A deep learning method for high dimensional PDE's

An application to crowd motion

by

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Abstract

Nada

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A mi lulú y mi pancita.

Contents

Chapter 1

Introduction

Las ecuaciones en derivadas parciales aparecen comúnmente como herramientas útiles para la modelación en múltiples disciplinas. Se encuentran frecuentemente aplicaciones en ciencias naturales como la física y biología, en diseño en ingeniería , y también en áreas como la economía y finanzas. Sin embargo, las propiedades matemáticas de las ecuaciones que aparecen son tan diversas como las áreas en que se aplican, y aunque se pueden clasificar parcialmente según algunas de sus características, no podría existir una teoría completa que describa nuestro conocimiento sobre estas.

Por otro lado, las soluciones analíticas a estos modelos generalmente no están a nuestro alcance, por lo que es necesario recurrir a métodos numéricos para obtener aproximaciones. Para esto, usualmente se recurre a métodos clásicos como diferencias finitas, elementos finitos, volúmenes finitos o métodos espectrales, para los cuales existe una amplia teoría que soporta y justifica rigurosamente su funcionamiento.

No obstante, la aplicación de estos métodos a problemas particulares a veces se restringe por propiedades especificas de la ecuación que se resuelve. Por ejemplo, los métodos mencionados sufren de la maldición de la dimensionalidad (*"the curse of dimentionality"*), esto es, su complejidad computacional escala exponencialmente en la dimensión del problema, por lo que su uso se restringe a problemas de dimensión baja ($n = 1, 2, 3, 4$). Lo anterior dificulta su implementación en aplicaciones como valoración en matemática financiera, donde la dimensión del problema está determinada por el número de activos considerados . También, su eficiencia computacional se reduce considerablemente conforme se aumenta la complejidad de los dominios en que se resuelven, o por las no-linealidades que aparecen, como es el caso de la ecuación de Navier-Stokes modelando flujos turbulentos.

Otra área en donde estos inconvenientes aparecen es en el análisis de datos y aprendizaje de maquinas. Por ejemplo, la complejidad de algunos modelos de regresión no lineal crece exponencialmente con el tamaño de los datos subyacentes. Para este tipo de problemas se han desarrollado herramientas poderosas que permiten modelar problemas en altas dimensiones y con posibles no linealidades. Entre estas, las redes neuronales han demostrado ser de gran utilidad como modelo para representar funciones con estas complejidades[1].

En consecuencia, intentando replicar el éxito obtenido con estas herramientas en aprendizaje de máquinas, recientemente han surgido nuevas perspectivas para aproximar soluciones de ecuaciones en derivadas parciales usando estas mismas herramientas. Entre estas se encuentran las PINNs (Physics Informed Neural Networks)[**PINNs**, **PINNS2**], FNO (Fourier Neural Operators)[2], y DGM (Deep Garlekin Method)[3]. La evidencia práctica muestra que estos métodos pueden proporcionar soluciones en casos donde los clásicos no [4, 5], a pesar de usualmente no competir con su eficiencia en las situaciones donde los últimos sí aplican. Además, se ha venido desarrollando un marco teórico riguroso que permite justificar su aplicación en situaciones específicas.

Chapter 2

Backward stochastic differential equations and PDEs

When addressing deterministic optimal control problems of dynamical systems, there are two approaches, one involving Bellman's dynamic programming principle, and the other relying on the Pontryagin's maximum principle. The former approach leads to a partial differential equation, the Hamilton-Jacobi-Bellman equation, to be solved for the value function and the optimal control of the process. The latter leads to a system of ordinary differential equations, one equation forward in time for the state and one backward in time for its adjoint.

The stochastic version of these problems is solved by methods analogous to those of the deterministic case. However, there are issues with desirable mathematical properties of solutions when we state them extending directly the ones proposed by deterministic methods. That is the case of the stochastic version of the Pontryagin's maximum principle, in which the backward differential equation cannot be stated directly as an SDE with terminal condition, as the solution is not guaranteed to be adapted to the filtration generated by the brownian motion.

The theory of backward stochastic differential equations (BSDEs) emerged in Bismut's [6] early work, and later generalized by Pardoux and Peng[7], as an attempt to formalize the application of the stochastic maximum principle. Here we give an introduction and compilation of results about them based on [8, 9, 10, 11], including its relation with a certain class of nonlinear parabolic partial differential equations, which will be the main tool for the method explained in the following chapters.

