$ *for $t = T$.*

(ii) $v \in LSC([0,T] \times \mathbb{R}^d)$ is called a viscosity supersolution of (8.1) *if for any $\varphi \in C^{1,2}([0,T] \times \mathbb{R}^d)$ and $(t,x) \in [0,T] \times \mathbb{R}^d$ which is a local minimum of $v - \varphi$ we have*

$$\min\Big\{ -\partial_t\varphi(t,x) - \mathcal{L}\varphi(t,x) - f(t,x,\varphi(t,x),\sigma^\top(t,x)\partial_x\varphi(t,x))\ ,\ H\Big(\partial_x\varphi(t,x)\Big)\Big\} \geq 0\ ,$$

for $t \in [0,T)$, and $\min\Big\{v(T,x) - g(x)\ ,\ H\Big(\partial_x\varphi(T,x)\Big)\Big\} \geq 0$, *for $t = T$.*

(iii) A locally bounded function v is called a viscosity solution of (8.1) *if v^* is a viscosity subsolution and and v_* is a viscosity supersolution.*

We notice that in the previous definition the terminal condition $v(T,.) = g$ is relaxed to take into account the effect of the constraint.

Theorem 8.2. *Under **(H**b,σ**)**, **(H**b,σ**)'**, **(H**f,g**)** and **(H**f,g**)'**, the function v defined by*

$$v(t,x) \;=\; Y_t^{t,x}\ , \quad (t,x) \in [0,T] \times \mathbb{R}^d\ , \tag{8.2}$$

where $(Y^{t,x}, Z^{t,x}, K^{t,x})$ is the minimal solution to (5.3)-(5.4)*, is a is a viscosity solution of* (8.1).

We refer to [24, Theorem 3.4] for a proof of the viscosity solution property on $[0,T) \times \mathbb{R}^d$. The viscosity solution property on $\{T\} \times \mathbb{R}^d$ is much more involved and can be proved by the same arguments as in [15, Theorem 4.2]. For the uniqueness, we have the following weaker result given by [24, Proposition 5].

Theorem 8.3. ***(H**b,σ**)**, **(H**b,σ**)'**, **(H**f,g**)** and **(H**f,g**)'** the function v defined by* (8.2) *is the smallest viscosity solution to* (8.1) *satisfying a polynomial growth condition.*

Again, the proof of minimality consists in using a comparison result for semilinear PDEs. This allows to show that all the penalized solutions are smaller than any solution to (8.1). By sending the penalization parameter to $+\infty$ we get that the function v is smaller than any other solution to (8.1).

Part III: Neural network approximation of PDEs

In this last part, we present some algorithms based on neural networks for the approximation of the value $v(t,x)$ at a given point $(t,x)\in[0,T]\times\mathbb{R}^d$ of a solution v to one of the PDEs presented in the previous part. In the sequel the approximations are presented for $t=0$, but they can be extended to any $t\in[0,T]$ by replacing the diffusion X defined bellow in (9.1) by $X^{t,x}$.

9 The semi-linear case

We consider the semi-linear PDE (6.1). We recall that it takes the following form

$$\begin{cases} -\partial_t v(t,x) - \mathcal{L}v(t,x) - f\Big(t,x,v(t,x),\sigma^\top(t,x)\partial_x v(t,x)\Big) = 0 \\ \text{ for } (t,x)\in[0,T)\times\mathbb{R}^d\ , \\ v(T,x) = g(x) \qquad \text{for } x\in\mathbb{R}^d\ , \end{cases}$$

with $\mathcal{L}$ the second order local operator related to the diffusion X and defined by

$$\mathcal{L}\varphi(t,x) \;=\; b(t,x).\partial_x\varphi(t,x) + \frac{1}{2}\mathrm{Tr}\Big(\sigma\sigma^\top(t,x)\partial^2_{xx}\varphi(t,x)\Big)$$

for $\varphi\in C^{1,2}([0,T]\times\mathbb{R}^d)$ and $(t,x)\in[0,T]\times\mathbb{R}^d$.

We provide two kind of numerical schemes for the approximation of $v(t=0,x)$ for $x\in\mathbb{R}^d$. We fix a deterministic initial condition $X_0 = x\in\mathbb{R}^d$ and we denote by $X\in\Big(S^2_{\mathbb{F},c}[0,T]\Big)^d$ the process defined by

$$X_t \;=\; X_0 + \int_0^t b(r,X_r)dr + \int_0^t \sigma(r,X_r)dW_r, \quad t\geq 0\ . \tag{9.1}$$

We also fix a time grid $\pi=\{t_0=0<t_1<\cdots<t_N=T\}$ of the time interval $[0,T]$ and we denote by $\bar{X}^\pi$ the related Euler-Maruyama scheme of X. $\bar{X}^\pi$ is defined by $\bar{X}^\pi_{t_0}=X_0$ and

$$\bar{X}^\pi_{t_{n+1}} \;=\; \bar{X}^\pi_{t_n} + b(t_n,\bar{X}^\pi_{t_n})\Delta t_n + \sigma(t_n,\bar{X}^\pi_{t_n})\Delta W_n$$

where

$$\Delta t_n = t_{n+1}-t_n \quad \text{and} \quad \Delta W_n = W_{t_{n+1}} - W_{t_n}$$

for $n=0,\ldots,N-1$. We also denote by $|\pi|$ the mesh of the grid π:

$$|\pi| \;=\; \max_{0\leq n\leq N-1}(t_{n+1}-t_n)\ .$$

9.1 Han-Jentzen-E algorithm

This algorithm was developed in the papers [8, 9]. If the PDE (6.1) admits a unique regular solution v, we have

$$\begin{aligned} v(t,X_t) \;=&\; v(0,X_0) - \int_0^t f\Big(s,X_s,v(s,X_s),\sigma^\top(s,X_s)\partial_x v(s,X_s)\Big)ds \\ &+ \int_0^t \partial_x v(s,X_s)^\top\sigma(s,X_s)dW_s \end{aligned} \tag{9.2}$$

for all $t\in[0,T]$. To derive a numerical algorithm to compute $v(0,X_0)$, we use the identity (9.2) and replace it by

