

Simulations numériques des problèmes
dépendant du temps

appliquées à l'épidémiologie, l'intelligence
artificielle et les finances

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nances

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11 mars 2024

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Chapitre 1

Motivations and Examples : Epidemiology, Finance, AI

The objective of this book is the numerical analysis of evolution problems and the computation of derivatives (and other intricacies) of a criterion in a computational graph (this will be applied to the control of evolution equations). For additional information, refer to [8].

We begin with some examples of applications.

1.1 Ordinary Differential Equations (ODE)

An important model in epidemiological modeling is the SIR model ; the initials denote S for the group of 'susceptible' individuals, I for the group of infected individuals, and R for the group of those recovered, see Figure 1.1 for an evolution diagram.

After a derivation (which will be presented later in Section

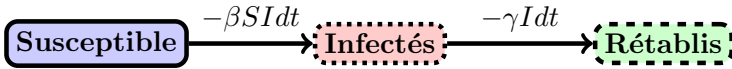


FIGURE 1.1 – Schematic representation of the SIR model in Equation (1.3).

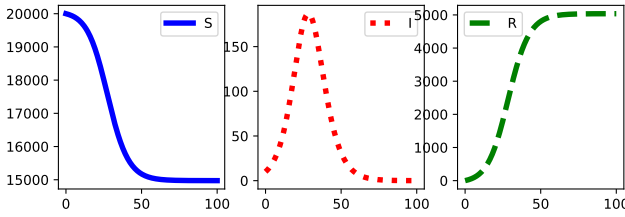


FIGURE 1.2 – Typical evolution of the system in Equation (1.3); data taken from [5].

2.9), we obtain the system of equations, called the SIR model

$$\frac{dS}{dt} = -\beta SI \quad (1.1)$$

$$\frac{dI}{dt} = \beta SI - \gamma I \quad (1.2)$$

$$\frac{dR}{dt} = \gamma I. \quad (1.3)$$

We assume $S(0) = S_0 \neq 0$, $I(0) = I_0 > 0$, $R(0) = R_0 \geq 0$, $S_0 + I_0 + R_0 = 1$ (it's about proportions). Here, β , γ are parameters of the model. A typical evolution is given in Figure 1.2.

In reality, the model needs to be adapted, as real data is not always compatible with simple models, see Figure 1.3. Therefore, we move beyond the domain of models with analytical solutions and must find accurate numerical approximations of their solutions.

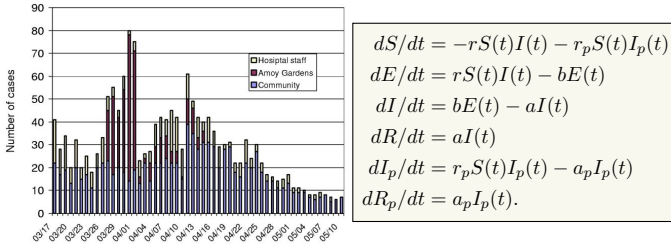


FIGURE 1.3 – Actual evolution of the number of infected individuals; image taken from [5]. To accurately reproduce real data, it is necessary to use a model like the one on the right.

1.2 Stochastic Differential Equations (SDE)

In financial applications (calculations for derivative products in different scenarios) or in physics (path integrals, etc.), there is a need to handle quantities that evolve over time and also contain an element of uncertainty. For instance, the yield $\frac{S_{t+\Delta t} - S_t}{S_t}$ of a financial asset contains a predictable part and another random part, which can be modelled, like in the Black-Scholes model, as a normal variable $\mathcal{N}(\mu\Delta t, \sigma^2\Delta t)$ ¹. The following stochastic differential equation (SDE) is obtained (see [7] for details) :

$$dS_t = \mu S_t dt + \sigma S_t dW_t. \quad (1.4)$$

An illustration of solution scenarios for (1.4) is provided in Figure 1.4.

Reminder : derivative products are financial instruments whose value depends (according to a pre-established contract) on an underlying asset. Example : a European call option on S_t with a final value of $(S_T - K)_+$. However, the calculation

1. We do not discuss the justification of the validity of this model here; for real-life applications, this justification must be carefully validated!!

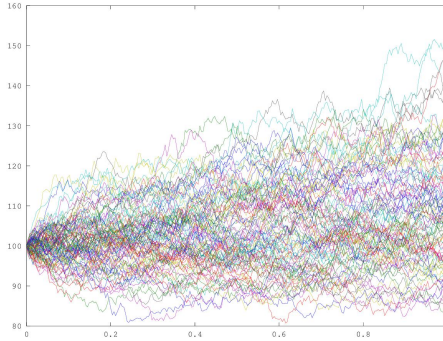


FIGURE 1.4 – Solution scenarios for (1.4).

of the value before expiration is unknown. Models need to be imposed, and quantities such as :

$$\mathbb{E}^{\mathbb{Q}}[e^{-r(T-t)}(S_T - K)_+ | (S_u)_{u \leq t}], \quad (1.5)$$

need to be calculated. As a reminder, S_t follows an SDE ; the goal is to calculate solutions, study the accuracy of numerical calculations, determine if precise scenario calculations are desired (strong convergence) or only averages (weak convergence), etc...

1.3 Derivative Computation on a Computational Graph, Control of Evolution Equations

The goal is to influence the evolution of a system by acting on various parameters called "controls". The same approach helps us study the sensitivity of a result obtained from an evolution with respect to various input parameters (see ODEs, for example, how the result $S(\infty)$ depends on β).

In general, whenever a result is obtained using sequential calculations on a computational graph, the derivative of the result with respect to the inputs can be calculated. This is

called backpropagation; in control theory, this gives rise to "adjoint states".

Example (adapted from [4], also see [2, chap 6.5]) : $f = 5 \cdot (x + y \cdot z)$. The graph has inputs x, y, z , and output $f = f(x, y, z)$. To calculate $\partial_x f, \partial_y f, \partial_z f$, write it as a computational graph (direct or "forward" calculation) :

$$u = y \times z$$

$$v = x + u$$

$$f = 5 \times v$$

Let $x = 1, y = 2, z = 3$; here are the relations obtained by elementary derivation of each calculation (adjoint or "backward" calculation) :

$$\partial_v f = 5$$

$$\partial_x f = \partial_v f \times \partial_x v = \partial_v f = 5$$

$$\partial_u f = \partial_v f \times \partial_u v = \partial_v f = 5$$

$$\partial_y f = \partial_u f \times \partial_y u = 5z = 15$$

$$\partial_z f = \partial_u f \times \partial_z u = 5y = 10.$$

We will study the relationship between the derivative and the computational graph and observe the emergence of an auxiliary variable called the adjoint state. It is crucial for the formalization of the calculation and allows the treatment of complex situations (cf. Figure 1.5 for the "Inception" network [6]).

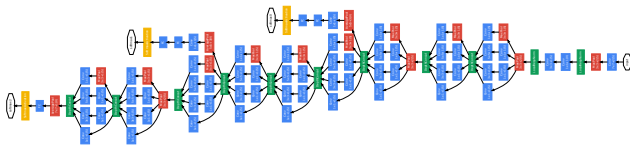


FIGURE 1.5 – "Inception" network architecture [6]. Each cell represents a multi-variable calculation such as matrix-vector multiplication followed by a non-linear operation like taking the positive part on each component.

Chapitre 2

Ordinary Differential Equations (ODE)

Let I be an open interval included in \mathbb{R}_+ . Consider the following ordinary differential equation (ODE) :

$$\frac{dX}{dt} = f(t, X(t)), \quad X(t_0) = X_0, \quad (2.1)$$

with the integral form

$$X(t) = X(t_0) + \int_{t_0}^t f(s, X(s)) ds. \quad (2.2)$$

2.1 Existence and Uniqueness of the Solution

To show the existence and uniqueness of the solution to the previous ODE, we use the following two theorems :

Theorem 2.1 (Local Lipschitz variant of Cauchy-Lipschitz). *Let $f : I \times \mathbb{R} \rightarrow \mathbb{R}$ be a locally Lipschitz continuous function at $X_0 \in \mathbb{R}$, $t_0 \in I$. In other words, there exist two balls $B_x(X_0, R_x)$, $B_t(t_0, R_t)$ and a constant $L > 0$ such that*

$\forall t \in B_t(t_0, R_t), \forall X_1, X_2 \in B_x(X_0, R_x) :$

$$|f(t, X_1) - f(t, X_2)| \leq L|X_1 - X_2|.$$

Then there exists $\varepsilon > 0$ such that the Cauchy problem (2.1) has a unique local solution : $X(t) : (t_0 - \varepsilon, t_0 + \varepsilon) \subset I \rightarrow \mathbb{R}$. Moreover, $X(\cdot)$ is a C^1 function.

Theorem 2.2 (Global Lipschitz variant of Cauchy-Lipschitz). Under the same assumptions as in Theorem (2.1), if L is the same for all R_x (radius of the ball) and initial condition X_0 , then a global solution exists and is unique.

Remark 2.3. Global existence also holds if we can find a continuous function $\alpha : \mathbb{R} \rightarrow \mathbb{R}_+$ such that

$$|f(t, X_1) - f(t, X_2)| \leq \alpha(t)|X_1 - X_2|.$$

This allows L to depend on time.

Example 2.4 (linear function). Let $f(t, X) = rX$ with $r \in \mathbb{R}$ constant. Then $|f(t, X_1) - f(t, X_2)| = |r| \cdot |X_1 - X_2|$, so we obtain global existence with $L = |r|$.

Example 2.5 (non-linear function that blows up). Let $f(t, X) = \frac{5}{X-3}$. An immediate calculation gives $|f(t, X_1) - f(t, X_2)| = \frac{5}{|(X_1-3)(X_2-3)|} \cdot |X_1 - X_2|$, so we obtain local existence for $L = \sup_{X_1, X_2 \in \mathcal{V}} \frac{5}{|(X_1-3)(X_2-3)|}$ in an open neighbourhood \mathcal{V} of any point $X_0 \neq 3$ (such that $3 \notin \bar{\mathcal{V}}$). However, as $\frac{5}{|(X_1-3)(X_2-3)|}$ is not bounded around $X_0 = 3$, the global existence theorem is not applicable at $X_0 = 3$.

2.2 Numerical Methods

If the solution to the Cauchy problem exists, it is unique (cf. Theorem 2.1). To numerically find the solution, it is approximated using different methods. The approximation is done, for example, on $[0, T]$ with N points.

Notations : - the equation to solve is (2.1) ;

- $h = T/N, t_n = n \cdot h, \forall n \leq N$;
- $X_n = X(t_n)$ is the exact solution.

We denote by U_n an approximation of X_n and $f_n = f(t_n, U_n)$. How to calculate the U_n ? For example, starting from the following formula :

$$X(t_{n+1}) = X(t_n) + \int_{t_n}^{t_{n+1}} f(s, X(s)) ds. \quad (2.3)$$

A one-step method is given by the formula :

$$U_{n+1} = U_n + h\phi(t_n, U_n, f_n, h). \quad (2.4)$$

Each function ϕ gives another numerical method. Note that ϕ can also depend on U_{n+1} or f_{n+1} ; in this case, we speak of implicit methods.

2.2.1 Definition of 4 methods :

We will explain some numerical methods for $f_1(t, X) = rX$ and $f_2(t, X) = rX^2$. We recall that for f_1 , the solution $X(t)$ of $\dot{X}(t) = f_1(t, X(t))$ is $X(t) = e^{rt}X_0$, while for f_2 , the solution $Y(t)$ of $\dot{Y}(t) = f_2(t, Y(t))$ is $Y(t) = \frac{Y_0}{1-rtY_0}$.

— **Explicit Euler (denoted EE from now on) :**

$$\begin{cases} U_{n+1} = U_n + hf(t_n, U_n) = U_n + hf_n \\ U(0) = X(0) \end{cases} \quad (2.5)$$

Here, $\phi = f_n$. Examples : for $f_1 : U_{n+1} = U_n + hrU_n = (1+rh)U_n$; for $f_2 : U_{n+1} = U_n + hrU_n^2 = (1+rhU_n)U_n$.

— **Implicit Euler (denoted EI from now on) :**

$$\begin{cases} U_{n+1} = U_n + hf_{n+1} \\ U(0) = X(0) \end{cases} \quad (2.6)$$

Here, $\phi = f_{n+1}$. Examples : for $f_1 : U_{n+1} = U_n + hrU_{n+1}$ so $U_{n+1} = \frac{U_n}{1-rh}$; for $f_2 : U_{n+1} = U_n + hrU_{n+1}^2$ so U_{n+1} is a solution of $rhU_{n+1}^2 - U_{n+1} + U_n = 0$.

When f is Lipschitz, for sufficiently small h , the value U_{n+1} , a solution of the implicit EI scheme definition equation, is unique, see exercise 2.5 page 41.

- **Crank-Nicolson (denoted CN from now on, implicit) :**

$$\begin{cases} U_{n+1} &= U_n + h \left[\frac{f_n + f_{n+1}}{2} \right] \\ U(0) &= X(0) \end{cases} \quad (2.7)$$

Examples : for $f_1 : U_{n+1} = U_n + hr \frac{U_n + U_{n+1}}{2}$ so $U_{n+1} = \frac{1 + \frac{rh}{2}}{1 - \frac{rh}{2}} U_n$; for $f_2 : U_{n+1} = U_n + hr \frac{U_n^2 + U_{n+1}^2}{2}$ so U_{n+1} is a solution of $\frac{rh}{2} U_{n+1}^2 - U_{n+1} + (1 + \frac{rh}{2} U_n) U_n = 0$.

- **Heun (denoted H from now on, explicit) :**

$$\begin{cases} U_{n+1} &= U_n + \frac{h}{2} [f_n + f(t_{n+1}, U_n + hf_n)] \\ U(0) &= X(0) \end{cases} \quad (2.8)$$

Examples : for $f_1 : U_{n+1} = U_n + \frac{h}{2} [rU_n + r(U_n + hrU_n)]$; for $f_2 : U_{n+1} = U_n + \frac{h}{2} [rU_n^2 + r(U_n + hrU_n)^2]$.

Intuition 2.5.1. *The relation (2.3) indicates that we need to find a way to approximately calculate the integral of $f(t, X(t))$ between t_n and $t_{n+1} = t_n + h$. The EE scheme takes an approximation using the method of rectangles by using the value at t_n , the EI scheme uses the value at $t_n + h$, and the CN scheme takes the average of the two, i.e., it uses the trapezoidal rule. As for the Heun scheme, it uses an approximation of X_{n+1} that it reintroduces into a CN-type scheme but with the idea of keeping it explicit.*

2.3 Error, Consistency, and Order

2.3.1 Error

When introducing the exact solution into the formula (2.4) for one-step methods, we obtain "truncation errors" $\tau_{n+1}(h)$:

$$\underbrace{X(t_{n+1}) = X(t_n) + h\phi(t_n, X_n, f(t_n, X_n), h)}_{\text{true for the numerical scheme, i.e., } U_n \text{ instead of } X_n, \text{ etc.}} + h\tau_{n+1}(h).$$

true for the numerical scheme, i.e., U_n instead of X_n , etc.

or

$$\begin{aligned}\tau_{n+1}(h) &:= \frac{X(t_{n+1}) - X(t_n) - h\phi(t_n, X_n, f(t_n, X_n), h)}{h} \\ &= \frac{X(t_{n+1}) - X(t_n)}{h} - \phi(t_n, X_n, f, h).\end{aligned}\quad (2.9)$$

Definition 2.6. *The remainder that appears when the true solution is placed into the relation defining the numerical scheme (similar in form to the initial equation) is called the truncation error. For one-step methods (2.4), it is $\tau_{n+1}(h)$ defined in (2.9), which is called the local truncation error at step $n + 1$. The global truncation error is defined by the relation : $\tau(h) = \max_{n=1, \dots, N} |\tau_n(h)|$.*

Remark 2.7. *The truncation error here is the same as the error (divided by h) between X_{n+1} and the U_{n+1}^* obtained starting from $U_n = X_n$.*

Examples :

Explicit Euler : Using the Taylor series formula to the 2nd order :

$$X(t+h) = X(t) + h\dot{X}(t) + \frac{1}{2}h^2\ddot{X}(\xi), \quad \xi \in [t, t+h]$$

For ($t = t_n$ and $t_n + h = t_{n+1}$), we get : $\tau_{n+1}(h) = \frac{1}{2}h\ddot{X}(\xi_n)$.