2.1 Backward stochastic differential equations

2.1.1 Motivation

Let's introduce the necessity for a different formulation of stochastic differential equations through an example [10]. In the usual setting for a stochastic differential equation (SDE), we specify the evolution of a $\mathbb{R}^d$-valued stochastic process X_t through its dynamics and an initial value $x_0 \in \mathbb{R}^d$(possibly random), in the form

$$X_t = x_0 + \int_0^t \mu(t, X_t)dt + \int_0^t \sigma(t, X_t)dW_t, \tag{2.1}$$

or equivalently,

$$\begin{aligned} dX_t &= \mu(t, X_t)dt + \sigma(t, X_t)dW_t \\ X_0 &= x_0, \end{aligned} \tag{2.2}$$

where W_t is a m-dimensional Brownian motion process and the stochastic integral is defined in the Ito sense.

We know that, under some Lipschitz and boundedness conditions for the drift μ and the volatility σ, the equation with initial condition (2.2) has a unique solution which is adapted with respect to the filtration $\mathbb{F} = (\mathcal{F}_t)_t$ generated by W_t.

Now, what happens if we consider the problem (2.2) with a terminal condition at time $T > 0$? Consider, for instance, the particular case with $\mu(t, X_t) = \sigma(t, X_t) = 0$, and a square-integrable $\mathcal{F}_T$-measurable random variable $\xi \in L^2(0, T)$ for which we try to solve the problem of finding a process Y_t such that

$$\begin{aligned} dY_t &= 0 \\ Y_t(T) &= \xi. \end{aligned} \tag{2.3}$$

This equation has a unique solution given by $Y(t) = \xi$, which is not necessarily $\mathcal{F}_t-$measurable for every $0 \le t \le T$, and therefore (2.3) may not have solution in the usual SDE sense.

Despite this, we can try to solve this problem reinterpreting the solution to (2.3) based on the following representation theorem.

Theorem 2.1.1 (Martingale representation theorem [12])**.** *Let $(M_t)_{0 \le t \le T}$ be a continuous $\mathbb{R}^d$-valued square-integrable martingale with respect to $\mathcal{F}_t$, the augmented filtration generated by an m-dimensional Brownian motion $(W_t)_t$. Then, there is a unique $\mathbb{R}^{d\times m}$-valued $\mathcal{F}_t$-adapted stochastic process $f(s)$, with $\mathbb{E}[\int_0^T |f|^2 dt] < \infty$, such that*

$$M_t = M_0 + \int_0^t f(s)dW_s \quad \textit{for} \quad t \in [0, T], \tag{2.4}$$

where the uniqueness is interpreted in the mean squared norm.

We can intend to enforce the solution Y_t to be $\mathcal{F}_t-$measurable for every $0 \le t \le T$ by taking its conditional expectation with respect to the evolving σ-algebra

$$Y(t) := \mathbb{E}[\xi|\mathcal{F}_t], \tag{2.5}$$

which satisfies the terminal condition $Y(T) = \xi$, since ξ is $\mathbb{F}_T$-measurable. Thus, as a consequence of the Martingale representation theorem 2.1.1, we conclude that there exist a square-integrable $\mathcal{F}_t$-measurable process Z_t such that

$$Y(t) = Y(0) + \int_0^t Z_s dW_s \quad \text{for} \quad t \in [0, T], \tag{2.6}$$

which can be written as

$$\begin{aligned} dY_t &= Z_t dW_t \\ Y(T) &= \xi \end{aligned} \tag{2.7}$$

Therefore, problem (2.3) can be reinterpreted as in problem (2.7), that we will denote as a bacward stochastic differential equation (BSDE) , in which we seek a pair of processes (Y_t, Z_t) that will provide an adapted solution to our original problem. Indeed, the process Z_t will "steer" the system so that the process Y_t remains adapted, and is thus called a control process. It is not possible to revert time as $t \to T - t$ as the filtration goes only in one direction [13].