$$\begin{aligned} v(t_{n+1},\bar{X}^\pi_{t_{n+1}}) \;\approx&\; v(t_n,\bar{X}^\pi_{t_n}) - f\Big(t_n,\bar{X}^\pi_{t_n},v(t_n,\bar{X}^\pi_{t_n}),\sigma^\top\partial_x v(t_n,\bar{X}^\pi_{t_n})\Big)\Delta t_n \\ &+\partial_x v(t_n,\bar{X}^\pi_{t_n})^\top\sigma(t_n,\bar{X}^\pi_{t_n})\Delta W_n \\ \approx&\; F\Big(t_{n+1},\bar{X}^\pi_{t_{n+1}},v(t_n,\bar{X}^\pi_{t_n}),\sigma^\top\partial_x v(t_n,\bar{X}^\pi_{t_n}),\Delta t_n,\Delta W_n\Big) \end{aligned} \tag{9.3}$$

for $n = 0, \ldots, N-1$, where the function F is defined by

$$F(t, x, y, z, h, \Delta) \quad = \quad y - f(t, x, y, z)h + z^\top \Delta \tag{9.4}$$

for $(t, x, y, z, h, \Delta) \in [0, T] \times \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d$.

The next key step is to approximate the function $v(0, .)$ by a neural network $NN^{\theta_{v_0}}$ and the functions $\sigma(t_n, .)^\top \partial_x v(t_n, .)$ by neural networks NN^{θ_n} for $n = 0, \ldots, N-1$. Here, we request the activation function ρ to be measurable, bounded and nonconstant, so that we can apply Theorem 3.1. We notice that, for $n = 0, \ldots, N-1$, the approximation of $v(t_n, .)$ given by this algorithm depends on the parameters $(\theta_{v_0}, \theta_0, \ldots, \theta_n)$ and we denote it by $\hat{v}_n(., \theta_{v_0}, \theta_0, \ldots, \theta_n)$. The total set of parameters $\theta = (\theta_{v_0}, \theta_0, \ldots, \theta_{N-1})$ is chosen so as to minimize the square error between the terminal condition $g(\bar{X}_T^\pi)$ and $\hat{v}_N(\bar{X}_T^\pi, \theta_{v_0}, \theta_0, \ldots, \theta_N)$:

$$\hat{\theta} = (\hat{\theta}_{v_0}, \hat{\theta}_0, \ldots, \hat{\theta}_{N-1}) \quad \in \underset{(\theta_{v_0}, \theta_0, \ldots, \theta_{N-1})}{\operatorname{argmin}} \mathbb{E}\left[\left|g\Big(\bar{X}_T^\pi\Big) - \hat{v}_N\Big(\bar{X}_T^\pi, \theta_{v_0}, \theta_0, \ldots, \theta_N\Big)\right|^2\right].$$

This last minimization is done using a stochastic gradient descent type algorithm.

Algorithm 1: HJE algorithm.

Initialize the approximation $\hat{v}_0$ of $v(0, .)$ as $\hat{v}_0 = NN^{\theta_{v_0}}$.
for $n = 0, \ldots, N-1$ **do**

$$\sigma^\top(t_n, .)\widehat{\partial_x v_n} \quad = \quad NN^{\theta_n^*}$$

and

$$\hat{v}_{n+1}(\bar{X}_{t_{n+1}}^\pi) \quad = \quad F\Big(t_{n+1}, \bar{X}_{t_{n+1}}^\pi, v_n(\bar{X}_{t_n}^\pi), \sigma^\top(t_n, \bar{X}_{t_n}^\pi)\widehat{\partial_x v_n}(\bar{X}_{t_n}^\pi), \Delta t_n, \Delta W_n\Big)$$

end

$$\hat{\theta} = (\hat{\theta}_{v_0}, \hat{\theta}_0, \ldots, \hat{\theta}_{N-1}) \quad \in \underset{(\theta_{v_0}, \theta_0, \ldots, \theta_{N-1})}{\operatorname{argmin}} \mathbb{E}\left[\left|g\big(\bar{X}_T^\pi\big) - \hat{v}_N\left(\bar{X}_T^\pi, \theta_{v_0}, \theta_0, \ldots, \theta_N\right)\right|^2\right].$$

We put as an input the parameters $(\theta_{v_0}, \theta_0, \ldots, \theta_n)$. We then compute the related function $\hat{v}_N(., \theta_{v_0}, \theta_0, \ldots, \theta_N)$. As an output, we get the parameters $(\hat{\theta}_{v_0}, \hat{\theta}_0, \ldots, \hat{\theta}_n)$ minimizing the quadratic error between $\hat{v}_N(., \theta_{v_0}, \theta_0, \ldots, \theta_N)$ and g. The related approximation of $v(0, X_0)$ is given by $NN^{\hat{\theta}_{v_0}}(X_0)$.

In [8], the authors provide examples illustrating the efficiency of their algorithm. They test their algorithm on three PDEs: Black and Scholes with default risk, linear quadratic HJB equation and Allen-Cahn equation in dimension $d = 100$. They obtain a relative error of 0,46%, 0,17% and 0,30% in a runtime of 1607, 330 and 647 seconds respectively (on a Mac book Pro computer).

9.2 Huré-Pham-Warin algorithm

In [11], the authors propose a new kind of algorithm and provide a theoretical bound of the error approximation. Contrary to the previous algorithm which writes in a forward form, the Huré-Pham-Warin algorithm computes the solution in a backward way using the approximation (9.3). To proceed in this way, one needs to approximate the unknown function v and its gradient $\sigma^\top \partial_x v$. Two algorithms are then developed in [11] to compute an approximation $\hat{v}_n$ of $v(t_n, .)$ for $n = 0, \ldots, N$.

First algorithm The first algorithm consists in approximating in a backward way the functions $v(t_n, .)$ and $\sigma^\top(t_n, .)\partial_x v(t_n, .)$ by two different neural networks NN^{θ_n} and $NN^{\partial\theta_n}$. As in the HJE algorithm, we request the activation function ρ to be measurable bounded and nonconstant.

Algorithm 2: First HPW algorithm.