Implicit Euler : ...

2.3.2 Consistency and Order

Definition 2.8. *A scheme is said to be consistent if :*

$$\lim_{h \rightarrow 0} \tau(h) = 0, \quad (2.10)$$

i.e., for small h , the exact solution satisfies the scheme.

A scheme is of order "p" if : $\tau(h) = O(h^p)$ for $h \rightarrow 0$.

2.4 Stability and Convergence

2.4.1 Zero-Stability

To study stability with respect to perturbations, we check if Z_n^h defined by :

$$\begin{aligned} Z_{n+1}^{(h)} &= Z_n^{(h)} + h[\phi(t_n, Z_n^{(h)}, f(t_n, Z_n^{(h)}), h) + \delta_{n+1}] \\ Z_0^{(h)} &= \delta_0 + X_0, \end{aligned} \quad (2.11)$$

is close to U_{n+1} .

To know more 2.8.1. *Numerical inaccuracies do not appear during an addition but mostly in the computation, often complex, of the function ϕ ; that's why the perturbations δ_n are placed where indicated in the formula (2.11). For example, if $f(t, X) = X^2 - 1$ needs to be calculated at $t = 0$, $X = \sqrt{2}$, the value $\sqrt{2}^2 - 1 = 1$ is often affected by errors. Python calculation example :*

```
In [2]: numpy.sqrt(2)**2 -1
Out [2]: 1.0000000000000004
```

Definition 2.9. *The scheme given by ϕ is called zero-stable if there exists h_0 and a constant C (independent of ε) such that if $h \leq h_0$ and $|\delta_n| < \varepsilon$ ($\forall n$) : then*

$$|Z_{n+1}^{(h)} - U_{n+1}| \leq C\varepsilon, \quad \forall n \geq 0. \quad (2.12)$$

Theorem 2.10. *Assuming f and ϕ are Lipschitz with respect to their second variable, meaning that there exist $\Lambda > 0$, $h_0 > 0$ such that $\forall h < h_0$*

$$|\phi(t, X, f(t, X), h) - \phi(t, Y, f(t, Y), h)| < \Lambda|X - Y|, \quad \forall X, Y.$$

Then the numerical scheme given by ϕ is zero-stable.

Démonstration. Let's denote : $W_n = Z_n^{(h)} - U_n$. Then

$$W_{n+1} = Z_n^{(h)} - U_n + h[\phi(t_n, Z_n^{(h)}, f, h) - \phi(t_n, U_n, f, h)] + h\delta_{n+1}$$

so $|W_{n+1}| \leq |W_n| + h\Lambda|W_n| + h|\delta_{n+1}|$ thus by summing these inequalities and simplifying terms :

$$|W_{n+1}| \leq |W_0| + h\Lambda \sum_{s=0}^n |W_s| + \sum_{s=1}^{n+1} h|\delta_s|.$$

This allows us to conclude using the discrete Gronwall's lemma (see exercise 2.3 page 40) :

$$|W_{n+1}| \leq |W_0| + h\Lambda \exp(h\Lambda n) \leq (1 + T)\varepsilon \exp(\Lambda T).$$

□

Important technique 2.10.1. *Question : which methods among EE, EI, CN, H satisfy the assumptions of theorem 2.10 ?*

- EE : $\phi = f_n$, Lipschitz when f is.
- H : similar techniques
- For general implicit methods, see exercise 2.5 page 41.
- Intuition for EI : by definition, ϕ has the property : $\phi(t_n, U_n, f_n, h) = f(t_{n+1}, U_{n+1})$ (assuming the existence of a unique solution). Then for two initial points U_n, V_n , we need to bound $f(t_{n+1}, U_{n+1}) - f(t_{n+1}, V_{n+1})$: $|f(t_{n+1}, U_{n+1}) - f(t_{n+1}, V_{n+1})| \leq L|U_{n+1} - V_{n+1}|$ and $|U_{n+1} - V_{n+1}| \leq |U_n - V_n| + h|f(t_{n+1}, U_{n+1}) - f(t_{n+1}, V_{n+1})| \leq |U_n - V_n| + hL|U_{n+1} - V_{n+1}|$ thus $|U_{n+1} - V_{n+1}| \leq |U_n - V_n|/(1 - hL) \dots$
- CN : similar techniques

2.4.2 Convergence

Definition 2.11. A scheme is said to be convergent of order p if, with the previous notations, $|U_n - X_n| = O(h^p)$. A scheme convergent of order 1 is simply called "convergent."

Theorem 2.12. Under the same assumptions as in Theorem 2.10, we have :

$$|U_n - X_n| \leq (|U_0 - X_0| + nh\tau(h)) \exp(\lambda nh).$$

In particular, if for $p \geq 1$: $|U_0 - X_0| = O(h^p)$ and $\tau(h) = O(h^p)$, then $|U_n - X_n| = O(h^p)$ (the scheme converges of order p).

Démonstration. We follow the same steps as in the proof of Theorem 2.10, with $\delta_j = \tau_j(h)$ (using the discrete Gronwall's lemma). Here, the exact solution X_n plays the role of the perturbation $Z_n^{(h)}$. \square

To know more 2.12.1. The previous theorem can be rewritten as stating that **consistency and stability imply convergence**. This is a principle often encountered.

Corrolary 2.13. The schemes EE and EI converge of order 1. The schemes CN and H converge of order 2.

Démonstration. I will provide detailed reasoning only for the Crank-Nicholson scheme :

$$X_{n+1} = X_n + \frac{h}{2} \left[f(t_n, X_n) + f(t_{n+1}, X_{n+1}) \right] + h\tau_{n+1}(h) \quad (2.13)$$

so (for now, treating it as if it were explicit, see exercise 2.5 for details) :

$$X_{n+1} = X_n + \frac{h}{2} \left[X'_n + X'_{n+1} \right] + h\tau_{n+1}(h). \quad (2.14)$$

Also, the Taylor series at order 2 for X' and at order 3 for

X provide :

$$X'_{n+1} = X'_n + hX''_n + \frac{h^2}{2}X_n^{(3)}(\eta) \quad (2.15)$$

$$X_{n+1} = X_n + hX'_n + \frac{h^2}{2}X''_n + \frac{h^3}{6}X_n^{(3)}(\xi) \quad (2.16)$$

Replacing (2.15) and (2.16) into (2.14) gives :

$$h\tau_{n+1}(h) = \frac{h^3}{6}X_n^{(3)}(\xi) - \frac{h^3}{4}X_n^{(3)}(\eta) \quad (2.17)$$

which leads to $\tau_{n+1}(h) = O(h^2)$ (after some calculations to transfer the implicit version into an explicit one). \square

To know more 2.13.1. *So, we have several methods, each with its convergence order. Which one to choose then ? A naive answer would be to pick the scheme with the highest order. However, as we saw with CN, for the order to be effective, we need to use higher derivatives of f (meaning f needs to be smooth), and on the other hand, the higher the order of the scheme, the more intermediate calculations of the f function are required (EE/EI have only one f calculation, while CN uses two), which can be costly. In practice, one rarely goes beyond order 4 or 5 (and sometimes sticks to order 1).*

2.4.3 Absolute Stability

Here, stability is considered from the perspective of the solution over a long time $T = Nh$ (as $T \rightarrow \infty$), but for a fixed step size h (so $N \rightarrow \infty$). For $\lambda \in \mathbb{C}$, $t \geq 0$, we consider the test problem :

$$\dot{Y}(t) = \lambda Y(t) \quad (2.18)$$

$$Y(0) = 1 \quad (2.19)$$

with the solution $Y(t) = e^{\lambda t}$. For $Re(\lambda) < 0$, we obtain $\lim_{t \rightarrow +\infty} Y(t) = 0$. So, any local perturbation in time is "era-

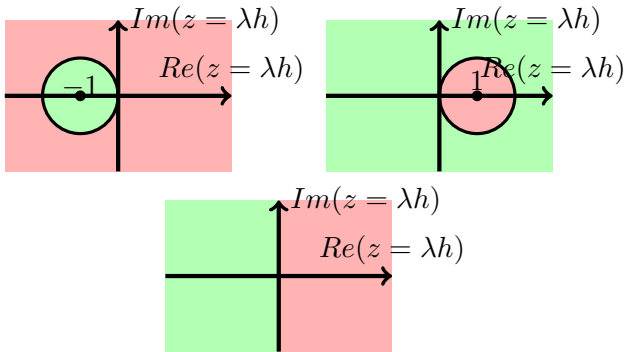


FIGURE 2.1 – The stability of Explicit Euler (top left), Implicit Euler (top right), and Crank-Nicholson (bottom) : in green stability region, in red instability region.

sed” in the long run. This is a very desirable property for numerical schemes that have to combat rounding errors, etc. We want to preserve this property.

Definition 2.14. *A scheme is said to be absolutely stable if, for $f(t, x) = \lambda x$ and $\forall h, \lambda, U_n \rightarrow 0$. Otherwise, its region of absolute stability is :*

$$\{h\lambda \in \mathbb{C} | U_n \rightarrow 0\}.$$

To know more 2.14.1. *Choosing f to be linear is not so surprising because at first order $f(t, x) \simeq f(t, X_0) + \frac{\partial f}{\partial x}(t, X_0)(x - X_0)$ so, apart from a constant, we have a linear function.*

Example 2.15 (Explicit Euler). $U_n = (1 + h\lambda)^n U_0$. We defines its stability region by imposing the stability condition : $|1 + h\lambda| < 1$. This corresponds to the interior of $B((-1, 0), 1)$, see figure (2.1) for an illustration.

Example 2.16 (Implicit Euler). $U_{n+1} = \frac{U_n}{1 - h\lambda} = \frac{U_0}{(1 - h\lambda)^{n+1}}$.

To find the stability region, limit the time step h by imposing the stability condition :

$$|1 - h\lambda| > 1$$

So, here it is the exterior of $B((1,0),1)$, see figure 2.1 for an illustration.

Example 2.17 (Crank-Nicholson).

$$U_{n+1} = \left(\frac{1 + \frac{h\lambda}{2}}{1 - \frac{h\lambda}{2}} \right)^{n+1} U_0. \quad (2.20)$$

The stability region is defined by imposing the stability condition :

$$\left\{ z = h\lambda \in \mathbb{C} : \left| \frac{1 + \frac{h\lambda}{2}}{1 - \frac{h\lambda}{2}} \right| < 1 \right\} = \{z \in \mathbb{C} : \operatorname{Re}(z) < 0\},$$

see figure 2.1 for an illustration.

Example 2.18 (Heun). The stability region is (after calculations) $\{z \in \mathbb{C} : |1 + z + \frac{z^2}{2}| < 1\}$.

2.5 Higher-Order Methods : Runge-Kutta

These are methods that evaluate the function at intermediate steps :

$$U_{n+1} = U_n + hF(t_n, U_n; h, f). \quad (2.21)$$

with the function F of the scheme defined by

$$F(t_n, U_n; h, f) = \sum_{i=1}^s b_i K_i \quad (2.22)$$

$$K_i = f(t_n + c_i h, U_n + h \sum_{j=1}^s a_{ij} K_j), i = 1, 2, \dots, s, c_i \geq 0. \quad (2.23)$$

A method of this kind is called a Runge-Kutta (R-K) method. For a simpler presentation, we introduce the **Butcher tableau of the scheme**

$$\frac{c \mid A}{b^T} \text{ or}$$

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \dots & \dots & \dots & \dots & \dots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array} \quad (2.24)$$

We will always assume $\sum_{j=1}^s a_{ij} = c_i$.

Definition 2.19. *If A is strictly lower triangular, then the method is called explicit; if A is only lower triangular, then the method is semi-explicit. In all other cases, it is an implicit method.*

Intuition 2.19.1. • *When A is lower triangular with zero diagonal, the calculation of K_1 is done explicitly. Then this allows the explicit calculation of K_2 and so on. The scheme is thus explicit.*

- *When A is triangular with a non-zero diagonal, the method requires the sequential solution of s equations (not necessarily linear) to find the K_i , $i \leq s$.*
- *When A is full, the method requires the simultaneous solution of s equations (a system of equations) to find the K_i , $i \leq s$.*

Remark 2.20. *For implicit methods, one would also need to show the existence of a solution for the time steps. Assuming f is Lipschitz, this follows from Picard's fixed-point theorem by taking a recurrence as in Exercise 2.5.*

Example 2.21 (4th-order R-K method). Consider the scheme :

$$U_{n+1} = U_n + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4) \quad (2.25)$$

$$K_1 = f_n = f(t_n, U_n), \quad (2.26)$$

$$K_2 = f\left(t_n + \frac{h}{2}, U_n + \frac{h}{2}K_1\right), \quad (2.27)$$

$$K_3 = f\left(t_n + \frac{h}{2}, U_n + \frac{h}{2}K_2\right), \quad (2.28)$$

$$K_4 = f(t_{n+1}, U_n + hK_3). \quad (2.29)$$

The associated Butcher tableau is

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array} . \quad (2.30)$$

This scheme is of order 4.

2.5.1 Construction of Second-Order Methods (Explicit)

Proposition 2.22. *Explicit methods with $s = 2$ that are second-order (in terms of convergence) satisfy $b_1 + b_2 = 1$ and $b_2c_2 = 1/2$.*

Démonstration. Take $s = 2$. Since the method is explicit, the matrix A in the Butcher tableau is strictly lower triangular, i.e., $A = \begin{pmatrix} 0 & 0 \\ a_{21} & 0 \end{pmatrix}$. Let $a := a_{21}$, then $c_1 = 0+0 = 0$ and $c_2 = a + 0 = a$.

The corresponding Butcher tableau is :

$$\begin{array}{c|cc} 0 & 0 & 0 \\ a & a & 0 \\ \hline & b_1 & b_2 \end{array}$$

Then $U_{n+1} = U_n + hF$ with : $F = b_1K_1 + b_2K_2$, $K_1 = f(t_n, U_n) = f_n$, $K_2 = f(t_n + ah, U_n + haK_1) = f(t_n +$

$ah, U_n + haf_n$).

So, $U_{n+1} = U_n + h(b_1 f_n + b_2 f(t_n + ah, U_n + ahf_n))$. For it to be of order 2, the truncation error $\tau_{n+1}(h)$ must satisfy $\tau_{n+1}(h) = O(h^2)$.