Finally, we can write this equation in another form. Note that (2.7) is a forward SDE problem, hence we can solve for $Y(0)$ in the integral form , and so we have

$$Y(0) = \xi - \int_0^T Z_s dW_s, \tag{2.8}$$

that is inserted in (2.6) to obtain

$$Y(t) = \xi - \int_0^T Z_s dW_s + \int_0^t Z_s dW_s = \xi - \int_t^T Z_s dW_s \quad \forall t \in [0, T], \tag{2.9}$$

which is the standard way to write the BSDE in integral form.

2.1.2 An existence and uniqueness theorem

Now that we have motivated the use of BSDEs, we follow [14] to provide a formal definition and prove that under certain regularity conditions, we can ensure the existence of a solution for that kind of equation.

Let be $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space and $T > 0$ a fixed horizon time. We consider a d-dimensional Brownian motion $W = (W_t)_{t\in[0,T]}$ and let $\mathbb{F} = (\mathcal{F}_t)_{t\in[0,T]}$ be the corresponding natural augmented filtration (i.e with the completeness and right continuity conditions).

Denote by $\mathbb{S}^2(0, T)$ the set of real-valued progressively measurable processes Y_t such that

$$\mathbb{E}\left[\sup_{0\le t\le T} |Y_t|^2\right] < \infty, \tag{2.10}$$

and by $\mathbb{H}^2(0, T)^d$ the set of $\mathbb{R}^d$-valued progressively measurable processes Z_t such that

$$\mathbb{E}\left[\int_0^T |Z_t|^2 dt\right] < \infty. \tag{2.11}$$

Here we consider the backward stochastic differential equation

$$\begin{aligned} dY_t &= -f(t, Y_t, Z_t)dt + Z_t \cdot dW_t \\ Y(T) &= \xi \end{aligned} \tag{2.12}$$

Definition 2.1.1. *A solution to the BSDE (2.12) is a pair* $(Y, Z) \in \mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d$ *such that*

$$Y_t = \xi + \int_t^T f(s, Y_s, Z_s)\, ds - \int_t^T Z_s \cdot dW_s, \quad 0 \le t \le T \tag{2.13}$$

And now we establish an existence and uniqueness theorem for $\mathbb{R}$-valued process, which can be extended to $\mathbb{R}^d$-valued processes

Theorem 2.1.2 (Existence and uniqueness of solutions to BSDEs [14])**.** *Given a pair* (ξ, f)*, called the terminal condition and the driver of the BSDE, that satisfy the following assumptions*

I. $\xi \in L^2(\Omega, \mathcal{F}_T, \mathbb{P}; \mathbb{R})$

II. $f : \Omega \times [0,T] \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ *such that*

a) $f(\cdot, t, y, z)$*, written* $f(t, y, z)$ *for simplicity, is progressively measurable for all* y, z

b) $f(t, 0, 0) \in \mathbb{H}^2[0,T]$

c) f *is uniformly Lipschitz in* (y, z)*, i.e ,there exist a constant* C_f *such that for all* $y_1, y_2 \in \mathbb{R} \times \mathbb{R}$ *and* $z_1, z_2 \in \mathbb{R}^d \times \mathbb{R}^d$ *we have*

$$|f(t, y_1, z_1) - f(t, y_2, z_2)| \le C_f \left(|y_1 - y_2| + |z_1 - z_2|\right) \quad a.s \tag{2.14}$$

There exist a unique solution (Y, Z) *to the equation (2.12).*

To give a demonstration we will need the following inequalities about SDEs, whose proofs will be omitted.

Theorem 2.1.3 (Doob's martingale inequality [12])**.** *Let* $\{M_t\}_t \ge 0$ *be a* $\mathbb{R}^d$*-valued martingale in* $L^p(\Omega; \mathbb{R}^d)$*. Let* $[0,T]$ *be a bounded interval with* $T > 0$ *and let* $p > 1$*. Then*

$$\mathbb{E}\left[\sup_{0 \le t \le T} |M_t|^p\right] \le \left(\frac{p}{p-1}\right)^p \mathbb{E}[|M_T|^p], \tag{2.15}$$

in particular, if $p = 2$*,*

$$\mathbb{E}\left[\sup_{0 \le t \le T} |M_t|^2\right] \le 4\mathbb{E}[|M_T|^2]. \tag{2.16}$$