Initialize the approximation $\hat{v}_N^1$ of $v(t_N,.)$ as $\hat{v}_N^1 = g$.
for $n = N-1, \ldots, 0$ **do**

$$\begin{aligned} \hat{v}_n^1 &= NN^{\theta_n^*} \\ \sigma^\top(t_n,.)\widehat{\partial_x v_n^1} &= NN^{\partial\theta_n^*} \end{aligned}$$

where

$$(\theta_n^*, \partial\theta_n^*) \in \operatorname*{argmin}_{(\theta_n,\partial\theta_n)\in\Theta_m^{d+1}} \mathbb{E}\Big[\Big|\hat{v}_{n+1}^1\big(\bar{X}_{t_{n+1}}^\pi\big) - F\big(t_n, \bar{X}_{t_n}^\pi, NN^{\theta_n}(\bar{X}_{t_n}^\pi), NN^{\partial\theta_n}(\bar{X}_{t_n}^\pi), \Delta t_n, \Delta W_n\big)\Big|^2\Big].$$

end

At each loop, the pair is the couple $(\theta_n, \partial\theta_n)$ and the output is the couple $(\theta_n^*, \partial\theta_n^*)$ obtained by a SGD and minimizing the square error between NN^{θ_n} and $F(., NN^{\theta_n}, NN^{\partial\theta_n}, .)$. The related approximations of $v(t_n,.)$ and $\sigma^\top(t_n,.)\partial_x v(t_n,.)$ are given by $NN^{\theta_n^*}$ and $NN^{\partial\theta_n^*}$ respectively.

Second algorithm The second algorithm consists in approximating in a backward way the functions $v(t_n,.)$ and $\partial_x v(t_n,.)$ by the same neural network and its derivative NN^{θ_n} and $\partial_x NN^{\theta_n}$. As we need the neural network to be differentiable, we use a continuously differentiable activation function.

Algorithm 3: Second HPW algorithm.

Initialize the approximation $\hat{v}_N^1$ of $v(t_N,.)$ as $\hat{v}_N^2 = g$.
for $n = N-1, \ldots, 0$ **do**

$$\begin{aligned} \hat{v}_n^2 &= NN^{\theta_n^*} \\ \widehat{\partial_x v_n^2} &= \partial_x NN^{\theta_n^*} \end{aligned}$$

where

$$\theta_n^* \in \operatorname*{argmin}_{\theta_n\in\Theta_m} \mathbb{E}\Big[\Big|\hat{v}_{n+1}^2\big(\bar{X}_{t_{n+1}}^\pi\big) - F\big(t_n, \bar{X}_{t_n}^\pi, NN^{\theta_n}(\bar{X}_{t_n}^\pi), \sigma(t_n, \bar{X}_{t_n}^\pi)\partial_x NN^{\theta_n}(\bar{X}_{t_n}^\pi), \Delta t_n, \Delta W_n\big)\Big|^2\Big].$$

end

At each loop, the input is the parameter θ_n and the output is the parameter θ_n^* minimizing the square error between NN^{θ_n} and $F(., NN^{\theta_n}, \sigma(t_n,.)\partial NN^{\theta_n}, .)$ (a SGD can be performed to get θ_n^*). The related approximation of $v(0, X_0)$ is given by $NN^{\theta_0^*}(X_0)$.

We introduce $(Y, Z) \in S^2_{\mathbb{F},c}[0,T] \times H^2_{\mathbb{F}}[0,T]$ the solution to the backward SDE with coefficients $(0, X_0, f, g)$:

$$Y_t = g(X_T) + \int_t^T f(r, X_r, Y_r, Z_r)dr - \int_t^T Z_r.dW_r$$

for all $t \in [0,T]$. We recall that under $(\mathbf{H}b,\sigma)$ and $(\mathbf{H}f,g)$, we have existence and uniqueness of such a solution from Theorem 5.1.

The following additional regularity assumption on the coefficients f and g is used in [11] to study the convergence of these schemes.

$(\mathbf{H}f,g)$**"** The functions f and g satisfy the following regularity conditions: there exists two constants L_f and L_g such that

$$\begin{aligned} |f(t,x,y,z) - f(t',x',y,z)| &\leq L_f|x-x'| + \sqrt{|t-t'|} \\ |g(x) - g(x')| &\leq L_g|x-x'| \end{aligned}$$

for all $t \in [0,T]$, $x, x' \in \mathbb{R}^d$, $y \in \mathbb{R}$ and $z \in \mathbb{R}^d$.

We then have the following result. We recall that the definition of $m \to +\infty$, where m is the neural network dimensions, is given by (4.2).

Theorem 9.1. *Under* **(H**b,σ**)**, **(H**f,g**)** *and* **(H**f,g**)”** *we have the following convergence*

$$\lim_{|\pi|\to 0}\lim_{m\to+\infty}\max_{n=0,\ldots,N}\mathbb{E}\Big[\Big|Y_t-\hat{v}^1_n(\bar{X}^\pi_{t_n})\Big|^2\Big]+\mathbb{E}\Big[\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\Big|Z_t-\sigma^\top\widehat{\partial_x v_n}^{\,1}(t_n,\bar{X}^\pi_{t_n})\Big|^2dt\Big] \;=\; 0$$

Proof. (Sketch) Under Assumptions **(H**b,σ**)**, **(H**f,g**)** and **(H**f,g**)”**, we can apply Theorem 4.1 in [11] which provides an estimate of the square error depending on two terms.

(i) The first is the square error due to the neural network error approximation of some intermediary functions.

(ii) The second term is the path regularity square error of the component Z of the solution (Y,Z) to the BSDE.

From Theorem 3.1, we first get that the error (i) goes to zero as $m\to+\infty$. Then using the regularity assumptions on the coefficients given by the standing assumptions, we get that the error (ii) also goes to zero as $|\pi|$ goes to 0. ☐

Corollary 9.2. *Under* **(H**b,σ**)**, **(H**f,g**)**, **(H**f,g**)’** *and* **(H**f,g**)”** *we have the following convergence*

$$\lim_{|\pi|\to 0}\lim_{m\to+\infty}\max_{n=0,\ldots,N}\mathbb{E}\Big[\Big|v(t_n,X_{t_n})-\hat{v}^1_n(\bar{X}^\pi_{t_n})\Big|^2\Big] \;=\; 0$$

Moreover, if $v\in C^0([0,T]\times\mathbb{R}^d)\cap C^{1,2}([0,T)\times\mathbb{R}^d)$ *we also have the convergence on the gradients*

$$\lim_{|\pi|\to 0}\lim_{m\to+\infty}\mathbb{E}\Big[\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\Big|\sigma^\top\partial_x v(t,X_t)-\sigma^\top\widehat{\partial_x v_n}^{\,1}(t_n,\bar{X}^\pi_{t_n})\Big|^2dt\Big] \;=\; 0\,.$$

Proof. The first convergence is a direct consequence of Theorems 6.3 and 9.1. The second convergence, follows from Theorems 9.1 and 6.1. ☐

A study of the convergence of the second algorithm is also done in [11]. However, as this algorithm aims at approximating the function v and its gradient by the same neural network and its derivative, one needs to add regularity (differentiability) assumptions on the coefficients and to impose boundary conditions on the neural network coefficients to avoid explosion of the derivatives. We refer to Theorem 4.2 in [11] for the detailed statement of the result and the related conditions.