Recalling that $\tau_{n+1}(h) = \frac{X_{n+1} - U_{n+1}^*}{h}$, where U_{n+1}^* is the scheme starting from the exact solution $X(t_n) = X_n$, here, $U_{n+1}^* = X_n + h[b_1 f(t_n, X_n) + b_2 f(t_n + ah, X_n + ahf(t_n, X_n))]$.

We will need the 2D Taylor formula : let G be a \mathcal{C}^2 function, then

$$\begin{aligned} G(\alpha + h_1, \beta + h_2) &= G(\alpha, \beta) + \underbrace{\frac{\partial G}{\partial \alpha}(\alpha, \beta)}_{\text{notation : } G_\alpha} h_1 + \underbrace{\frac{\partial G}{\partial \beta}(\alpha, \beta)}_{G_\beta} h_2 \\ &+ O\left(\left(\sqrt{h_1^2 + h_2^2}\right)^2\right). \end{aligned} \quad (2.31)$$

So, by the 2D Taylor formula,

$$\begin{aligned} &f(t_n + ah, X_n + ahf(t_n, X_n)) \\ &= f(t_n, X_n) + ah[f_t(t_n, X_n) + f_X(t_n, X_n)f(t_n, X_n)] + O(h^2) \\ &= f(t_n, X_n) + ah[f_t(t_n, X_n) + f_X(t_n, X_n)f(t_n, X_n)] + O(h^2) \end{aligned}$$

On the other hand, as $X'(t) = f(t, X(t))$, we also have

$$\begin{aligned} X''(t) &= \frac{d}{dt} X'(t) = \frac{d}{dt} f(t, X(t)) \\ &= f_t(t, X(t)) + f_X(t, X(t))f(t, X(t)). \end{aligned}$$

So,

$$\begin{aligned} f(t_n + ah, X_n + ahf(t_n, X_n)) &= f(t_n, X_n) + ahX''(t_n) + O(h^2) \\ &= X'(t_n) + ahX''(t_n) + O(h^2) \end{aligned} \quad (2.32)$$

The truncation error thus satisfies :

$$\begin{aligned}
 \tau_{n+1}(h) &= \frac{X_{n+1} - U_{n+1}^*}{h} \\
 &= \frac{\overbrace{X(t_{n+1}) - X(t_n)}^{\text{Taylor-Lagrange}} - hb_1X'(t_n) - hb_2(X'(t_n) + ahX''(t_n)) + O(h^3)}{h} \\
 &= \frac{hX'(t_n) + \frac{h^2}{2}X''(t_n) + O(h^3) - hb_1X'(t_n) - hb_2(X'(t_n) + ahX''(t_n)) + O(h^3)}{h} \\
 &= X'(t_n)(1 - b_1 - b_2) + h \left(\frac{X''(t_n)}{2} - ab_2X''(t_n) \right) + O(h^2) \\
 &= X'(t_n)(1 - b_1 - b_2) + hX''(t_n) \left(\frac{1}{2} - ab_2 \right) + O(h^2).
 \end{aligned}
 \tag{2.33}$$

For the method to be of order 2, it is necessary and sufficient that $b_1 + b_2 = 1$ and $ab_2 = 1/2$, which gives the conclusion. \square

Example 2.23 (Heun as a Second-Order RK Method).

In the case where $b_1 = b_2$, then $b_1 = b_2 = \frac{1}{2}$ and $a = 1$:

$$\begin{array}{c|cc}
 0 & 0 & 0 \\
 1 & 1 & 0 \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}$$

So : $K_1 = f(t_n, U_n) = f_n$ and $K_2 = f(t_n+h, U_n+hf(t_n, U_n)) = f(t_{n+1}, U_n+hf_n)$, thus $U_{n+1} = U_n + \frac{h}{2}[f_n + f(t_{n+1}, U_n+hf_n)]$, giving us the Heun method.

2.5.2 Consistency

Proposition 2.24. *Let f be a Lipschitz function. Then the Runge-Kutta method (explicit) is consistent if and only if $\sum_{i=1}^s b_i = 1$.*

Démonstration. by Taylor expansions. \square

2.6 Adaptive Time Steps for Runge-Kutta

Motivation : Sometimes the solution is almost constant, but other times it is highly variable. We would like to take advantage of the "calm" regions and use a large step h , which

will be adjusted later in highly oscillatory regions. For this, we need to employ **adaptive step** (i.e., variable and adjusted) methods. To determine how to choose this step, we need **error estimations**.

How to estimate the error in practice? The easiest way would be to double the step. One idea would be to perform a calculation with a step $2h$ and compare it with two consecutive calculations with step h . Let Y_{2h} be the value obtained after a single step of size $2h$ and $Y_{h,h}$ after two steps of size h . Both are assumed to start from X_n or close to it within a tolerance. We know that, if the method is of order $p > 1$:

$$\begin{aligned} X(t_n + 2h) &= Y_{2h} + (2h)^{p+1}\psi_n + O(h^{p+2}) \\ X(t_n + 2h) &= Y_{h,h} + 2h^{p+1}\psi_n + O(h^{p+2}). \end{aligned}$$

The quantity $\Delta = Y_{2h} - Y_{h,h} = (2^{p+1} - 2)h^{p+1}\psi_n$ helps us adjust the h .

Remark 2.25. *The formulas provide an approximation of order $p + 1$ for $X(t_n + 2h)$. However, the error would then be unknown.*

Although in principle the method above would be interesting, it uses too many evaluations of f . We will refine it by constructing two methods that use the same evaluations (thus same K_i) but whose linear combinations involving b_i yield different orders. We then talk about **embedded schemes** of Runge-Kutta-Fehlberg (R-K-F). Notation :

$$\begin{array}{c|c} c & A \\ \hline & \hat{b}^T \\ & \hat{b}^T \\ \hline & E^T \end{array}$$

where c, A, b give a scheme of order p while c, A, \hat{b}^T give a scheme of order $p + 1$. The difference $E = b - \hat{b}$ serves to estimate the truncation error $\Delta = h \sum_{i=1}^s E_i K_i$.

The most popular are the R-K-F schemes of orders 4-5 or 5-6 or even 2-3. In practice, the algorithm is as follows :

- At the beginning, we specify a tolerance Δ_0 .
- If $\Delta > \Delta_0$ then we redo the calculation with the step $\tilde{h} = h \sqrt[p+1]{\frac{\Delta_0}{\Delta}}$.
- If $\Delta \leq \Delta_0$, the step h is kept constant.

2.7 Systems of ODEs

Let $I \subset \mathbb{R}_+$ be an open interval and $F : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$. The problem is to solve the following Cauchy problem :

$$\begin{cases} Y'(t) = F(t, Y(t)) \\ Y(t=0) = Y_0 \in \mathbb{R}^n \end{cases} \quad (2.34)$$

Example 2.26. $X'' = f(X)$ is not an ODE, but it can be written as a system, by setting : $Y_1 = X, Y_2 = X'$, and we get :

$$\begin{cases} Y_1' = Y_2 \\ Y_2' = f(Y_1) \end{cases}$$

Theorem 2.27 (existence and uniqueness). *Let $F :]-\infty, \infty[\times \mathbb{R}^n \rightarrow \mathbb{R}^n$ be a continuous function and Lipschitz with respect to the second variable*

$$\|F(t, y) - F(t, \tilde{y})\| \leq L\|y - \tilde{y}\| \quad \forall t \in \mathbb{R}, \forall y \in \mathbb{R}^n,$$

with an L not depending on $y \in \mathbb{R}^n$. Then the Cauchy problem (2.34) has a unique global solution (i.e., defined for all $t \geq 0$). If F is Lipschitz only around $(t_0 = 0, Y_0)$, then the solution is only locally defined.

Particular case : $F(t, y) = Ay$ with A being an $n \times n$ matrix. The problem

$$\begin{cases} Y' = AY \\ Y(0) = Y_0 \end{cases}$$

has the (unique) solution $Y(t) = e^{At}Y_0$ where we recall the definition of $e^{At} = \sum_{n=0}^{\infty} \frac{(At)^k}{k!}$.

If A is diagonalizable, i.e. :

- 1) $\exists Q$ invertible such that $A = QDQ^{-1}$, D diagonal

2) or equivalently $\exists V_i, \lambda_i$, such that $AV_i = \lambda_i V_i$, $\|V_i\| = 1$,
 and $\{V_i; i = 1, \dots, n\}$ is a basis of \mathbb{R}^n
 then, $Y(t) = \sum_{i=1}^n e^{\lambda_i t} V_i \langle y_0, V_i \rangle$.

2.7.1 System Stability :

By setting $Z = Q^{-1}Y$, we obtain :

$$Y' = AY \implies Y' = QDQ^{-1}Y \implies Q^{-1}Y' = DQ^{-1}Y \quad (2.35)$$

And, since $Z' = (Q)^{-1}Y'$, we derive the following differential equation : $Z' = DZ$, and the problem :

$$\begin{cases} Z'_1 = \lambda_1 Z_1 \\ \vdots \\ Z'_n = \lambda_n Z_n \end{cases}$$

The solutions to this problem are given by : $Z_i(t) = e^{\lambda_i t} Z_i(0)$,
 and the stability of the system is equivalent to the stability
 of all the ODEs in the problem.

Example 2.28 (Explicit Euler). $U_{n+1} = U_n + hf(t_n, U_n)$.
 Let $f(y) = Dy$.

Applying Explicit Euler to this example, we have : $U_{n+1} = U_n + hDU_n = (1 + hD)U_n$. Therefore, the scheme is stable if $|1 + h\lambda_i| < 1$ for all $i = 1, \dots, n$.

Example 2.29 (Implicit Euler). $U_{n+1} = U_n + hf(t_{n+1}, U_{n+1})$;
 for the previous example, we have : $U_{n+1} = U_n + hDU_{n+1}$, so
 $U_{n+1} = (1 - hD)^{-1}U_n$. The scheme is stable if $|1 - h\lambda_i| > 1$
 for all $i = 1, \dots, n$.

To know more 2.29.1 (Implementation). We always consider the case $f(t, y) = Ay$.

- For explicit schemes $U_{n+1} = U_n + hAU_n$, so it's a direct calculation.

- For implicit schemes $U_{n+1} = U_n + hAU_{n+1}$, $U_{n+1} = (I - hA)^{-1}U_n$; a linear system must be solved. For

more complicated functions f , methods like Newton's or Picard's approximation are needed (cf. exercise 2.5) etc. ...

2.7.2 Stiff Systems

We have seen that implicit schemes are sometimes challenging to implement ; why use them then ? Consider the following differential system :

$$\begin{aligned} u' &= 998u + 1998v \text{ with } u(0) = 1 \\ v' &= -999u - 1999v \text{ with } v(0) = 0 \end{aligned}$$

We make the change of variables $u = 2y - z$ and $v = -y + z$, which gives us :

$$\begin{cases} y' = -y \\ z' = -1000z \end{cases} \Rightarrow \begin{cases} y(t) = e^{-t}y_0 \\ z(t) = e^{-1000t}z_0 \end{cases}$$

(so $\lambda_1 = -1$, $\lambda_2 = -1000$). Returning to our initial variables, we obtain the desired solution :

$$\begin{aligned} u &= 2e^{-t} - e^{-1000t}, \\ v &= e^{-t} + e^{-1000t}. \end{aligned}$$

For the stability of Explicit Euler, $|1 + h\lambda_1| < 1$ and $|1 + h\lambda_2| < 1$ are required, so $h \leq \frac{2}{1000}$.

For Implicit Euler stability, $|1 - h\lambda_i| > 1$, which is always satisfied ($\forall h > 0$). Assuming we are only interested in the e^{-t} part of the solution (treating e^{-1000t} as a perturbation, which it is), the precision of both schemes could be good for sufficiently large steps h ; however, for Explicit Euler, we must use a small h as stability is not guaranteed otherwise. Conclusion : using implicit schemes allows solving with a larger h , hence more quickly.

2.8 Multi-step Methods

The idea behind these schemes is to use previous steps (values) that are available.

Vocabulary : These schemes are also known as predictor-corrector methods.

Definition 2.30. *The linear multi-step scheme of order s (with the notation $a_s = 1$) is given by the recurrence :*

$$\sum_{k=0}^s a_k y_{n+k} = h \sum_{k=0}^s b_k f(t_{n+k}, y_{n+k}). \quad (2.36)$$

Here y_{n+s} is unknown, and the previous values y_{n+s-1}, \dots, y_n are known.

We notice that if $b_s \neq 0$, then the method is implicit ; otherwise, it is explicit. Let's consider some examples.

Example 2.31. Explicit Euler For $s = 1, a_0 = -1, a_1 = b_0 = 1, b_1 = 0$,

$$1 \cdot y_{n+1} + (-1) \cdot y_n = 1 \cdot hf(t_n, y_n) + 0 \cdot hf(t_{n+1}, y_{n+1}).$$

Example 2.32. Adams-Bashforth Two-Step (explicit) Taking $s = 2, a_0 = 0, a_1 = -1, a_2 = 1, b_0 = -\frac{1}{2}, b_1 = \frac{3}{2}, b_2 = 0$, the scheme is defined by the relation :

$$y_{n+2} = y_{n+1} + \frac{3}{2}hf(t_{n+1}, y_{n+1}) - \frac{1}{2}hf(t_n, y_n). \quad (2.37)$$

Example 2.33. BDF Two-Step (implicit) Here $s = 2, a_0 = \frac{1}{3}, a_1 = -\frac{4}{3}, a_2 = 1, b_0 = 0, b_1 = 0, b_2 = \frac{2}{3}$, and thus :

$$y_{n+2} - \frac{4}{3}y_{n+1} + \frac{1}{3}y_n = \frac{2}{3}hf(t_{n+2}, y_{n+2}). \quad (2.38)$$

Definition 2.34. *The local truncation error is $\tau_{n+s}(h)$ defined by :*

$$\tau_{n+s}(h) := \frac{\sum_{k=0}^s a_k X(t_{n+k}) - h \sum_{k=0}^s b_k f(t_{n+k}, X_{n+k})}{h}. \quad (2.39)$$

Reminder : The global truncation error is $\tau(h) = \max_n |\tau_{n+s}(h)|$; the multi-step scheme $(a_k, b_k)_{k=0}^s$ is consistent if $\lim_{h \rightarrow 0} \tau(h) = 0$.

Theorem 2.35. *The multi-step scheme $(a_k, b_k)_{k=0}^s$ is consistent if and only if :*

$$\sum_{k=0}^s a_k = 0, \quad \sum_{k=0}^s b_k = \sum_{k=0}^s k a_k. \quad (2.40)$$

or, equivalently :

$$\sum_{k=0}^{s-1} a_k = -1, \quad \sum_{k=0}^s b_k = s + \sum_{k=0}^{s-1} k a_k. \quad (2.41)$$

Example 2.36 (EE as a Consistent Multi-step Scheme).

Taking the previous example where $a_0 = -1, a_1 = 1, b_0 = 1, b_1 = 0$, the conditions for the theorem are satisfied. Thus, the EE scheme is consistent.

Example 2.37 (Adam-Bashforth as a Consistent Multi-step Scheme). *The Adam-Bashforth scheme satisfies $\sum_{k=0}^2 a_k =$*

0 and $\sum_{k=0}^2 a_k k = \sum_{k=0}^2 b_k = 1$. Therefore, this scheme is consistent.

Example 2.38 (BDF as a Consistent Multi-step Scheme).