Theorem 2.1.4 (Burkholder-Davis-Gundy inequality [12])**.** *Let* $g \in L^2(\mathbb{R}^+; \mathbb{R}^{d \times m})$*. Define for* $t \ge 0$

$$x(t) = \int_0^t g(s) dW_s \quad \text{and} \quad A(t) = \int_0^t |g(s)|^2 ds$$

then, for every $p > 0$ *there exist universal positive constants* c_p, C_p*, depending only on* p*, such that the following inequalities hold*

$$c_p \mathbb{E}[|A(t)|^{\frac{p}{2}}] \le \mathbb{E}\left[\sup_{0 \le s \le t} |x(s)|^p\right] \le C_p \mathbb{E}[|A(t)|^{\frac{p}{2}}], \tag{2.17}$$

in particular, if $p = 1$*, we can take* $c_p = \frac{1}{2}$ *and* $C_p = 4\sqrt{2}$

Proof of theorem 2.1.2 . Here we give a fixed point argument. To do it, lets consider a pair of process $(U,V) \in \mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d$ and, as in the motivation example, consider the martingale

$$M_t = \mathbb{E}\left[\xi + \int_0^T f(s,U_s,V_s)ds \middle| \mathcal{F}_t\right], \tag{2.18}$$

which is square-integrable under the hypothesis on (ξ, f). Using to the martingale representation theorem 2.1.1, we deduce the existence and uniqueness of a process $Z_s \in \mathbb{H}^2(0,T)^d$ such that

$$M_t = M_0 + \int_0^t Z_s \cdot dW_s. \tag{2.19}$$

Now, define the process Y_t for $0 \leq t \leq T$ as

$$\begin{aligned} Y_t &= \mathbb{E}\left[\xi + \int_t^T f(s,U_s,V_s)ds \middle| \mathcal{F}_t\right] = \mathbb{E}\left[\xi + \int_0^T f(s,U_s,V_s)ds - \int_0^t f(s,U_s,V_s)ds \middle| \mathcal{F}_t\right] \\ &= M_t - \int_0^t f(s,U_s,V_s)ds \end{aligned} \tag{2.20}$$

and note that from this and using (2.19), Y_t satisfies

$$\begin{aligned} Y_t &= M_0 + \int_0^t Z_s \cdot dW_s - \int_0^t f(s,U_s,V_s)ds \\ &= \xi + \int_t^T f(s,U_s,V_s)ds - \int_t^T Z_s \cdot dW_s. \end{aligned} \tag{2.21}$$

Thus, consider the function $\Phi : \mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d \to \mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d$ that maps the pair (U,V) to the pair (Y,Z) constructed as above, $\Phi(U,V) = (Y,Z)$. Note that it is well-defined as the Z process is unique, and by Doob's martingale inequality 2.1.3 we have

$$\mathbb{E}\left[\sup_{0\leq t\leq T}\left|\int_t^T Z_s \cdot dW_s\right|^2\right] \leq 4\mathbb{E}\left[\int_0^T |Z_s|^2 ds\right] < \infty, \tag{2.22}$$

and therefore, by assumptions I, $IIa)$ and $IIb)$, Y_t lies in $\mathbb{S}^2(0,T)$. Also note that a solution to the BSDE (2.12) is a fixed point of Φ. We will show that such fixed point exist by showing it is a contraction if we endow the $\mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d$ space with the metric

$$\|(Y,Z)\|_\beta = \left(\mathbb{E}\left[\int_0^T e^{\beta s}(|Y_s|^2 + |Z_s|^2)ds\right]\right)^{\frac{1}{2}}, \tag{2.23}$$

where $\beta > 0$ is a parameter to be chosen later.

To show that Φ is a contraction, let $(U,V),(U',V') \in \mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d$ and $(Y,Z) = \Phi(U,V)$, $(Y',Z') = \Phi(U',V')$. We denote $(\bar{U},\bar{V}) = (U-U', V-V')$, $(\bar{Y},\bar{Z}) = (Y - Y', Z-Z')$ and $\bar{f}_t = f(t,U_t,V_t) - f(t,U'_t,V'_t)$.