Some numerical tests are also done in [11]. The authors consider a PDE with trigonometrical nonlinearity f and several dimensions d. Let us mention the case of bounded solutions in dimension $d=50$ for which their first and second algorithm provide a relative error of 0,03% and 0,06% respectively.

10 Obstacle problems

We turn to the approximation of the obstacle problem (7.1). We recall that it takes the following form

$$\begin{cases}\min\Big\{-\partial_t v(t,x)-\mathcal{L}v(t,x)-f\Big(t,x,v(t,x),\sigma^\top\partial_x v(t,x)\Big)\,,\\ \qquad v(t,x)-h(t,x)\Big\}=0 \text{ for } (t,x)\in[0,T)\times\mathbb{R}^d\,,\\ v(T,x)=g(x) \qquad \text{for } x\in\mathbb{R}^d\,.\end{cases}$$

10.1 Huré-Pham-Warin algorithm

In [11], the authors extend their first algorithm for semi-linear PDEs to the obstacle problem (7.1) by correcting the approximation to keep it over the function h. In this algorithm, we take a measurable bounded and nonconstant activation function ρ.

Algorithm 4: HPW algorithm for obstacle problems.

Initialize the approximation $\hat{v}_N$ of $v(t_N,.)$ as $\hat{v}_N = g$.
for $n = N-1,\ldots,0$ **do**

$$\begin{aligned}\hat{v}_n &= \max\{NN^{\theta_n^*}, h(t_n,.)\}\\ \sigma^\top(t_n,.)\widehat{\partial_x v_n} &= NN^{\partial\theta_n^*}\end{aligned}$$

where

$$(\theta_n^*,\partial\theta_n^*) \in \operatorname{argmin}_{(\theta_n,\partial\theta_n)\in\Theta_m^{d+1}}\mathbb{E}\Big[\Big|\hat{v}_{n+1}\big(\bar{X}^\pi_{t_{n+1}}\big) - F\big(t_n,\bar{X}^\pi_{t_n},NN^{\theta_n}(\bar{X}^\pi_{t_n}),NN^{\partial\theta_n}(\bar{X}^\pi_{t_n}),\Delta t_n,\Delta W_n\big)\Big|^2\Big]\,.$$

end

At each loop, the input is the pair $(\theta_n,\partial\theta_n)$ and the output is the couple $(\theta_n^*,\partial\theta_n^*)$ minimizing the square error between NN^{θ_n} and $F(.,NN^{\theta_n},NN^{\partial\theta_n},.)$. The related approximations of $v(t_n,.)$ and $\sigma^\top(t_n,.)\partial_x v(t_n,.)$ are given by $\max\{NN^{\theta_n^*},h(t_n,.)\}$ and $NN^{\partial\theta_n^*}$ respectively. The minimization can be done by a SGD.

We introduce $(Y,Z,K)\in S^2_{\mathbb{F},c}[0,T]\times H^2_{\mathbb{F}}[0,T]\times A^2_{\mathbb{F},c}[t,T]$ the solution to the reflect BSDE with coefficients $(0,X_0,f,g,h)$:

$$Y_t = g(X_T) + \int_t^T f(r,X_r,Y_r,Z_r)dr - \int_t^T Z_r.dW_r + K_T - K_t\,, \tag{10.1}$$

$$Y_t \geq h(t,X_t) \tag{10.2}$$

for $t\in[0,T]$ and

$$\int_0^T \Big((Y_s - h(s,X_s)\Big)dK_s = 0\,. \tag{10.3}$$

We recall that under $(\mathbf{H}b,\sigma)$, $(\mathbf{H}f,g)$ and $(\mathbf{H}h)$, we have existence and uniqueness of such a solution from Theorem 5.2.

To prove the convergence of the functions $\hat{v}_n$ to v, we strenthen the assumption on the obstacle function h.

(Hh)' There exists a constant L_h such that

$$|h(t,x)-h(t',x')| \leq L_h\Big(\sqrt{t-t'}+|x-x'|\Big)$$

for all $t\in[0,T]$ and $x,x'\in\mathbb{R}^d$.

We then have the following convergence result.

Theorem 10.1. *Suppose that the function f does not depend on the variable z. Under* **(H**b,σ**)**, **(H**f,g**)**, **(H**f,g**)"** *and* **(H**h**)'** *we have the following convergence*

$$\lim_{|\pi|\to 0}\lim_{m\to+\infty}\max_{n=0,\ldots,N}\mathbb{E}\Big[\Big|Y_t - \hat{v}_n(\bar{X}^\pi_{t_n})\Big|^2\Big] = 0$$

Proof. (Sketch) Under Assumptions $(\mathbf{H}b,\sigma)$, $(\mathbf{H}f,g)$, $(\mathbf{H}f,g)$", $(\mathbf{H}h)$ and $(\mathbf{H}h)$' and since f does not depend on the variable z, we can apply Theorem 4.3 in [11] which provides an estimate of the square error depending on two terms.

(i) The first is the square error due to the neural network error approximation of some intermediary functions.

(ii) The second term is related to the path regularity square error of the component Y of the solution (Y,Z,K) to the reflected BSDE. It is then $O(|\pi|)$ under the regularity assumptions on the coefficients given by the standing assumptions.

From Theorem 3.1, we first get that the error (i) goes to zero as $m\to+\infty$. We therefore get the convergence as $|\pi|$ goes to 0 from the behavior of the term (ii). □

Corollary 10.2. *Suppose that the function f do not depend on the variable z. Under **(Hb,σ)**, **(Hf,g)**, **(Hf,g)"**, **(Hh)** and **(Hh)'** we have the following convergence*

$$\lim_{|\pi|\to 0}\lim_{m\to+\infty}\max_{n=0,\dots,N}\mathbb{E}\Big[\Big|v(t_n,X_{t_n})-\hat{v}_n(\bar{X}^{\pi}_{t_n})\Big|^2\Big] \;=\; 0$$

Proof. This convergence is a direct consequence of Theorem 8.2 and Theorem 10.1. □

Under additional regularity assumptions on the coefficients b, σ, f, g and h, an approximation result for the component Z of the reflected BSDE and hence for the function $\sigma^\top\partial_x v$ is provided in [11] (see their Theorem 4.4).