The BDF scheme ($s = 2$) satisfies $\sum_{k=0}^2 a_k = 0$ and $\sum_{k=0}^2 a_k k = \sum_{k=0}^2 b_k = 2/3$. Hence, this scheme is also consistent.

2.9 Application in Epidemiology : SIR Model

We quickly present the modeling leading to the SIR system. We refer to [5, 3] and similar references for a more de-

tailed presentation (just to change, we took a reference prior to the COVID-19 pandemic...). The variables are :

- S = the number of people susceptible to infection (the population not yet affected by the epidemic).
- I = the number of infected people.
- R = the number of people who have had the disease, died, or can no longer transmit it (having acquired immunity or being in quarantine, etc.).

Let $N = S(0) + I(0) + R(0)$ be the initial population (which will be conserved).

Model assumptions :

1. The number of infections (transition from S to I) is proportional to the number of individuals in S , the infection rate $I(t)/N$, and the duration Δt . We denote β as the proportionality factor. Since the number of new infections between t and $t + \Delta t$ is $S(t) - S(t + \Delta t)$, we obtain $S(t) - S(t + \Delta t) \simeq \beta SI \Delta t / N$
2. The transition $I \rightarrow R$ is proportional to the number of individuals in I ; it depends on the recovery rate γ (here $1/\gamma$ is the average number of days before leaving the I compartment).

By taking the limit $\Delta t \rightarrow 0$, we obtain the system of equations, called the SIR model :

$$\frac{dS}{dt} = -\beta SI/N \quad (2.42)$$

$$\frac{dI}{dt} = \beta SI/N - \gamma I \quad (2.43)$$

$$\frac{dR}{dt} = \gamma I \quad (2.44)$$

We assume $S(0) = S_0 \neq 0$, $I(0) = I_0 > 0$, $R(0) = R_0 = 0$.

Remark 2.39. Since $\frac{d}{dt}(S + I + R) = 0$, then $S(t) + I(t) + R(t) = N = cst$.

A first question to ask is when I will be increasing or decreasing. Fortunately, this can be read directly from the equation for I : $I' = I(\beta S/N - \gamma)$, so there will be growth when S/N is greater than $\frac{1}{\mathcal{R}_0}$, where $\mathcal{R}_0 = \beta/\gamma$ is known as

the "reproduction rate." Note that \mathcal{R}_0 depends only on the characteristics of the disease and transmission and not on the state $S(t), I(t), R(t)$. In particular, if initially $S(0) \simeq N$, there will be no epidemic (in the sense that I will always be decreasing) if $\mathcal{R}_0 < 1$, and conversely, there will be an epidemic with exponential growth if $\mathcal{R}_0 > 1$.

Therefore, \mathcal{R}_0 is an important number, and in particular, it is the target of most epidemic containment policies; to make it sub-unitary, you can :

1. Make β small by reducing contacts (lockdown, etc.).
2. Make γ large by isolating the sick (so they are no longer contagious).
3. Otherwise, finally, make $S(0)$ smaller through vaccination if it is **effective and without side effects** (otherwise, it won't work).

In this (constant parameter!) model, the typical evolution of I , illustrated in Figure 1.2 on page 10, is as follows : it grows until a maximum value (corresponding to the "epidemic peak") and then decreases. Of course, in practice, it's more complicated because β will change depending on the preventive measures implemented, which in turn will fluctuate, etc.

The total number of infected individuals is

$$R_\infty := \lim_{t \rightarrow \infty} R(t) = I_0 + S_0 - \lim_{t \rightarrow \infty} S(t).$$

Note that $\lim_{t \rightarrow \infty} S(t)$ exists because $S(t), I(t), R(t) \geq 0, \forall t$ and S is decreasing).

Let ζ be the size of the epidemic. It can be shown (see [3]) that ζ is a solution of $1 - \frac{\zeta}{S(0)} = e^{-\mathcal{R}_0(\zeta + I(0))}$.

Remark 2.40. *Note that $S_\infty := \lim_{t \rightarrow \infty} S(t) \neq 0$; therefore, even in the absence of any protective measures, the epidemic will not affect everyone. It is then called the phenomenon of herd immunity in the SIR model. However, 'not everyone' can still include too many people, and in practice, epidemic containment measures must be taken.*

In practice : β and γ are unknown, so we proceed in 2 steps

- 1) Inversion : find β, γ from observations $R(n), n = 1, \dots, N_{max}$
- 2) Prediction : calculate $S(t), I(t), t \geq N_{max}$

Remark 2.41. *Sometimes more complicated models are necessary, such as : $S \rightarrow E \rightarrow I \rightarrow R$ or as in [1].*

2.10 Ordinary Differential Equations Exercises

Exercise 2.1. (Gronwall's Lemma : Integral Variant)

Let $T > 0$ (it can also be ∞), $a(t)$, $b(t)$, $\lambda(t)$ be continuous functions on $[0, T]$, where $\lambda(t) \geq 0$ for all t . Define $\Lambda(t) = \int_0^t \lambda(\tau) d\tau$.

1. If for all $t > 0$:

$$a(t) \leq b(t) + \int_0^t \lambda(s)a(s)ds, \quad (2.45)$$

then

$$a(t) \leq b(t) + \int_0^t e^{\Lambda(t)-\Lambda(s)} \lambda(s)b(s)ds. \quad (2.46)$$

Indication : Estimate the derivative of $A(t) = e^{-\Lambda(t)} \int_0^t \lambda(s)a(s)ds$.

Alternative : Let ξ be the right-hand side of (2.46). It also satisfies $\xi(t) = b(t) + \int_0^t \lambda_s \xi_s ds$ (direct calculation or use $V(t) = \int_0^t \lambda \xi$, i.e., (2.45) with equality). It is then natural to want to show that $a(t) \leq \xi(t)$ for all t ; this is done by bounding $\xi - a$ using (2.45) and the equation for ξ .

2. If b is differentiable with an integrable derivative on $[0, T]$, then

$$a(t) \leq e^{\Lambda(t)} \left(b(0) + \int_0^t e^{-\Lambda(s)} b'(s) ds \right). \quad (2.47)$$

3. If, in addition, b is monotonically increasing, then

$$a(t) \leq e^{\Lambda(t)} b(t). \quad (2.48)$$

4. Verify that in the absence of the assumption $\lambda(t) \geq 0$, a counterexample is $\lambda(t) = \lambda < 0$, $b(t) = b + \omega(t)$, $\text{supp}(\omega) \subset]0, T[$, $a(t) = be^{\lambda t}$.

Exercise 2.2. (*Gronwall : Differential Variant without the sign assumption*)

Let $T > 0$ (it can also be ∞), $g(t)$, $\lambda(t)$ be continuous functions on $[0, T]$, and $a(t)$ a differentiable function with a continuous derivative on $[0, T]$. Define $\Lambda(s) = \int_0^t \lambda(\tau) d\tau$.

If for all $t > 0$:

$$a'(t) \leq g(t) + \lambda(t)a(t) \quad (2.49)$$

then

$$a(t) \leq e^{\Lambda(t)} a(0) + \int_0^t e^{\Lambda(t)-\Lambda(s)} g(s) ds. \quad (2.50)$$

Indication : Estimate the derivative of $A(t) = e^{-\Lambda(t)} a(t)$.

Exercise 2.3. (*Gronwall : Discrete Variant*)

Let k_n be a sequence of positive real numbers and $\phi_n \geq 0$ a sequence such that

$$\phi_0 \leq g_0 \quad (2.51)$$

$$\phi_n \leq g_0 + \sum_{s=0}^{n-1} p_s + \sum_{s=0}^{n-1} k_s \phi_s, \quad n \geq 1. \quad (2.52)$$

If $g_0 \geq 0$ and $p_n \geq 0$ for all $n \geq 0$, then

$$\phi_n \leq \left(g_0 + \sum_{s=0}^{n-1} p_s \right) \exp \left(\sum_{s=0}^{n-1} k_s \right) \quad (2.53)$$

Exercise 2.4. *Consider the Cauchy problem :*

$$x'(t) = 2|x(t)|^{1/2} \quad (2.54)$$

$$x(0) = 0 \quad (2.55)$$

1. Show that for any constant $\lambda \in [0, \infty]$, this problem has the solution $x_\lambda(t) = (t-\lambda)^2$ if $t \geq \lambda$ and $x_\lambda(t) = 0$ otherwise. Comment on uniqueness.

2. Write an explicit/implicit Euler scheme and explain towards which solution $x_\lambda(t)$ it converges numerically.

Exercise 2.5 (Existence of Implicit Schemes). Let $\Psi : \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ be Lipschitz with respect to all arguments, and let $h > 0$.

1. Show that the equation

$$y = x + h\Psi(t, x, y), \quad (2.56)$$

has a unique solution for small enough h and provide a numerical method to compute it. Hint : Picard iterations can be used. Notation : the solution will be denoted by $y = s(t, x, h)$.

2. Now, let y be a solution of (2.56), and ϕ be the function defined by

$$y = x + h\phi(t, x). \quad (2.57)$$

Provide the formula for ϕ in terms of $s(\cdot)$ and $\Psi(\cdot)$ and show that ϕ is well-defined and Lipschitz for sufficiently small h .

Exercise 2.6 (Stability of Implicit Schemes). By using possibly Exercise 2.5, show that the Crank-Nicholson scheme satisfies the assumptions of Theorem 2.10 (page 20) for zero-stability.

Exercise 2.7 (Theoretical Convergence). Provide a convergence result for the Euler scheme without using the discrete Gronwall's lemma.

Hints : Start without round-off errors and establish a recurrence formula for the error.

Exercise 2.8 (RK Writing). Verify that the Heun's method is indeed a two-step Runge-Kutta method and write down the corresponding Butcher tableau.

Do the same for the modified Euler method :

$$u_{n+1} = u_n + hf\left(t_n + \frac{h}{2}, u_n + \frac{h}{2}f_n\right)$$

Exercise 2.9 (θ -Scheme). Consider the " θ -scheme" :

$$u_{n+1} = u_n + h \{(1 - \theta)f(t_n, u_n) + \theta f(t_{n+1}, u_{n+1})\}.$$

1. Write down the Butcher tableau of the scheme.
2. Show that the stability region of this scheme includes $\{z = h\lambda; \operatorname{Re}(z) < 0\}$ if and only if $\theta \geq 1/2$.

Exercise 2.10 (Multi-Step Methods). 1. Show that the BDF-2 scheme (2.38) satisfies the consistency conditions.

2. Show that for BDF-2, the truncation error is indeed of order 2.
3. Determine the order of the truncation error for the Adam-Bashforth scheme (2.37).

Exercise 2.11 (SIR Model). Write one step of the implicit Euler method for the system

$$\begin{aligned} \frac{dS}{dt} &= -rSI, \\ \frac{dI}{dt} &= rSI - aI, \\ \frac{dR}{dt} &= aI. \end{aligned}$$

Exercise 2.12 ((Identification of ODE Schemes)). With the notations from the lecture, a student intends to numerically solve the Lorenz system : $x'(t) = \sigma(y(t) - x(t))$, $y'(t) = x(t)(\rho - z(t)) - y(t)$, $z'(t) = x(t)y(t) - \beta z(t)$. He has three programs L1, L2, and L3, each implementing a different scheme in the list : Explicit Euler, Implicit Euler, Crank-Nicholson. He performs the following tests : he runs the three programs with $\sigma = 10$, $\beta = 8/3$, and $\rho = 28$. $h = 10^{-2}$, starting from $(x_0, y_0, z_0) = (1, 2, 3)$. He obtains vectors representing the numerical solution after **TWO time steps** (to 1×10^{-3} accuracy) :

Program L1 : $\mathbf{v}_1 = [1.228, 2.511, 2.893]$

Program L2 : $\mathbf{v}_2 = [1.213, 2.483, 2.886]$

Program L3 : $\mathbf{v}_3 = [1.244, 2.543, 2.900]$

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1. Recall the definitions of the three schemes.
2. Find the values that the Explicit Euler scheme obtains after **ONE** time step.
3. Determine which scheme each program uses. Rigorously justify your answer.

Note : It is possible to solve the problem without excessive calculations or a calculator. If necessary, approximate to 3-4 decimal places. Correction on page 99.

Various other exercises (Additional ODE)

Exercise 2.13. Consider the Cauchy problem :

$$x' = 2y, \quad (2.58)$$

$$y' = -2x - 4x^3 - y, \quad (2.59)$$

with initial values $(x(0), y(0)) = (x_0, y_0) \neq (0, 0)$. Show that this problem has a maximal solution over the interval $]\alpha, \beta[$ (with $-\infty \leq \alpha < \beta \leq \infty$).

Exercise 2.14. Consider the Cauchy problem :

$$x' = 2y(z - 1), \quad (2.60)$$

$$y' = -x(z - 1), \quad (2.61)$$

$$z' = -xy, \quad (2.62)$$

with initial values $(x(0), y(0), z(0)) = (x_0, y_0, z_0)$. Show that this problem has a maximal solution over the interval $[0, \infty[$.

Exercise 2.15 (Autonomous systems). Consider the system $x' = f(x)$ with f being C^1 class. The state x is a vector in \mathbb{R}^d .

1/ Let x_1 and x_2 be two solutions of this system. Then if these solutions touch at a point, they are equal.

2/ So, let x be a solution. Then either $t \mapsto x(t)$ is injective, or it is periodic.

2.11 Python TP

Exercise 2.16 (Numerical precision). *Implement exercise 2.4 in order to observe all the behaviours described in the lecture for EE and EI with finite precision or not.*

Exercise 2.17 (SIR model, scheme order). *Write a program that solves the SIR system (2.42)-(2.44) using the Euler Explicit, Heun, and Runge-Kutta schemes of order 4 with Butcher table (2.30). Take as an example $S_0 = 10.0^6$, $I_0 = 10$, $R_0 = 0$ (but work with the proportions of the total population), $r = 0.5$, $a = 0.33$, $T = 150.0$, $N = 150$ ($h = T/N$).*

1. *Implement it using the "odeint" function in python (without any scheme).*
2. *Study the order of the schemes by varying h and comparing it with the solution found by 'odeint' at time T (take the error on "S"). For this study, take $T_0 = 52$, $T = 60$ (get the initial values at time T_0 from the previous calculation) and $h = 0.05, 0.01, 0.1, 0.5, 1, 2, 4$. The result should be similar to that in figure 2.2.*
3. *Study the impact of control policies that will change r and a .*

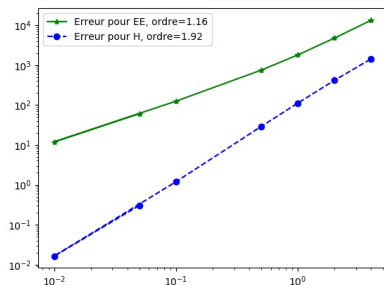


FIGURE 2.2 – Results for exercise 2.17

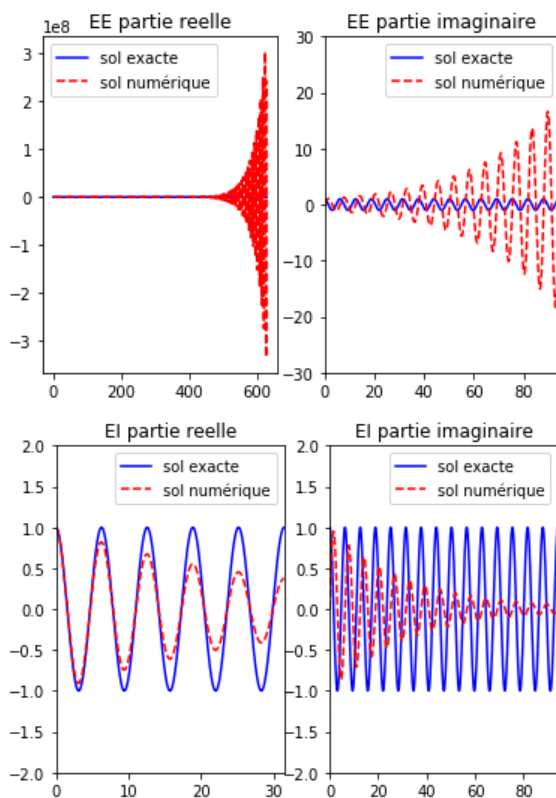


FIGURE 2.3 – Stability of EE and EI schemes.