Using equation (2.21), we know that $\bar{Y}_s$ satisfies

$$\bar{Y}_s = -\int_0^t \bar{f}_s ds + \int_0^t \bar{Z}_s \cdot dW_s \tag{2.24}$$

So let's apply Ito's formula to the process $e^{\beta s}|\bar{Y}_s|^2$ between 0 and T to obtain

$$\begin{aligned} e^{\beta T}|\bar{Y}_T|^2 = |\bar{Y}_0|^2 &+ \int_0^T (\beta e^{\beta s}|\bar{Y}_s|^2 - 2e^{\beta s}\bar{Y}_s \cdot \bar{f}_s + e^{\beta s}|\bar{Z}_s|^2)ds \\ &+ \int_0^T 2e^{\beta s}\bar{Y}_s\bar{Z}_s \cdot dW_s. \end{aligned} \tag{2.25}$$

Observe that we can apply the Burkholder-Davis-Gundy inequality 2.1.4 with $p = 1$ to the following expectation of the supremum associated with the last term

$$\begin{aligned} \mathbb{E}\left[\sup_{0\le t\le T}\left|\int_0^t 2e^{\beta s}\bar{Y}_s\bar{Z}_s \cdot dW_s\right|\right] &\le 4\sqrt{2}\,\mathbb{E}\left[\left(\int_0^T 4e^{2\beta s}|\bar{Y}_s|^2|\bar{Z}_s|^2 ds\right)^{\frac{1}{2}}\right] \\ &\le 4\sqrt{2}e^{\beta T}\,\mathbb{E}\left[\sup_{0\le t\le T}|Y_t|^2 + \int_0^T |\bar{Z}_s|^2 ds\right] \\ &< \infty, \end{aligned} \tag{2.26}$$

which shows that the local martingale $\int_0^t 2e^{\beta s}\bar{Y}_s\bar{Z}_s \cdot dW_s$ is actually a uniformly integrable martingale and therefore its expected value remains constant zero. Also, note that $\bar{Y}_T = Y_T - Y'_T = \xi - \xi = 0$.

Using these facts, take the expected value to (2.25) and reorder terms to obtain

$$\begin{aligned} \mathbb{E}\left|\bar{Y}_0\right|^2 + \mathbb{E}\left[\int_0^T e^{\beta s}\left(\beta\left|\bar{Y}_s\right|^2 + \left|\bar{Z}_s\right|^2\right)ds\right] &= 2\mathbb{E}\left[\int_0^T e^{\beta s}\bar{Y}_s \cdot \bar{f}_s ds\right] \\ \le 2C_f\mathbb{E}\left[\int_0^T e^{\beta s}\left|\bar{Y}_s\right|\left(\left|\bar{U}_s\right| + \left|\bar{V}_s\right|\right)ds\right] \quad &\text{(by condition } IIc)) \\ \le 4C_f^2\mathbb{E}\left[\int_0^T e^{\beta s}\left|\bar{Y}_s\right|^2 ds\right] + \frac{1}{2}\mathbb{E}\left[\int_0^T e^{\beta s}\left(\left|\bar{U}_s\right|^2 + \left|\bar{V}_s\right|^2\right)ds\right]&, \end{aligned} \tag{2.27}$$

so if we choose $\beta = 1 + 4C_f^2$ and ignore the $\mathbb{E}\left|\bar{Y}_0\right|^2$ term, we obtain

$$\mathbb{E}\left[\int_0^T e^{\beta s}\left(\left|\bar{Y}_s\right|^2 + \left|\bar{Z}_s\right|^2\right)ds\right] \le \frac{1}{2}\mathbb{E}\left[\int_0^T e^{\beta s}\left(\left|\bar{U}_s\right|^2 + \left|\bar{V}_s\right|^2\right)ds\right], \tag{2.28}$$

which is $\|(\Phi(U,V))\|_\beta \le \frac{1}{2}\|(U,V)\|_\beta$, that means Φ is a contraction in a Banach space, as $\mathbb{S}^2(0,T) \times \mathbb{H}^2(0,T)^d$ is the product of Banach spaces, and therefore has a unique fixed point.

■

2.1.3 Forward-Backward stochastic differential equations

2.2 The Feynman-Kac formulas

2.2.1 The linear Feynman-Kac formula

2.2.2 The non-linear Feynman-Kac formula

Chapter 3

The Deep BSDE method

Chapter 4

Crowd motion modeling

Chapter 5

An application

Chapter 6

Conclusion

Appendix A

Neural Networks

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