10.2 Becker-Cheridito-Jentzen algorithm

As shown by Theorem 8.2 and Remark 5.3, the obstacle problem (7.1) is related to an optimal stopping problem. In [4], a machine learning algorithm for the approximation of such an optimal stopping problem is proposed.

More precisely, the considered optimal stopping problem is of the following form:

$$V_n \;=\; \operatorname*{ess\,sup}_{\tau\in\mathcal{T}^\pi_n}\mathbb{E}\Big[g\Big(\bar{X}^\pi_\tau\Big)\mathbb{1}_{\tau=T}+h\Big(\tau,\bar{X}^\pi_\tau\Big)\mathbb{1}_{\tau<T}\Big|\mathcal{F}_{t_n}\Big]$$

where $\mathcal{T}^\pi_n$ stands for the set of stopping times τ w.r.t. the natural filtration of $\bar{X}^\pi$ and valued in π such that $\tau\geq t_n$.

The key idea is to reduce the optimal stopping problem to an optimization problem over stopping decisions of the form $\tau_N=N\xi_N(\bar{X}^\pi_T)$ with $\xi_N\equiv 1$ and

$$\tau_n \;=\; \sum_{j=n}^{N} j\xi_j(\bar{X}^\pi_{t_j})\prod_{k=n}^{j-1}\Big(1-\xi_k(\bar{X}^\pi_{t_k})\Big)$$

for $n=0,\dots,N-1$, where $\xi_0,\dots,\xi_{N-1}$ are measurable functions from $\mathbb{R}$ to $\{0,1\}$. Then, if we denote by $\tilde{\mathcal{T}}^\pi_n$ the set of such stopping times τ_n, we get from [4, Theorem 1 and Remark 2], that

$$V_n \;=\; \operatorname*{ess\,sup}_{\tau\in\tilde{\mathcal{T}}^\pi_n}\mathbb{E}\Big[g\Big(\bar{X}^\pi_\tau\Big)\mathbb{1}_{\tau=T}+h\Big(\tau,\bar{X}^\pi_\tau\Big)\mathbb{1}_{\tau<T}\Big|\mathcal{F}_{t_n}\Big]$$

for all $n=0,1,\dots,N-1$. Then, the neural network approximation consists in replacing the functions ξ_n by functions ξ^{θ_n} of the form

$$\xi^{\theta_n}(x) \;=\; \mathbb{1}_{[0,+\infty)}\Big(NN^{\theta_n}(x)\Big)\;,\quad x\in\mathbb{R}^d\;,\;\; n=0,\dots,N\;,$$

and choosing the parameter θ^*_n which maximizes

$$\mathbb{E}\Big[g(n,X_n)\Xi^{\theta_n}(X_n)+g(\tau_{n+1},X_{\tau_{n+1}})\Big(1-\Xi^{\theta_n}(X_n)\Big)\Big]$$

over θ_n, where

$$\Xi^{\theta_n}(x) \;=\; \psi\Big(NN^{\theta_n}(x)\Big)\;,\quad x\in\mathbb{R}^d\;,\;\; n=0,\dots,N\;,$$

with $\psi:\ \mathbb{R}\to(0,1)$ the standard logistic function defined by $\psi(u)=e^u/(1+e^u)$ for $u\in\mathbb{R}$. The function Ξ^{θ_n} can be interpreted as a stopping probability. We then define $\Theta^*=(\theta^*_0,\dots,\theta^*_N)$ and the stopping time

$$\tau^{\Theta^*} \;=\; \sum_{j=n}^{N} j\xi^{\theta^*_j}(\bar{X}^\pi_{t_j})\prod_{k=n}^{j-1}\Big(1-\xi^{\theta^*_k}(\bar{X}^\pi_{t_k})\Big)\;.$$

We took in this algorithm the ReLU activation function defined by $\rho(x)=\max\{x,0\}$ for any $x\in\mathbb{R}$.

Algorithm 5: BCJ deep optimal stopping algorithm.

Initialize $\xi_N \equiv 1$.
for $n = N-1, \ldots, 0$ **do**

$$\xi_n(x) \;=\; \mathbb{1}_{[0,+\infty)}\Big(NN^{\theta_n^*}(x)\Big)\,, \quad x \in \mathbb{R}^d\,, \quad n = 0, \ldots, N\,,$$

where

$$\theta_n^* \;\in\; \underset{\theta_n \in \Theta_m}{\arg\min}\; \mathbb{E}\Big[g(n, X_n)\Xi^{\theta_n}(X_n) + g(\tau_{n+1}, X_{\tau_{n+1}})\big(1 - \Xi^{\theta_n}(X_n)\big)\Big]\,.$$

with

$$\Xi^{\theta} \;=\; \psi\big(NN^{\theta}\big)$$

Set

$$\tau^{\Theta^*} \;=\; \sum_{j=n}^{N} j\xi^{\theta_j^*}(\bar{X}_{t_j}^{\pi}) \prod_{k=n}^{j-1}\Big(1 - \xi^{\theta_k^*}(\bar{X}_{t_k}^{\pi})\Big)\,.$$

end

At each loop, the input is the parameter θ_n and the output is θ_n^* minimizing (by a SGD) the presented mean value. Once all the output parameters $\Theta^* = (\theta_0^*, \ldots, \theta_{N-1}^*)$ are obtained, the related approximated optimal stopping time is given by τ^{Θ^*}.
We can state the following result.

Theorem 10.3. *We have the following convergence*

$$\lim_{m\to+\infty} \mathbb{E}\Big[g\Big(\bar{X}^{\pi}_{\tau^{\Theta^*}}\Big)\mathbb{1}_{\tau^{\Theta^*}=T} + h\Big(\tau^{\Theta^*}, \bar{X}^{\pi}_{\tau^{\Theta^*}}\Big)\mathbb{1}_{\tau^{\Theta^*}<T}\Big] \;=\; V_0\,.$$

Proof. The proof is a direct consequence of [4, Corollary 5]. □

The efficiency of the algorithm is illustrated in [4] by numerical examples. Let us mention the example of max-call options on $d = 5$ symmetric assets, for which they need about 30 seconds as computation time. Their results improved the precision of existing methods by a factor 2.