Exercise 2.18. Numerically study the stability of Euler Explicit for the case of the system $x'(t) = \lambda x(t)$ with $\lambda = i$, $T = 100 \cdot 2\pi$, $h = 2\pi/100$. Typical results are in figure 2.3.

Chapitre 3

Automatic Differentiation, Backpropagation, Optimization, Control

3.1 Introduction

The goal of this chapter is to provide some insights into how to automatically compute gradients (given the code that computes the function). This is known as *automatic differentiation*; one way to implement it is through *backpropagation*, which is used in optimization and control problems. Let's start with some examples.

3.1.1 Example 1 : Explicit function

Calculating the gradient of a function with 3 variables $f(x, y, z) = (3x^2 + y)z - x$. This case is quite simple; we can perform the operations manually to calculate $\nabla f = (\partial_x f, \partial_y f, \partial_z f)$. This will serve as a textbook case and verification.

3.1.2 Example 2 : Optimization in an epidemiological model

We now consider a current context with the SIR system, seen previously. The system is of the form $X' = f(X(t), u(t))$

$$\begin{cases} \dot{S} = -\beta SI \\ \dot{I} = \beta SI - \gamma I \\ \dot{R} = \gamma I \end{cases}$$

with $u(t) = \beta(t) = \beta$ the control.

Thus, the goal is to minimize the cost of containment ($\int_0^T c(\beta(t))dt$) and the number of infected people ($S(0) - S(T)$) over the period $[0, T]$. In other words, we seek :

$$\min_{\beta} J[\beta] := S(0) - S(T) + \int_0^T c(\beta(t))dt$$

We have initially :

$$\frac{\partial}{\partial \beta} \left[\int_0^T c(\beta(t))dt \right] = c'(\beta(t)).$$

However, the difference $S(0) - S(T)$ is much less obvious to differentiate because β does not appear explicitly, although it does appear in this function.

3.1.3 Example 3 : Neural networks (NN)

Suppose we have a database Ω ; we then wish to define a neural network, *Neural Network* (NN), that will "learn" based on certain results from this database, $\omega \in \Omega$.

We will then seek to optimize certain parameters X , so that the output of our network is as close as possible to the chosen examples ω . Thus, it is an optimization problem :

$$\arg \min_X \{ \mathbb{E}_{\omega} (\mathcal{L}(X, \omega)) \}$$

We will be concerned with neural network of which we give an example below. The principle is as follows : we have

an input layer, called the *Input Layer*, a certain number of hidden layers, the *Hidden Layers*, and an output layer, the *Output Layer*, see figure 3.1 for an illustration.

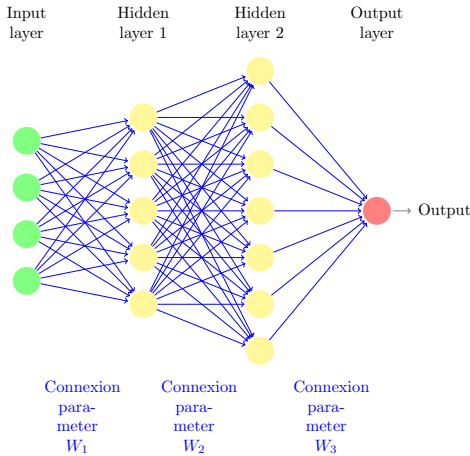


FIGURE 3.1 – Example of a neural network

Each of the hidden layers (\tilde{Y}, Y) performs the following calculation : We take all the results from the previous layer, we assign them a weight (a vector W , and a bias b). We then obtain \tilde{Y} and finally apply an activation function \mathcal{A} (for example, the ReLU function which is the positive part : $ReLU(x_1, \dots, x_N) = ((x_1)_+, \dots, (x_N)_+)$), we get Y .

Finally, we apply an output function g to the last layer (for example, a sigmoid-type function $x \mapsto \frac{1}{1+e^{-x}}$ which transforms the input into an output of type 'probability', i.e., a number between 0 and 1). If we have to choose between K classes, we can use the softmax function

$$x \in \mathbb{R}^K \mapsto s(x) := \left(\frac{e^{x_k}}{\sum_{\ell=1}^K e^{x_\ell}} \right)_{k=1}^K \in \mathbb{R}^K, \quad (3.1)$$

which returns a probability distribution, and in particular the component $s(x)_k = \frac{e^{x_k}}{\sum_{\ell} e^{x_\ell}}$ of the result can be interpreted as the probability that label k is correct one.

In general, we can describe the output Y_{n+1} of a given layer $n + 1$, with respect to the output Y_n of the previous layer n , as follows :

$$\begin{cases} \tilde{Y}_{n+1} = W_{n+1}Y_n + b_{n+1} \\ Y_{n+1} = \mathcal{A}_{n+1}(\tilde{Y}_{n+1}) \end{cases}$$

We then seek to optimize the weights W as well as the biases b , that is, to optimize :

$$X = (W_1, b_1, \dots, W_n, b_n)$$

To minimize a loss function : $\mathcal{L}(X, \omega)$ which describes "the difference between the estimation by the neural network with parameters X , and the examples ω ". This minimization can then be performed with gradient descent.

3.2 Finite Difference Approach

A first idea would be to use the formula

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h). \quad (3.2)$$

This formula is derived using the Taylor series. It is called the formula of finite differences (non-centered). There is also another more accurate formula

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2). \quad (3.3)$$

It is also derived with the Taylor series (exact to order 2 with remainder of order 3). The approximation (3.3) is called centered finite differences of order 2.

Now let's analyze the cost of such a formula for a general function $G(y_1, \dots, y_N)$. It should be noted that in general, the most expensive part is the evaluation of the function G . Thus the cost will be expressed in terms of the number of evaluations of the function G needed to calculate $\nabla_X G$.

For example, if we want to obtain $\partial_{y_k} G$ we can use the approximation (3.3) for the function $f(x) := G(y_1, \dots, y_{k-1}, x, y_k, \dots, y_N)$. This means that calculating $\partial_{y_k} G$ will cost two evaluations of G . So calculating $\nabla_X G$ as a whole will cost $2N$ evaluations of G which is prohibitive when N is large (for neural networks N can be of the order of 10^9 !). Another approach is needed.

To know more 3.0.1. *However, finite differences are used to independently verify the implementation that will be done with automatic differentiation detailed later on.*



Warning 3.0.1. *Generally, one also needs to pay attention to numerical precision. If we assume that the numerical precision of the function f calculation is 10^{-16} , then we will have an error of $\frac{10^{-16}}{2h} + h^2$; this can be minimized with respect to h to obtain the optimal error order which will be $O(10^{-10.66})$ (achieved for $h = O(10^{-16/3})$). Note that in particular, we never achieve the order of 10^{-16} for the derivative calculation (this can be slightly improved by using higher-order formulas than 2 ... but which have an even greater cost).*

3.3 Computational Graphs, Notions of *Forward* and *Backward*

3.3.1 Direct Computational Graphs

We now delve into the heart of the matter : computational graphs.

Definition 3.1. Computational Graph. *A computational graph is a directed, connected, acyclic graph, in which the nodes correspond to operations that create new variables using the values of variables from incoming nodes.*

Each variable can thus be used by a target node, and each operation takes as input the result of previous operations. Its own result can then be used by other target operation nodes.

Let's take the example of the function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ defined by :

$$f(x, y, z) = (3x^2 + y)z - x. \quad (3.4)$$

We can associate with this function f the computational graph in figure 3.2.

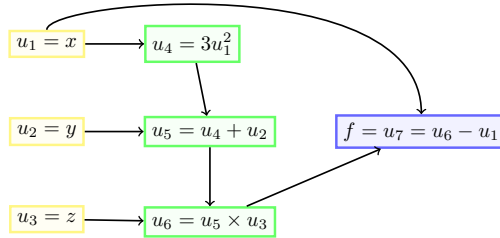


FIGURE 3.2 – Computational graph of f in equation (3.4).

Remark 3.2. *the yellow nodes (u_1, u_2, u_3) have no incoming degrees, they are nodes that contain only the input variables to our function f . The blue node u_7 constitutes the output of the function f . This graph is said to be direct : it performs the same operations as those of the function.*

Definition 3.3 (Input, Output). *The Input of a direct computational graph consists of all nodes with zero incoming degree. The Output of a computational graph consists of all nodes with zero outgoing degree.*

Example 3.4. *Taking again figure 3.2, the yellow nodes (u_1, u_2, u_3) are Inputs, the blue node u_7 is an output.*

In table 3.1 we specify the functions that define each node of the graph in figure 3.2. In an optimization problem, we will seek to obtain the gradient of the function computed by

	U_4	U_5	U_6	U_7
number of variables	1	2	2	2
function	$3U_1^2$	$U_4 + U_2$	$U_5 \times U_3$	$U_6 - U_1$

TABLE 3.1 – Functions of the nodes of the graph in figure 3.2.

the graph. This is where the notion of inverse computational graph comes in.

3.3.2 Backward Computational Graphs

We begin with some reminders concerning the computation of derivatives of composite functions. We assume all functions to be sufficiently regular. Let $f : \mathbb{R}^L \rightarrow \mathbb{R}$ be a function and g_1, \dots, g_L functions from \mathbb{R}^N to \mathbb{R} , and let $\forall X \in \mathbb{R}^N$:

$$F(X) := f(g_1(X), \dots, g_L(X))$$

The derivative of the function F with respect to X_k is given by :

$$\frac{\partial F}{\partial X_k} = \sum_{l=1}^L \frac{\partial f}{\partial g_l}(g_1(X), \dots, g_L(X)) \frac{\partial g_l}{\partial X_k}. \quad (3.5)$$

We recall that the gradient of the function F is the vector :

$$\nabla_X F = \left(\frac{\partial F}{\partial X_1}, \dots, \frac{\partial F}{\partial X_L} \right). \quad (3.6)$$

Sometimes the notation " $\nabla_X F$ " is also seen as " $J_X F$ ".

To know more 3.4.1. *We recall the definition of the first-order derivative (Jacobian) :*

Definition 3.5 (Jacobian). *Let $H : \mathbb{R}^N \rightarrow \mathbb{R}^P$ with*

the notations, for $X = (X_1, \dots, X_N) \in \mathbb{R}^N$:

$$H(X) = \begin{pmatrix} H_1(X) \\ \dots \\ H_P(X) \end{pmatrix}. \quad (3.7)$$

The Jacobian matrix of H is the matrix of the derivatives of H written as follows

$$J_X H = \begin{pmatrix} \frac{\partial H_1}{\partial X_1} & \dots & \frac{\partial H_1}{\partial X_N} \\ \vdots & \dots & \vdots \\ \frac{\partial H_P}{\partial X_1} & \dots & \frac{\partial H_P}{\partial X_N} \end{pmatrix} \in \mathbb{R}^{P \times N}. \quad (3.8)$$

In particular $(J_X H)_{ij} = \frac{\partial H_i}{\partial X_j}$. Sometimes the transpose is also used $\frac{DH}{DX} = D_X H = (J_X H)^T$.

Remark 3.6. The function $F : \mathbb{R}^N \rightarrow \mathbb{R}$ is in fact the composite function $f \circ g$. We have :

$$\left(\frac{\partial F}{\partial X_1}, \dots, \frac{\partial F}{\partial X_L} \right) = J_X F = J_X (f \circ g) = J_g f \times J_X g, \quad (3.9)$$

where " \times " denotes the usual matrix-vector product. This is a formula for deriving composite functions.

Returning to the graph 3.2; we employ the following notation :

$$\delta U_k = \frac{\partial f}{\partial U_k}. \quad (3.10)$$

Obviously, $\delta U_7 = \delta f = 1$. For the others it is not as immediate but we can see immediately that this calculation seems to be easier to develop **in reverse**, which is why it will be called backward. Let's be more precise.

To use the formula (3.5), the calculation must be put in this form. This is not possible with the initial graph but with a 'layered' version as in figure 3.3. where each *layer* contains

all the variables necessary to calculate the values of the next layer : the last layer contains only U_7 , its derivative is already calculated. The penultimate layer contains only U_6 and $U_{1,4}$ (which propagates the value of x). We can use the composite derivation to obtain $\delta U_6 = \frac{\partial U_7}{\partial U_6} = 1$, according to the formula of U_7 in table 3.1 ; similarly $\delta U_{1,4} = \frac{\partial U_7}{\partial U_{1,4}} = -1$.

So we continue backwards ; this new layer contains $U_{1,3}$, U_5 and $U_{3,3}$. The idea is to see $U_{1,3}$, U_5 and $U_{3,3}$ as inputs, the next layer U_6 and $U_{1,4}$ as intermediate variables and U_7 as the output. We then apply the composite derivation formula, for example :

$$\delta U_5 = \frac{\partial f}{\partial U_5} = \frac{\partial f}{\partial U_6} \cdot \frac{\partial U_6}{\partial U_5} + \frac{\partial f}{\partial U_{1,4}} \cdot \frac{\partial U_{1,4}}{\partial U_5} = \delta U_6 \cdot U_{3,3} + 0 = U_{3,3}.$$

The calculation can thus continue. Pay attention to the final calculation of δU_1 which will have two non-zero terms.

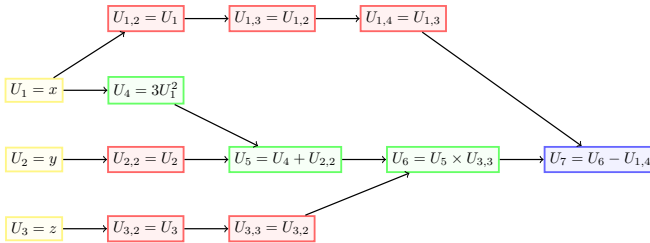


FIGURE 3.3 – Layered computational graph of f in equation (3.4). It was built by adding variables that will be necessary later in the form of new trivial variables, such as $U_{1,2} = U_1$, etc.

Remark 3.7. *This 'layered' representation introduces additional variables, here in red, but has the advantage of having a block structure where each block uses only the block that directly precedes it. This solution has the advantage of being rigorous but the disadvantage of complicating the calculations.*

To simplify the calculations, the idea is to keep the initial graph but to follow the following rule : going backward from

the output to the inputs, we calculate the derivative corresponding to a variable U_a only when all the derivatives δU_b of the boxes U_b such that an arrow between U_a and U_b exists have been calculated. Put simply : when everyone downstream of U_a in the graph has its derivative calculated, then we can also calculate the derivative δU_a . In our case, for example, this means attempting to calculate δU_1 only once δU_4 and $\delta U_{1,2}$ are known. The calculation results in the figure 3.4.