11 Variational inequalities

We end by the approximation of the variational inequality (8.1). We recall that it takes the following form

$$\begin{cases} \min\Big\{ -\partial_t v(t,x) - \mathcal{L}v(t,x) - f\Big(t, x, v(t,x), \sigma^\top(t,x)v(t,x)\Big)\,, \\ \qquad H\Big(\partial_x\partial_x v(t,x)\Big)\Big\} = 0 \text{ for } (t,x) \in [0,T) \times \mathbb{R}^d\,, \\ v(T,x) = g(x) \qquad \text{for } x \in \mathbb{R}^d\,, \end{cases}$$

where H is defined by

$$H(p) \;=\; \inf_{|u|=1}\Big(\delta_{\mathcal{C}}(u) - p.u\Big)$$

for all $p \in \mathbb{R}^d$ and $\mathcal{C}$ is the closed, convex and bounded set defined in (5.7).

We recall that from Theorems (8.2) and 8.3, there exists a unique minimal viscosity solution v to (8.1) and it is given by

$$v(t,x) \;=\; Y_t^{t,x}\,, \quad (t,x) \in [0,T] \times \mathbb{R}^d\,,$$

where $(Y^{t,x}, Z^{t,x}, K^{t,x})$ is the minimal solution to (5.3)-(5.8). In the sequel we describe an algorithm provided by [14] for the approximation of the function v using this BSDE representation.

We denote by $(Y, Z, K) \in S^2_{\mathbb{F}}[0,T] \times H^2_{\mathbb{F}}[0,T] \times A^2_{\mathbb{F}}[0,T]$ the minimal solution to the constrained BSDE

$$\begin{aligned} Y_t &= g(X_T) + \int_t^T f(r, X_r, Y_r, Z_r)dr - \int_t^T Z_r.dW_r \\ &\quad + K_T - K_t \,, \qquad t \in [0,T] \,, \end{aligned} \tag{11.1}$$

$$Z_t \in \sigma(t, X_t)^\top \mathcal{C} \,, \qquad d\mathbb{P} \otimes dt - a.e. \text{ on } \Omega \times [0,T] \,. \tag{11.2}$$

We recall that from Theorem 5.4, such a minimal solution exists and is unique under **(H**b, σ**)**, **(H**b, σ**)'**, **(H**f, g**)** and **(H**f, g**)'**.

11.1 Discretely constrained BSDE

We fix a constraint grid $\mathcal{R} = \{r_0 = 0 < r_1 < \ldots < r_\kappa = T\}$, with $\kappa \in \mathbb{N}^*$, of the time interval $[0,T]$. We denote by $|\mathcal{R}|$ its mesh:

$$|\mathcal{R}| = \max_{0 \le \ell \le \kappa - 1} (r_{\ell+1} - r_\ell) \,.$$

For a random variable R of the form $R = \varphi(X_s)$ with $\varphi : \mathbb{R}^d \to \mathbb{R}$, we define $\mathfrak{F}_{\mathcal{C},s}[R]$ by

$$\mathfrak{F}_{\mathcal{C},s}[R] = \sup_{y \in \mathbb{R}^d} \{\varphi(X_s + y) - \delta_{\mathcal{C}}(y)\} \,.$$

We also define the set $\tilde{S}^2_{\mathbb{F}}[0,T]$ of set of $\mathbb{R}$-valued $\mathbb{F}$-adapted *càglàd*[3] processes $Y = (Y_s)_{s\in[0,T]}$ such that $\mathbb{E}\Big[\sup_{s\in[t,T]} |Y_s|^2\Big] < +\infty$.

We then consider the discretely constrained BSDE: find $(Y^{\mathcal{R}}, \tilde{Y}^{\mathcal{R}}, Z^{\mathcal{R}}, K^{\mathcal{R}}) \in S^2_{\mathbb{F}}[0,T] \times \tilde{S}^2_{\mathbb{F}}[0,T] \times H^2_{\mathbb{F}}[0,T] \times A^2_{\mathbb{F}}[0,T]$ such that

$$Y^{\mathcal{R}}_T = \tilde{Y}^{\mathcal{R}}_T = \mathfrak{F}_{\mathcal{C},T}[g(X_T)] = \sup_{y \in \mathbb{R}^d} \{g(X_T + y) - \delta_{\mathcal{C}}(y)\} \tag{11.3}$$

and

$$\tilde{Y}^{\mathcal{R}}_u = Y^{\mathcal{R}}_{r_{k+1}} + \int_u^{r_{k+1}} f(s, X_s, \tilde{Y}^{\mathcal{R}}_s, Z^{\mathcal{R}}_s)ds - \int_u^{r_{k+1}} Z^{\mathcal{R}}_s.dW_s \tag{11.4}$$

$$Y^{\mathcal{R}}_u = \tilde{Y}^{\mathcal{R}}_u \mathbb{1}_{(r_k, r_{k+1})}(u) + \mathfrak{F}_{\mathcal{C},r_k}[\tilde{Y}^{\mathcal{R}}_u]^{t,x} \mathbb{1}_{\{r_k\}}(u) \tag{11.5}$$

for $u \in [r_k, r_{k+1})$, $k = 0, \ldots, \kappa - 1$, and

$$K^{\mathcal{R}}_u = \sum_{k=0}^{n} (Y^{\mathcal{R}}_{r_k} - \tilde{Y}^{\mathcal{R}}_{r_k}) \mathbb{1}_{r_k \le u \le T}$$

for $u \in [0,T]$. Such a solution is constructed by a backward induction and we get from [14, Proposition 3.3] that this BSDE has a unique solution. This discretely constrained BSDE can be used to approximate the continuously constrained BSDE as shown by the following result.

Theorem 11.1. *Let* $(\mathcal{R}^\ell)$ *be nondecreasing sequence of grids such that*

$$\lim_{\ell \to +\infty} |\mathcal{R}^\ell| = 0 \,.$$

We have the following convergence result

$$\lim_{n \to +\infty} \mathbb{E}\Big[\sup_{[0,T)} \Big|Y^{\mathcal{R}^n} - Y\Big|^2\Big] + \mathbb{E}\Big[\sup_{[0,T)} \Big|\tilde{Y}^{\mathcal{R}^n} - Y\Big|^2\Big] + \mathbb{E}\Big[\int_0^T \Big|Z^{\mathcal{R}^n}_s - Z_s\Big|^2 ds\Big] = 0 \,.$$

We refer to [14, Theorem 3.1 and Corollary 3.2] for the proof of this result.

[3] French acronym for 'left-continuous and right-limited'.

11.2 Neural network approximation of the discretely constrained BSDE

We now provide a neural network approximation of the discretely constrained BSDE (11.3)-(11.4)-(11.5). For that sake, we need to compute the facelift operator $\mathfrak{F}_{\mathcal{C},s}[\varphi(X_s)]$ of a given function φ. We face here an issue since we need to know all the values of the function φ to compute the facelift $\mathfrak{F}_{\mathcal{C},s}[\varphi(X_s)]$. To overcome this difficulty, we use the characterization of the facelift as the envelop $\hat{\varphi}$ of φ, *i.e.* the smallest function $\hat{\varphi}$ greater than φ, such that $\partial_x\hat{\varphi} \in \mathcal{C}$. This leads to approximate the facelift by a neural network greater than φ with derivatives in $\mathcal{C}$. As these constraints might be numerically too strong, we relax them and consider the following approximation:

$$\mathfrak{F}_{\mathcal{C},s}[\varphi(X_s)] \quad \approx \quad NN^{\theta^*_{m,\varepsilon}}(X_s)$$

$$\text{with } \theta^*_{m,\varepsilon} \quad \in \quad \arg\min_{\theta\in\Theta_m} \left\{ \mathbb{E}\Big[\big|(NN^\theta - \varphi)(X_s)\big|^2 \mathbb{1}_{B_\varepsilon}(X_s) \Big] \ , \ \theta \ \text{ s.t. } \mathbb{P}(\partial_x NN^\theta(X_s) \in \mathcal{C}_\varepsilon; \ (NN^\theta - \varphi_\ell)(X_s) \geq -\varepsilon \ \big| \ X_s \in B_\varepsilon) = 1 \right\}$$

where $\mathcal{C}_\varepsilon = \{y \in \mathbb{R}^d \ : \ \exists x \in \mathcal{C}, \ |x-y| \leq \varepsilon\}$, and B_ε stands for the ball $B(0, \frac{1}{\varepsilon})$. This approximation is combined with the previous first HPW algorithm for semi-linear PDEs to approximate the discretely constrained BSDEs. Since we need our neural networks to be differentiable, we use a continuously differentiable activation function.

Recall the definition of $\mathcal{R}$ in the previous subsection. We suppose that $\mathcal{R} \subset \pi$. More precisely, we suppose that π is of the form $\pi = \{\pi_k, \ k = 0, \ldots, \kappa - 1\}$ where π_k is a grid of $[r_k, r_{k+1}]$ of the form $\pi_k = \{t_{k,0} = r_k < \cdots < t_{k,n_k} = r_{k+1}\}$. We set $|\pi_k| = \max_{i=0,\ldots,n_k-1}(t_{k,i+1} - t_{k,i})$.

We define $\{\mathcal{V}^{\mathcal{R},\pi,\varepsilon,m}_{k,i}\}^{0\leq k\leq\kappa-1}_{0\leq i\leq n_k}$ and $(\tilde{\mathcal{V}}^{\mathcal{R},\pi,\varepsilon,m}_{k,i})^{0\leq k\leq\kappa-1}_{0\leq i\leq n_k}$ as follows.

Algorithm 6: Global approximation scheme for constrained BSDEs.

$$\mathcal{V}_{\kappa,0}^{\mathcal{R},\pi,\varepsilon,m} = \tilde{\mathcal{V}}_{\kappa,0}^{\mathcal{R},\pi,\varepsilon,m} = NN^{\theta^*_{\kappa,0}} \wedge (-M) \vee M$$

where

$$\theta^*_{\kappa,0} \in \arg\min \mathbb{E}\Big[\Big|NN^\theta(X_T^\pi) - g(X_T^\pi)\Big|^2 \;\Big|\; X_T^\pi \in B_{\varepsilon_\kappa}\Big]$$
$$\theta \in \Theta_{m^1_\kappa} \text{ s.t. } \mathbb{P}\Big(DNN^\theta(X_T^\pi) \in \mathcal{C}_{\varepsilon_\kappa}; NN^\theta(X_T^\pi) \geq g(X_T^\pi) - \varepsilon_\kappa \;\Big|\; X_T^\pi \in B_{\varepsilon_\kappa}\Big) = 1 .$$

for $k = \kappa - 1, \ldots, 0$ **do**

$$\mathcal{V}_{k,n_k}^{\mathcal{R},\pi,\varepsilon,m} = \mathcal{V}_{k+1,0}^{\mathcal{R},\pi,\varepsilon,m} \quad \text{and} \quad \tilde{\mathcal{V}}_{k,n_k}^{\mathcal{R},\pi,\varepsilon,m} = \tilde{\mathcal{V}}_{k+1,0}^{\mathcal{R},\pi,\varepsilon,m} .$$

for $i = n_k - 1, \ldots, 1$ **do**

$$\tilde{\mathcal{V}}_{k,i}^{\mathcal{R},\pi,\varepsilon,m} = \mathcal{V}_{k,i}^{\mathcal{R},\pi,\varepsilon,m} = NN^{\theta^*_{k,i}}$$

where

$$(\theta^*_{k,i}, \hat{\theta}^*_{k,i}) \in \underset{(\theta,\hat{\theta}) \in \Theta_{m^3_k} \times \Theta^d_{m^3_k}}{\arg\min} \mathbb{E}\Big[\Big|NN^{\theta^*_{k,i+1}}(X^\pi_{t_{k,i+1}}) - F\Big(t_{k,i}, X^\pi_{t_{k,i}}, NN^\theta(X^\pi_{t_{k,i}}), NN^{\hat{\theta}}(X^\pi_{t_{k,i}}), \Delta t_{k,i}, \Delta B_{t_{k,i}}\Big)\Big|^2\Big] .$$

end

$$\mathcal{V}_{k,0}^{\mathcal{R},\pi,\varepsilon,m} = NN^{\theta^*_{k,0}} \wedge (-M) \vee M \quad \text{and} \quad \tilde{\mathcal{V}}_{k,0}^{\mathcal{R},\pi,\varepsilon,m} = NN^{\tilde{\theta}^*_{k,0}}$$