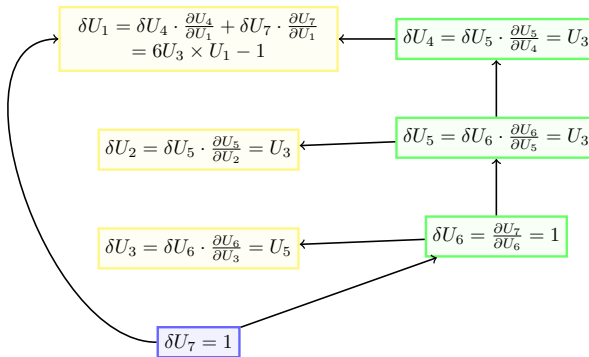


FIGURE 3.4 – Backward computational graph of f in equation (3.4).

In summary, it is possible to create a **direct** computational graph (which performs the same operations as our function) or a **backward** computational graph (which contains the derivatives).

3.4 Example 1 : Neural Networks

Suppose we have a training dataset Ω , and we want to define a neural network (NN) that will "learn" from this dataset, $\omega \in \Omega$.

We will then seek to optimize certain parameters X , so that the output of our network is as close as possible to the (known) output for the examples ω in the dataset Ω (for all $\omega \in \Omega$ the correct output is known; we are thus in the

context of so-called supervised learning). It is therefore an optimization problem :

$$\arg \min_X \{ \mathbb{E}_\omega (\mathcal{L}(X, \omega)) \} \quad (3.11)$$

We propose to study the neural network defined by the schema illustrated in figure 3.1.

3.4.1 Problem Definition

The network consists of an input layer, called *Input Layer*, a number of hidden layers, the *Hidden Layers*, and an output layer, the *Output Layer*. Each of the hidden layers (\tilde{Y}, Y) performs the following calculation : we take all the results from the previous layer, we assign them a weight (a vector W , and a bias b). We then obtain \tilde{Y} and finally apply an activation function \mathcal{A} , to obtain Y . Finally, we apply an output function g to the last layer. In general, we can describe the output Y_{n+1} of a given layer $n + 1$, relative to the output Y_n of the previous layer n as follows :

$$\begin{cases} \tilde{Y}_{n+1} = W_{n+1}Y_n + b_{n+1} \\ Y_{n+1} = \mathcal{A}_{n+1}(\tilde{Y}_{n+1}) \end{cases}$$

We then seek to optimize the weights W as well as the biases b , i.e., to optimize :

$$X = (W_1, b_1, \dots, W_n, b_n)$$

To minimize a loss function : $\mathcal{L}(X, \omega)$ which describes "the difference between the estimation by the neural network with the parameters X , for the examples ω ". This minimization can then be performed, for example, with a stochastic gradient descent algorithm (SGD).

3.4.2 Computational Graph of the Neural Network

In our example defined by the graph in Figure 3.1, we have :

- An *Input Layer*, $Y_0 \in \mathbb{R}^4$;
- A first *Hidden Layer*, $(\tilde{Y}_1, Y_1) \in \mathbb{R}^5$;
- A second *Hidden Layer*, $(\tilde{Y}_2, Y_2) \in \mathbb{R}^7$;
- An *Output Layer*, $O = g(Y_2) \in \mathbb{R}$.

Therefore, we have the computational graph presented in Figure 3.5.

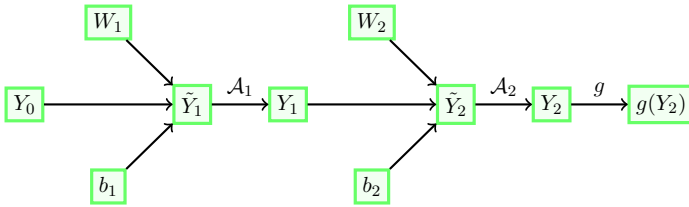


FIGURE 3.5 – Forward propagation graph of the neural network

3.4.3 Gradient Calculation of the Loss Function

We will now focus on the backward graph of this neural network as well as on the gradient calculation :

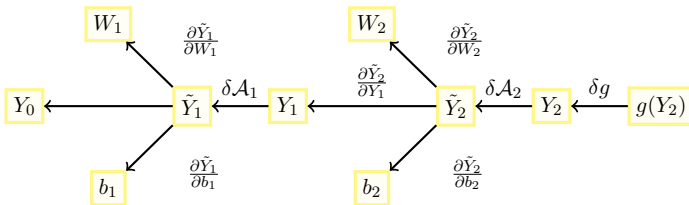


FIGURE 3.6 – Backward propagation graph of the neural network

We then have (note that this is a symbolic representation, for rigor it is necessary to employ the Jacobian matrix, see

the sidebar 3.4.1 page 54) :

$$\left\{ \begin{array}{l} \frac{\partial g}{\partial W_2} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial W_2} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial \tilde{Y}_2} \cdot \frac{\partial \tilde{Y}_2}{\partial W_2} \\ \\ \frac{\partial g}{\partial b_2} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial \tilde{Y}_2} \cdot \frac{\partial \tilde{Y}_2}{\partial b_2} \\ \\ \frac{\partial g}{\partial W_1} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial W_1} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial \tilde{Y}_2} \cdot \frac{\partial \tilde{Y}_2}{\partial W_1} \\ = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial \tilde{Y}_2} \cdot \frac{\partial \tilde{Y}_2}{\partial Y_1} \cdot \frac{\partial Y_1}{\partial W_1} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial \tilde{Y}_2} \cdot \frac{\partial \tilde{Y}_2}{\partial Y_1} \cdot \frac{\partial Y_1}{\partial \tilde{Y}_1} \cdot \frac{\partial \tilde{Y}_1}{\partial W_1} \\ \\ \frac{\partial g}{\partial b_1} = \frac{\partial g}{\partial Y_2} \cdot \frac{\partial Y_2}{\partial \tilde{Y}_2} \cdot \frac{\partial \tilde{Y}_2}{\partial Y_1} \cdot \frac{\partial Y_1}{\partial \tilde{Y}_1} \cdot \frac{\partial \tilde{Y}_1}{\partial b_1} \end{array} \right.$$

It is then possible to compute the quadruplet : $\left[\frac{\partial g}{\partial W_1}, \frac{\partial g}{\partial b_1}, \frac{\partial g}{\partial W_2}, \frac{\partial g}{\partial b_2} \right]$ which gives us the gradient of g with respect to $X = (W_1, b_1, W_2, b_2)$. We can then optimize g with respect to X using gradient descent.

Remark 3.8. *Note that in reality, we mainly need the derivative of the loss function \mathcal{L} in (3.11) ; it directly results from the derivative of g . Moreover, the construction of the loss function takes into account both objectives (reproduction of known results) as well as other considerations, for example generalization power ; indeed, overfitting must be prevented. To address this issue, we can introduce a penalty in the weight update at each iteration of gradient descent, or perform dropout, i.e., temporarily remove a neuron to force the algorithm not to overfit.*

Remark 3.9. *The gradient expressed above corresponds to the proposition shown earlier : each of the partial derivatives can be expressed as a sum.*

To know more 3.9.1 (Stochastic Gradient Descent).

We recall the formula for gradient descent for a multidimensional function $\mathcal{F} : \mathbb{R}^p \rightarrow \mathbb{R}$, with gradient $\nabla_x \mathcal{F}$:

$$x_{n+1} = x_n - \gamma_n \nabla_x \mathcal{F}(x_n).$$

Under certain assumptions (convexity, size of γ , ...), the sequence $(x_n)_{n \geq 1}$ converges to the nearest local minimum.

Here, γ_n is also called the "learning rate" in the case of statistical learning. In the case of high dimensions and when the function \mathcal{F} has the form of an average $\mathcal{F} = \mathbb{E}_\omega F(x, \omega)$ as in equation (3.11), computing the gradient at a point becomes very costly (and obtaining the average requires an expensive empirical average to calculate); this is where stochastic gradient descent (SGD) is used. We then take, among the different gradients $\nabla_x F(x, \omega)$, one value (or several, but in a small number) randomly selected.

$$x_{n+1} = x_n - \gamma_n \nabla_x F(x_n, \omega_n).$$

Several stochastic gradient descent algorithms combine different techniques (for learning rate variation as well as stochastic descent).

3.5 Example 2 : Control Problem

We now place ourselves in the context of the SIR system, seen previously. However, we will start with a more general presentation by considering that we use the Explicit Euler method to solve $x' = f(t, x(t), u(t))$ with the function $F(x(T))$ to optimize.

3.5.1 Computational Graphs

The first way to solve this problem is to create computational graphs. First, we obtain the direct computational graph in Figure 3.7 top. Subsequently, we obtain the backward computational graph in Figure 3.7 bottom.

However, these graphs represent only a part of the actual graph. Indeed, the complete direct graph is, for $n = 2$,

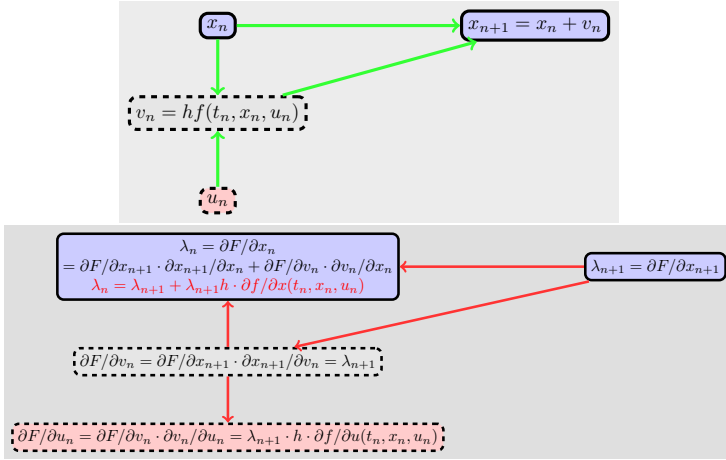


FIGURE 3.7 – Description of the "forward" mode (top image) and "backward" mode (bottom image) for a control problem ; the schema obtained for the adjoint state λ_n is an Explicit Euler type discretization of (3.14). Although this seems to correspond to Implicit Euler, it should be remembered that (3.14) is solved in reverse in time, which means that for example λ_{n+1} is known before λ_n .

presented in Figure 3.8.

3.5.2 Construction of a Discrete Version of an Euler-Lagrange Procedure

Direct and backward computational graphs allow us to construct a discrete version of an Euler-Lagrange procedure.

Consider a general framework where $x(t)$ satisfies the ODE : $x'(t) = f(t, x(t), u(t))$ At the discrete level, the EE scheme gives $x_{n+1} = x_n + hf(t_n, x_n, u_n)$. The computational

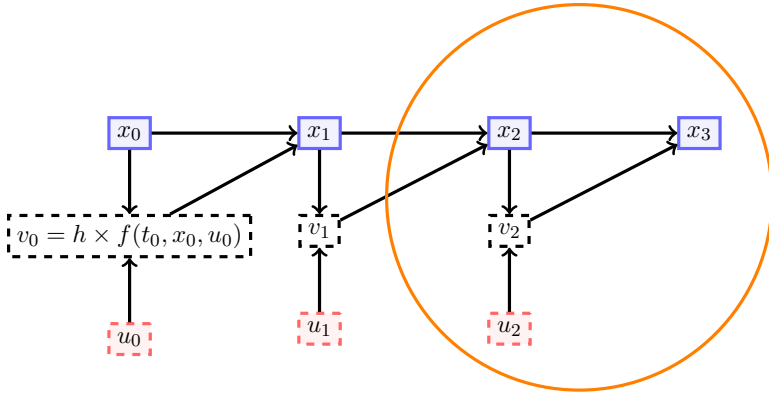


FIGURE 3.8 – Complete direct graph of the SIR system for $n = 2$; the orange circle represents the part that we had previously plotted in 3.7.

graph allows us to obtain :

$$\lambda_n = \lambda_{n+1} + \lambda_{n+1} \frac{\partial f}{\partial X}(t_n, x_n, u_n) h \quad (3.12)$$

$$\lambda_N = \frac{\partial F}{\partial x_N}. \quad (3.13)$$

The obvious peculiarity of this formula is that we know the end, namely λ_N , and we must construct the other values λ_n . This leads us to view $\lambda(t)$ as a solution of a **backward-in-time** equation and thus we find ourselves solving, by an Explicit Euler method, the equation :

$$\lambda'(t) = -\frac{\partial f}{\partial x}(t, x(t), u(t)) \lambda(t). \quad (3.14)$$

We also obtain a formula for the derivative :

$$\frac{\partial F}{\partial u_n} = \lambda_{n+1} h \frac{\partial f}{\partial u_n}(t_n, x_n, u_n). \quad (3.15)$$

In summary, the computational graph shows us that the derivative can be obtained with the help of solving the ODE (3.14) involving $\lambda(t)$, which will be called the adjoint state.

It is important to see that the cost of this calculation method is just 2 times the cost of calculating F , and thus independent of the number N of u_n values to optimize (to be compared with $2N$ evaluations that would be necessary if using a finite difference formula like (3.3)).

To know more 3.9.2. *The relation (3.15) is consistent with a formulation of the problem as an Euler-Lagrange type minimization; it is not a proof, rather a verification. The minimization to be done is written as $\min_{x'=f(t,x,u)} F(x(T))$. We apply the Lagrange multiplier method to the function $F(x(t))$ and introduce G :*

$$G(x, u, \lambda) = F(x(T)) - \int_0^T (x' - f(t, x, u))\lambda(t)dt,$$

where $\lambda(t)$ is the Lagrange multiplier. It is then appropriate to nullify the partial derivatives of G with respect to λ and x . As expected, the derivative with respect to the multiplier λ allows us to obtain the constraint :

$$\frac{\partial G}{\partial \lambda(t)} = 0 \Leftrightarrow x' = f(t, x, u).$$

The derivative with respect to the Lagrange multiplier $\lambda(t)$ will allow us to link our computational graph to the Euler-Lagrange procedure :

$$\begin{aligned} \frac{\partial G}{\partial x(t)} &= -\frac{\partial}{\partial x(t)} \int_0^T \lambda(x' - f(t, x, u))dt \\ &\stackrel{IPP}{=} -\frac{\partial}{\partial x(t)} \left[[\lambda x]_0^T - \int_0^T x\lambda' - \lambda f dt \right] \\ &= \lambda' - \lambda \frac{\partial f}{\partial x}(t, x(t), u(t)). \end{aligned}$$

We find equation (3.14) again. Thus, the computational graph allows us to obtain a discrete version of the

Euler-Lagrange procedure for our control variable. The derivative with respect to $x(T)$ allows us to find that $\lambda(T)$ should be set equal to $\frac{\partial F(x(T))}{\partial x(T)}$.