where

$$\theta^*_{k,0} \in \arg\min \mathbb{E}\Big[\Big|NN^\theta(X^\pi_{t_{k,0}}) - NN^{\check{\theta}^*_{k,0}}(X^\pi_{t_{k,0}}) \wedge (-M) \vee M\Big|^2 \;\Big|\; X^\pi_{t_{k,0}} \in B_{\varepsilon_k}\Big]$$
$$\theta \in \Theta_{m^1_k} \text{ s.t. } \mathbb{P}\Big(DNN^\theta(X^\pi_{t_{k,0}}) \in \mathcal{C}_{\varepsilon_k};$$
$$NN^\theta(X^\pi_{t_{k,0}}) \geq NN^{\check{\theta}^*_{k,0}}(X^\pi_{t_{k,0}}) \wedge (-M) \vee M - \varepsilon_k \;\Big|\; X^\pi_{t_{k,0}} \in B_{\varepsilon_k}\Big) = 1 ,$$
$$\check{\theta}^*_{k,0} \in \arg\min \mathbb{E}\Big[\Big|NN^\theta(X^\pi_{t_{k,0}}) \wedge (-M) \vee M - NN^{\tilde{\theta}^*_{k,0}}(X^\pi_{t_{k,0}})\Big|^2 \;\Big|\; X^\pi_{t_{k,0}} \in B_{\varepsilon_k}\Big]$$
$$\theta = (\lambda_i, \alpha_i)_{1 \leq i \leq m^2_k} \in \Theta_{m^2_k} \text{ s.t. } \Big|\sum_{i=1}^{m^2_k} \lambda_i \alpha_i\Big| \leq \frac{L+1}{|\rho'(0)|}$$
$$\tilde{\theta}^*_{k,0} \in \underset{(\theta,\hat{\theta}) \in \Theta_{m^3_k} \times \Theta^d_{m^3_k}}{\arg\min} \mathbb{E}\Big[\Big|NN^{\theta^*_{k,1}}(X^\pi_{t_{k,1}}) - F\Big(t_{k,0}, X^\pi_{t_{k,0}}, NN^\theta(X^\pi_{t_{k,0}}), NN^{\hat{\theta}}(X^\pi_{t_{k,0}}), \Delta t_{k,0}, \Delta B_{t_{k,0}}\Big)\Big|^2\Big] .$$

end

At each loop of the constraint grid, the input is the couple $(\theta_n, \hat{\theta}_n)$ and the output is the couple $(\theta^*_n, \hat{\theta}^*_n)$ minimizing the square error between NN^{θ_n} and $F(., NN^{\theta_n}, NN^{\hat{\theta}_n}, .)$ under the relaxed gradient and domination constraint. The related approximations of $v(t_n, .)$ and $\sigma^\top(t_n, .)\partial_x v(t_n, .)$ are given by $NN^{\theta^*_n}$ and $NN^{\hat{\theta}^*_n}$ respectively. For the loops that are not related to the constraint grid, the input is the same, and the output is a minimizer of the same quantity but without constraint. The minimizations are done by a SGD in the case without constraints. For the case with a constraint, the minimization can be turned to an unconstrained one by considering a penalized error.

We recall that the function F is defined in (9.4). We next define the error $\mathrm{Err}^{\pi,\mathcal{R}}$ related to the grids π and $\mathcal{R}$:

$$\mathrm{Err}^{\pi,\mathcal{R}}_{\varepsilon,m} = \max_{k=0,\ldots,\kappa-1} \max_{i=1,\ldots,n_k} \mathbb{E}\Big[\Big|Y^{\mathcal{R}}_{t_{k,i}} - \mathcal{V}^{\mathcal{R},\pi,\varepsilon,m}_{k,i}(\bar{X}^\pi_{t_{k,i}})\Big|^2\Big] + \max_{k=0,\ldots,\kappa-1} \max_{i=0,\ldots,n_k-1} \mathbb{E}\Big[\Big|\tilde{Y}^{\mathcal{R}}_{t_{k,i}} - \tilde{\mathcal{V}}^{\mathcal{R},\pi,\varepsilon,m}_{k,i}(\bar{X}^\pi_{t_{k,i}})\Big|^2\Big] .$$

We can state the convergence result.

Theorem 11.2. *We have the following convergence*

$$\lim_{n_0\to+\infty}\lim_{m_0^3\to+\infty}\lim_{\varepsilon_1\to 0}\lim_{m_1^1\to+\infty}\lim_{m_1^2\to+\infty}\lim_{n_1\to+\infty}\lim_{m_1^3\to+\infty}\cdots$$
$$\cdots\lim_{\varepsilon_{\kappa-1}\to 0}\lim_{m_{\kappa-1}^1\to+\infty}\lim_{m_{\kappa-1}^2\to+\infty}\lim_{n_{\kappa-1}\to+\infty}\lim_{m_{\kappa-1}^3\to+\infty}\lim_{\varepsilon_\kappa\to 0}\lim_{m_\kappa^1\to+\infty} Err_{\varepsilon,m}^{\pi,\mathcal{R}} \;=\; 0\,.$$

We refer to [14, Theorem 4.3] for the proof of this result. The algorithm is tested on the PDE related to a Black & Scholes model with differential interest rates in [14]. In dimension $d = 2$ and 3, the results provided by the algorithm are close to those obtained by other methods but they remain greater, which is a valuable fact as the results correspond to a super-hedging prices.

12 Conclusion

These lecture notes present up-to-date techniques to numerically solve some parabolic PDEs related to optimal control problems. The first part deals with general results on neural network approximation. The second part provides probabilistic representations of solutions to PDEs in terms of Backward SDE. Finally the third part focusses on the approximation of the BSDEs representing the considered PDEs by algorithms involving neural networks.

Many questions concerning the machine learning approximations of PDEs remain open in the literature. Let us mention two of them. The first is the speed of convergence of such algorithms which needs to be specified, *i.e.* an estimation of the approximation error depending on the number of neurons on each layer and on the time discretization mesh must be provided. The second question concerns the approximation of other kinds of frequently used PDEs as PDEs with boundary conditions (Dirichlet or Neumann conditions). For those PDEs, the additional constraints impose an adaptation of the approximating algorithms and a specific study of their convergence.

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