3.5.3 Problem Reminder

Let's now apply the described procedure to our situation of the SIR model. The problem can be represented by a system, which we call SIR. The system is of the form $x' = f(t, x(t), u(t))$

$$\begin{cases} \dot{S} = -\beta SI \\ \dot{I} = \beta SI - \gamma I \\ \dot{R} = \gamma I \end{cases}$$

with $u(t) = \beta(t) = \beta$ the control and $x = (S, I, R)$ the state. The goal is to minimize the cost of the confinement ($\int_0^T c(\beta(t))dt$) and the number of infected people ($S(0) - S(T)$) during the period $[0, T]$. In other words, we seek :

$$\min_{\beta} S(0) - S(T) + \int_0^T c(\beta(t))dt$$

Later on, we will denote $J(\beta) = S(0) - S(T) + \int_0^T c(\beta(t))dt$, with u being the set of time functions u_n that we will discretize :

$$\begin{array}{ccccccc} & u_1 & & u_2 & & u_3 & \\ | & | & | & | & | & | & \\ 0 & h & 2h & 3h & & & T = N \cdot h \end{array}$$

Initially, we have :

$$\frac{\partial}{\partial \beta} \left[\int_0^T c(\beta(t))dt \right] = c'(\beta(t)).$$

On the other hand, the difference $S(0) - S(T)$ is much less straightforward to derive because β does not appear explicitly, although it intervenes in this function. In general, we are

thus seeking to compute : $\frac{\partial}{\partial u_n} [F(x(T))]$, (for SIR $F(x(T)) = S(0) - S(T)$).

The methodology presented in 3.9.2 can be applied, and we obtain that, if we introduce λ and μ which satisfy :

$$\lambda'(t) = \beta(t)I(t)(\lambda(t) - \mu(t)), \quad \lambda(T) = -1, \quad (3.16)$$

$$\mu'(t) = \beta(t)S(t)(\lambda(t) - \mu(t)) + \gamma\mu(t), \quad \mu(T) = 0. \quad (3.17)$$

then $S(T) = \int_0^T -\beta(t)S(t)I(t)(\lambda(t) - \mu(t))dt - S(0)\lambda(0) - I(0)\mu(0)$, which can now be derived with respect to $\beta(t)$ to obtain $\frac{\partial}{\partial \beta(t)} S(T) = -S(t)I(t)(\lambda(t) - \mu(t))$.

3.6 Theoretical Appendix : Graph Theory

We will introduce some notions of graph theory.

Definition 3.10 (Directed Graph). A (oriented) graph is a pair $G = (V, E)$ consisting of :

- V a set of vertices ;
- E a set of edges, $E \subseteq V^2$, with $(a, b) \in E$ meaning that there is an edge between a and b . If the graph is considered oriented then the edge is **from** a to b .

Example 3.11. See figure 3.9 for an example of a directed graph.

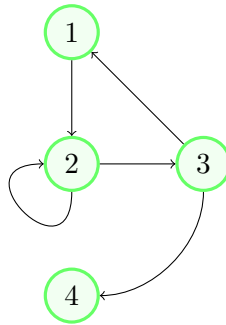


FIGURE 3.9 – Example of a directed graph

Each arc $\{x, y\}$ thus goes from node x to node y . The arc $\{x, y\}$ is not the same as the arc $\{y, x\}$. It is possible for an arc to point to the node from which it originates ($\{x, x\}$).

Remark 3.12. An undirected graph is a pair $G = (V, E)$ where $E \subseteq \{(x, y), (x, y) \in V^2, x \neq y\}$ is a set of edges that connect two different nodes together. An arc is thus an edge with a direction. We speak of a path from one node to another to refer to a consecutive sequence of edges connecting the two nodes.

Definition 3.13 (Connected Graph). A graph is said to be connected if it is in one piece, i.e., for any pair of nodes $v_1, v_2 \in V$ there exists a path from node v_1 to node v_2 .

Example 3.14. See figures 3.10 and 3.11 for an example of a connected or not connected graph.

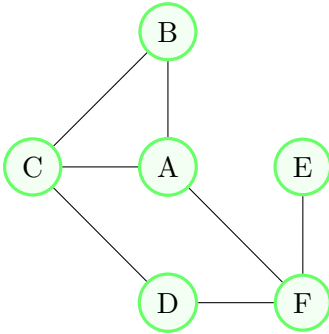


FIGURE 3.10
–
Connected
graph

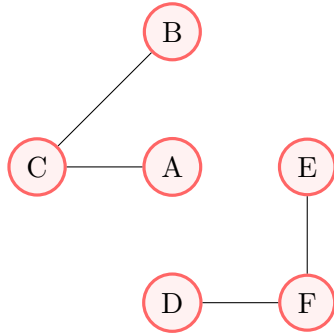


FIGURE 3.11
–
Non-
connected
graph

Definition 3.15. Graph without cycles. A graph without cycles is a graph that contains no path that has the same starting and ending node.

The graph in Figure 3.10 has several cycles (notably $\{A, F, D, C\}$), while the one in Figure 3.11 has none.

Definition 3.16 (Node Degrees). *Given an arc $\{x, y\}$ connecting nodes x and y , we call the starting node x the **source** and the ending node y the **target**. We then define :*

- *the **out-degree** of a node as the number of arcs that have this node as the source ;*
- *the **in-degree** of a node as the number of arcs that have this node as the target.*

A graph thus has as many in-degrees as out-degrees.

Example 3.17. *In the graph of Figure 3.9 :*

- *the out-degree of node $\{2\}$ is 2, the out-degree of node $\{4\}$ is zero.*
- *the in-degree of node $\{3\}$ is 1, the in-degree of node $\{2\}$ is 2.*
- *There are a total of 5 in-degrees and 5 out-degrees, which confirms our definition : there are as many in-degrees as out-degrees.*

3.7 Exercises

Exercise 3.1 (Finite differences of orders 3 and 4).

1. Show that

$$f'(x) = \frac{2f(x+3h) - 9f(x+2h) + 18f(x+h) - 11f(x)}{6h} + O(h^3). \quad (3.18)$$

2. Find a third-order formula of the form :

$$f'(x) = \frac{\alpha f(x+2h) + \beta f(x+h) + \gamma f(x) + \delta f(x-h)}{h} + O(h^3). \quad (3.19)$$

3. Show that

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4). \quad (3.20)$$

Exercise 3.2 (Reminder of Euler-Lagrange multipliers -1-).

Find the minimum of the function $x + y$ under the constraint $x^2 + y^2 = 1$ using the method of Euler-Lagrange multipliers.

Exercise 3.3 (Reminder of Euler-Lagrange multipliers -2-).

Let $f, g : \mathbb{R}^2 \rightarrow \mathbb{R}$ be C^2 functions. Suppose that the equation $g(x, y) = 0$ has a unique solution $y = \mathcal{Y}(x)$ for each given x , with \mathcal{Y} being C^1 . Also suppose that for all $x : \nabla_y g(x, \mathcal{Y}(x)) \neq 0$. Let $F : \mathbb{R} \rightarrow \mathbb{R}$ where $F(x) = f(x, \mathcal{Y}(x))$. We assume $\mathcal{Y}(\cdot)$ is difficult to obtain and we want to compute the gradient $\nabla_x F(x)$ without using $\mathcal{Y}(\cdot)$ too many times. Let $L(\lambda, x, y) = f(x, y) + \lambda g(x, y)$.

1. Show that for every x there exists λ_x such that :

$$\nabla_y L(\lambda_x, x, \mathcal{Y}(x)) = \nabla_\lambda L(\lambda_x, x, \mathcal{Y}(x)) = 0. \quad (3.21)$$

2. Show that : $\nabla_x F(x) = \nabla_x L(\lambda_x, x, \mathcal{Y}(x))$.

3. Generalize for functions $f : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$, $g : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n$.

Exercise 3.4 (example of computational graph).

1. Write the computational graph for the following computation : $z = x + \sin(x \cdot y) + x^2$. Then write the backward graph for computing the derivatives of z with respect to x and y . Explicitly calculate the values of these two graphs for $x = 2$, $y = \pi/6$.
2. Same for the function $(x, y, z) \mapsto xyze^{x^2+yz}$.

Exercise 3.5 (Backward mode EI, cf figure 3.7).

1. Find the formulas for forward and backward mode for a control problem as in figure 3.7 but with an Implicit Euler scheme.
2. Similarly, if the forward graph implements a general RK scheme, find the "adjoint" scheme, i.e., the one used by the backward propagation of the adjoint state. What do you observe ?

Exercise 3.6 (computational graph of projection). Let $P = \{(x, y, z)^T \in \mathbb{R}^3 \text{ such that } x + y + z = 1\} \subset \mathbb{R}^3$ and $\Pi : \mathbb{R}^3 \rightarrow P$ defined for any vector $v = (v_1, v_2, v_3)^T \in \mathbb{R}^3$ by $\Pi(v) = v - \lambda(v) \cdot (1, 1, 1)^T$ where $\lambda(v) \in \mathbb{R}$ is the only real number such that $\Pi(v) \in P$. Let $g : \mathbb{R}^3 \rightarrow \mathbb{R}$ be a C^1 function.

1. Find the formula for λ_v as a function of v ;
2. Write the direct computational graph that computes $v \mapsto g(\Pi(v))$;
3. Write the backward computational graph that computes the derivatives of $g(\Pi(v))$ with respect to the inputs (components of v).
4. Compute the derivatives for $v = (1, 2, 3)^T$ and $g(x, y, z) = x^2 + yz - 2$.

Reminder : for any vector a , a^T denotes its transpose.

Exercise 3.7 (computational graph of softmax/cross entropy). Compute the function g for the case of cross-entropy loss after a final "softmax" layer (output in \mathbb{R}^3) and architecture FC/ReLU 4 – 5 – 7 – 3; compute its derivatives.

Exercise 3.8 ("Layer Normalization"). A part of the work of the so-called "Layer Normalization" layer is the computation of the standard deviation of a data sample $x = (x_1, \dots, x_n)$. It is done as follows : first, calculate the empirical mean $\bar{\mu} = (\sum_{k=1}^n x_k)/n$, then the empirical variance $v = \sum_{k=1}^n (x_k - \bar{\mu})^2 / (n - 1)$ and finally the estimate of the standard deviation $\bar{\sigma} = \sqrt{v}$.

1. Draw the direct computational graph corresponding to the above calculations; for each node in the graph, explicitly specify, as in the lecture, the inputs/outputs and the operation performed by the node.
2. Similarly, draw the backward computational graph for the derivatives of the final output with respect to the inputs;
3. Compute the derivatives for $n = 3$, $x = (1, 2, 4)$ **with the help of the direct and backward computational graphs.**

3.8 Implementation session on backward chapter

Exercise 3.9. Implement exercise 3.5 for the case of the SIR model in section 3.1.2. Take the values $T = 150, N = 150, h = T/N, S(0) = 10^6, I(0) = 10, R(0) = 0, N_{total} = S(0) + I(0) + R(0), \beta = 0.5/N_{total}, \gamma = 1/3, c(\beta) = c_0/\beta$ with $c_0 = 10^{-2}$.

Exercise 3.10. Build and train a neural network with dense layers as described in section 3.1.3.

Chapitre 4

Équations différentielles stochastiques (EDS)

4.1 Rappels : mouvement brownien, martingales, intégrales et processus stochastiques, formule d'Ito

Pour les rappels de calcul stochastique voir le poly de M1 [7] d'où sont extraits ces résultats et les exercices 4.3, 4.1.

4.1.1 Mouvement brownien : définition

Definition 4.1 (mouvement brownien réel). *Soit $B = \{B_t, t \geq 0\}$ un processus défini sur l'espace de probabilité $(\Omega, \mathcal{F}, \mathbb{P})$ muni de la filtration naturelle (complétée) du processus B , filtration notée \mathbb{F} tel que :*

1. *B est un processus à trajectoires continues ;*
2. *B est un processus à accroissements indépendants, c'est-à-dire que pour tous $0 \leq s \leq t$ la variable aléatoire $B_t - B_s$ est indépendante de \mathcal{F}_s ;*

3. pour tous $0 \leq s \leq t$ la variable aléatoire $B_t - B_s$ suit la loi normale $\mathcal{N}(0, t - s)$.

Si de plus $B_0 = 0$ (respectivement $B_0 \neq 0$), on dit que B est un mouvement brownien standard (respectivement non-standard).

Quand la filtration \mathbb{F} est donnée a priori, un processus \mathbb{F} -adapté qui vérifie les conditions ci-dessus est dit \mathbb{F} -mouvement brownien.

Dans tout ce qui suit, sauf mention explicite du contraire nous supposons $B_0 = 0$.

Remark 4.2. Soit $B = \{B_t, t \geq 0\}$ un \mathbb{F} -mouvement brownien sur l'espace de probabilité filtré $(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{F})$. Alors B est un processus gaussien de fonction moyenne $e_B(t) = 0$ et d'opérateur de covariance $K_B(s, t) := \text{cov}(B_s, B_t) = \min(s, t)$.

Nous noterons par B ou W les mouvements browniens.

4.1.2 Variation quadratique

Definition 4.3. Soit $t > 0$ un réel donné et $\Delta := \{t_0 = 0 \leq t_1 \leq \dots \leq t_n = t\}$ une subdivision de l'intervalle $[0, t]$. On appelle module de la subdivision Δ et on note $|\Delta|$ la quantité $|\Delta| := \sup_i |t_i - t_{i-1}|$. Pour un processus X_t on note

$$V_t^{(2)}(X, \Delta) := \sum_{i=1}^n |X(t_i) - X(t_{i-1})|^2. \quad (4.1)$$

La fonction $t \mapsto V_t^{(2)}(X) := \overline{\lim}_{|\Delta| \rightarrow 0} V_t^{(2)}(X, \Delta) < \infty$ est appelée variation quadratique de X .

Proposition 4.4 (Variation quadratique du mouvement brownien). Soit B un mouvement brownien sur l'espace de probabilité $(\Omega, \mathcal{F}, \mathbb{P})$. Alors, pour tout $t \geq 0$

$$\lim_{|\Delta| \rightarrow 0} \mathbb{E} \left[|V_t^{(2)}(B, \Delta) - t|^2 \right] = 0. \quad (4.2)$$

Ceci peut s'écrire encore $V_t^{(2)}(B, \Delta) \xrightarrow[|\Delta| \rightarrow 0]{L^2} t$. On dit que la variation quadratique sur $[0, t]$ du mouvement brownien existe dans L^2 et $V_t^{(2)}(B) = t$.

Intuition 4.4.1. La variation quadratique somme les carrés des oscillations du mouvement brownien. Lorsque l'intervalle du temps devient de plus en plus petit nous obtenons une somme d'incrémentants indépendants qui convergera donc vers sa moyenne. Ceci peut se formaliser avec l'étude des variables χ^2 qui représentent la variation quadratique du Brownien.

4.1.3 Intégration des processus de $\mathcal{L}([0, T])$

On considère les ensembles $\mathcal{L}(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{F}; [0, T])$ (noté plus simplement $\mathcal{L}([0, T])$) et $\mathcal{L}^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{F}; [0, T])$ (noté plus simplement $\mathcal{L}^2([0, T])$) définis par :

$$\mathcal{L}([0, T]) := \left\{ (H_t)_{0 \leq t \leq T}, \text{ processus } \mathbb{F}\text{-adapté} \left| \left[\int_0^T H_u^2 du \right] < \infty \mathbb{P} - \text{p.s.} \right. \right\}.$$

$$\mathcal{L}^2([0, T]) = \left\{ \{H_t, 0 \leq t \leq T\}, \text{ processus } \mathbb{F}\text{-adapté} \left| \mathbb{E} \left[\int_0^T H_u^2 du \right] < \infty \right. \right\}.$$

Theorem 4.5 (Intégrale stochastique). *Il existe une unique application linéaire \mathcal{I} qui à tout processus $H \in \mathcal{L}([0, T])$ associe un processus $\mathcal{I}[H]$ à trajectoires continues sur $[0, T]$ tel que si H est continue et localement bornée et Δ^n est une suite de subdivisions de $[0, t]$ avec $|\Delta^n| \rightarrow 0$ alors (propriété de sommes de Riemann-Itô) :*

$$\mathbb{P} - \lim_{n \rightarrow \infty} \sum_{t_k \in \Delta^n} H_{t_k} (B_{t_{k+1}} - B_{t_k}) = \int_0^t H_s dB_s. \quad (4.3)$$

Si de plus $H \in \mathcal{L}^2([0, T])$ alors $\mathcal{I}[H]$ est une martingale.

Definition 4.6. Pour $H \in \mathcal{L}([0, T])$, le processus $\mathcal{I}[H]$ est appelé intégrale stochastique ou encore intégrale d'Itô de H par rapport au mouvement brownien B . On note $\int_0^t H_s dB_s := \mathcal{I}[H]_t$.

Exemple : exercice 4.1.

4.1.4 Processus d'Itô

Definition 4.7 (Processus d'Itô). *Un processus stochastique X est appelé processus d'Itô s'il s'écrit sous la forme*

$$X_t = X_0 + \int_0^t \alpha_u du + \int_0^t H_u dB_u \quad (4.4)$$

où X_0 est \mathcal{F}_0 -mesurable, $\{\alpha_t, t \in \mathbb{R}_+\}$ et $\{H_t, t \in \mathbb{R}_+\}$ sont deux processus \mathbb{F} -adaptés vérifiant les conditions d'intégrabilité

$$\int_0^T |\alpha_u| du < \infty \mathbb{P} - p.s. \text{ et } \int_0^T |H_u|^2 du < \infty \mathbb{P} - p.s. \quad (4.5)$$

On note également sous forme différentielle : $dX_t = \alpha_t dt + H_t dB_t$.



Warning 4.7.1. *La forme différentielle constitue juste une notation pour $\int_a^b dX_t = X_b - X_a$. Le mouvement brownien n'est pas différentiable pour autant (ce que laisserait penser le cas particulier $\alpha = 0, H = 1$!).*

Dorénavant on notera \mathfrak{I} l'ensemble des processus d'Itô et \mathfrak{I}^2 le sous-ensemble des processus d'Itô, $X_t = X_0 + \int_0^t \alpha_u du + \int_0^t H_u dB_u \in \mathfrak{I}$ tels que :

$$\mathbb{E} \left[\int_0^T |\alpha_u|^2 du \right] < \infty \text{ et } \mathbb{E} \left[\int_0^T |H_u|^2 du \right] < \infty. \quad (4.6)$$

4.1.5 Formule d'Itô

Intuition 4.7.1. L'exercice 4.1 page 92 montre que l'on a l'égalité suivante $\int_0^T 2B_s dB_s = B_T^2 - T$ que l'on peut aussi écrire en forme différentielle : $dB_s^2 = 2B_s dB_s + ds$. Nous voyons donc que la formule de dérivation composée "habituelle" $df(x) = f'(x)dx$ ne s'applique pas à $f(x) = x^2$ et $x = B_s$ car le terme $-T$ apparaît. Regardons cela de plus près : l'incrément infinitésimal entre t et $t + \Delta t$ d'un processus d'Itô est de l'ordre $\alpha_t \Delta t$ pour la partie continue et $H_t \sqrt{\Delta t} \mathcal{N}(0, 1)$ pour la partie brownienne. Pour Δt petit c'est clairement la partie brownienne qui domine. Faisons un petit calcul **formel** pour une fonction $f(x, y)$ et $x = t$, $y = \sqrt{t}$ dans la limite t petit :

$$f(t, \sqrt{t}) = f(0, 0) + \frac{\partial f}{\partial y}(0, 0)\sqrt{t} + \frac{\partial f}{\partial x}(0, 0)t + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} t^2 + \frac{\partial^2 f}{\partial x \partial y} t \sqrt{t} + \frac{1}{2} \frac{\partial^2 f}{\partial y^2} \sqrt{t}^2 + o(t^2 + \sqrt{t}^2) \quad (4.7)$$

Pour prendre en compte tous les termes d'ordre inférieur ou égal à t il faut nécessairement inclure le terme $\frac{1}{2} \frac{\partial^2 f}{\partial y^2} \sqrt{t}^2$, c'est-à-dire écrire :

$$f(t, \sqrt{t}) = f(0, 0) + \frac{\partial f}{\partial y}(0, 0)\sqrt{t} + \frac{\partial f}{\partial x}(0, 0)t + \frac{1}{2} \frac{\partial^2 f}{\partial y^2} t + o(t). \quad (4.8)$$

C'est ce terme additionnel qui constitue la nouveauté et doit être pris en compte. Il provient de la non-dérivabilité du mouvement brownien qui entraîne par ailleurs la non-différentiabilité de $t \mapsto f(t, \sqrt{t})$ en zéro et donc la présence d'un terme d'ordre \sqrt{t} et des termes \sqrt{t}^2 .

Theorem 4.8 (formule d'Itô). Soit $f : \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}$ une

fonction de classe $C^{1,2}$ (c'est-à-dire dérivable une fois en temps avec la dérivée continue et deux fois en espace avec dérivée seconde continue). Soit $X \in \mathfrak{I}$ un processus d'Itô $X_t = X_0 + \int_0^t \alpha_u du + \int_0^t H_u dB_u$. Alors, le processus $Y_t = f(t, X_t) \in \mathfrak{I}$ et

$$f(t, X_t) = f(0, X_0) + \int_0^t \frac{\partial f}{\partial t}(u, X_u) du + \int_0^t \frac{\partial f}{\partial x}(u, X_u) dX_u + \frac{1}{2} \int_0^t \frac{\partial^2 f}{\partial x^2}(u, X_u) H_u^2 du$$

ou encore, en formulation différentielle,

$$df(t, X_t) = \left\{ \frac{\partial f}{\partial t} + \alpha_t \frac{\partial f}{\partial x} + H_t^2 \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \right\} (t, X_t) dt + H_t \frac{\partial f}{\partial x}(t, X_t) dB_t. \quad (4.9)$$

Exemple : $Y_t = X_t^2$.

4.1.6 Équations différentielles stochastiques

Étant données deux applications a et b on se demande s'il existe un processus d'Itô $X = \{X_t, t \leq 0\}$ dont la décomposition (unique) vérifie

$$dX_t = a(t, X_t) dt + b(t, X_t) dB_t$$

en notation différentielle. Voir l'exercice 4.3 page 92 pour des exemples de telles équations apparaissant dans des modèles en finance.

Theorem 4.9. Soit $T > 0$ et $a(\cdot, \cdot), b(\cdot, \cdot) : [0, T] \times \mathbb{R} \rightarrow \mathbb{R}$ des fonctions mesurables telles qu'il existe des constantes $C, L > 0$ satisfaisant :

$$|a(t, x)| + |b(t, x)| \leq C(1 + |x|), \quad \forall x \in \mathbb{R}, t \in [0, T], \quad (4.10)$$

$$|a(t, x) - a(t, y)| + |b(t, x) - b(t, y)| \leq L|x - y|, \quad \forall x, y \in \mathbb{R}, t \in [0, T]$$

Soit Z une variable aléatoire indépendante de $\mathcal{F}^\infty = \sigma\{B_s, s \geq 0\}$ et telle que

$$\mathbb{E}[Z^2] < \infty.$$

Alors l'équation différentielle stochastique

$$X_t = Z + \int_0^t a(s, X_s) ds + \int_0^t b(s, X_s) dB_s, \quad t \in [0, T], \quad (4.12)$$

ou en notation différentielle

$$dX_t = a(t, X_t) dt + b(t, X_t) dB_t, \quad X_0 = Z, \quad t \in [0, T], \quad (4.13)$$

admet une unique solution $X = \{X_t, t \leq 0\}$ telle que :

1. X est continue par rapport à t ;
2. X est adaptée à la filtration \mathcal{F}_t^Z générée par \mathcal{F}_t et Z ;
3. $X \in \mathcal{L}^2([0, T])$ i.e., :

$$\mathbb{E} \left[\int_0^T X_t^2 dt \right] < \infty.$$

4.1.7 Résumé du cadre

Nous nous plaçons dans un cadre d'espace probabilisé filtré $(\Omega, \mathbb{P}, \mathcal{F}, (\mathcal{F}_t))$ et (W_t) est un mouvement brownien qui engendre la filtration (\mathcal{F}_t) .

On appelle processus d'Itô, un processus $(X_t)_{0 \leq t \leq T}$ à valeurs dans \mathbb{R} tel que :

$$\mathbb{P} - ps \quad \forall t \leq T : X_t = X_0 + \int_0^t K_s ds + \int_0^t H_s dW_s, \quad (4.14)$$

ou de manière équivalente :

$$dX_t = K_t dt + H_t dW_t, \quad (4.15)$$

avec X_0 donné \mathcal{F}_0 -mesurable, (H_t) et (K_t) adaptés à (\mathcal{F}_t) , $\int_0^T |K_s| ds < \infty$ et $\int_0^T H_s^2 ds < \infty$, $\mathbb{P} - ps$.

Lorsque K et H dépendent de X nous obtenons des Equations Différentielles Stochastiques (EDS) dont l'existence d'une solution est donnée par un résultat spécifique. L'approximation de leur solution est l'objet de ce chapitre.

4.2 Schéma d'Euler-Maruyama et Milshstein

Les méthodes que nous allons détailler portent sur la résolution du type d'équations suivant :

$$dX_t = a(t, X_t)dt + b(t, X_t)dW_t$$

Ou encore, en forme intégrale :

$$X_t = X_0 + \int_0^t a(s, X_s) ds + \int_0^t b(s, X_s) dW_s$$

Nous gardons les notations $0 = t_0 < t_1 < \dots < t_n < \dots < t_N = T$. En fait, sauf mention contraire, on supposera que $t_{n+1} - t_n$ est constant égal à h .

Schéma d'Euler-Maruyama (E-M) : Ce schéma propose d'approcher $X(t_n)$ par Y_n vérifiant :

$$Y_{n+1} = Y_n + a(t_n, Y_n)(t_{n+1} - t_n) + b(t_n, Y_n)(W_{t_{n+1}} - W_{t_n}).$$

Remark 4.10. Lorsque $t_{k+1} - t_k = h$ pour tout k et si on note $\Delta W_n := W_{t_{n+1}} - W_{t_n}$, $a_n := a(t_n, Y_n)$, $b_n := b(t_n, Y_n)$ alors le schéma E-M s'écrit :

$$Y_{n+1} = Y_n + a_n h + b_n \Delta W_n, \quad Y_0 = X(0).$$

Remark 4.11. a_n et b_n sont des variables aléatoires \mathcal{A}_{t_n} -mesurables, où $(\mathcal{A}_t)_{t \geq 0}$ est la filtration engendrée par $(W_t)_{t \geq 0}$.

Schéma de Milshstein : Il est donné par la relation :

$$Y_{n+1} = Y_n + a_n h + b_n \Delta W_n + \frac{1}{2} b_n b'_n [(\Delta W_n)^2 - h], \quad Y_0 = X(0).$$

To know more 4.11.1. *Supposons que $a(t, X) = \alpha X$ et $b(t, X) = \beta X$, existe-t-il des schémas implicites ? Une proposition pourrait être : $Y_{n+1} = Y_n + \alpha Y_{n+1}h + \beta Y_{n+1}\Delta W_n$ ce qui veut dire que $Y_{n+1} = \frac{Y_n}{1 - \alpha h - \beta \Delta W_n}$. Or, ceci est non borné puisque si $\xi \sim \mathcal{N}(0, 1)$ alors $\mathbb{E}(\frac{1}{|\xi|}) = +\infty$. Il faudrait donc plutôt : $Y_{n+1} = Y_n + \alpha h Y_{n+1} + \beta Y_n \Delta W_n$; pour Milshtein on pourrait utiliser tout au plus une implicite en gardant explicite ce terme $\frac{b_n b'_n}{2}(\Delta W_n^2 - h)$.*

4.3 Consistance faible et forte

Pour rappel, pour une EDO la consistance pouvait s'écrire sous la forme : erreur de troncature est nulle dans la limite $h \rightarrow 0$, ou encore $\tau(h) = o(1)$. Ceci motive la définition suivante :

Definition 4.12 (Consistance faible). *Un schéma qui permet d'obtenir $(Y_n)_{n \geq 1}$ est dit faiblement consistant si :*

$$(W1) \quad \lim_{h \rightarrow 0} \mathbb{E} \left[\left(\mathbb{E} \left[\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n} \right] - a_n \right)^2 \right] = 0.$$

$$(W2) \quad \lim_{h \rightarrow 0} \mathbb{E} \left[\left(\mathbb{E} \left[\frac{(Y_{n+1} - Y_n)^2}{h} \middle| \mathcal{A}_{t_n} \right] - b_n^2 \right)^2 \right] = 0.$$

Theorem 4.13. *Soit $T > 0$ et $a(.,.), b(.,.), b'(.,.) : [0, T] \times \mathbf{R} \rightarrow \mathbf{R}$ des fonctions bornées. Alors les schémas d'Euler-Maruyama (E-M) et Milstein (M) définis précédemment sont faiblement consistants.*

Démonstration. a) Schéma d'Euler-Maruyama (E-M)

Vérifions (W1) :

$$\begin{aligned}
& \mathbb{E} \left[\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n} \right] - a_n \\
&= \mathbb{E} \left[\frac{Y_n + a_n h + b_n \Delta W_n - Y_n}{h} \middle| \mathcal{A}_{t_n} \right] - a_n \\
&= \mathbb{E} \left[a_n + b_n \frac{\Delta W_n}{h} \middle| \mathcal{A}_{t_n} \right] - a_n \\
&= a_n + b_n \mathbb{E} \left[\frac{\Delta W_n}{h} \middle| \mathcal{A}_{t_n} \right] - a_n \quad (\text{car } a_n, b_n \widehat{\in} \mathcal{A}_{t_n}) \\
&= b_n \mathbb{E} \left[\frac{\Delta W_n}{h} \right] \quad (\text{car } \Delta W_n \perp\!\!\!\perp \mathcal{A}_{t_n}) = 0. \quad (4.16)
\end{aligned}$$

Vérifions (W2) :

$$\begin{aligned}
& \mathbb{E} \left[\frac{(Y_{n+1} - Y_n)^2}{h} \middle| \mathcal{A}_{t_n} \right] - b_n^2 = \mathbb{E} \left[\frac{(a_n h + b_n \Delta W_n)^2}{h} \middle| \mathcal{A}_{t_n} \right] - b_n^2 \\
&= \mathbb{E} \left[h a_n^2 + 2 a_n \Delta W_n b_n + b_n^2 \frac{(\Delta W_n)^2}{h} \middle| \mathcal{A}_{t_n} \right] - b_n^2 \\
&= h a_n^2 + 2 a_n b_n \mathbb{E}[\Delta W_n] + b_n^2 \frac{\mathbb{E}[\Delta W_n^2]}{h} - b_n^2 \\
&= h a_n^2 \quad (\text{car } \Delta W_n \sim \mathcal{N}(0, h)) \xrightarrow{L^2} 0. \quad (4.17)
\end{aligned}$$

b) Schéma de Milstein (M)

Vérifions (W1) :

On rappelle que $\Delta W_n \sim \mathcal{N}(0, h)$.

$$\begin{aligned}
& \mathbb{E} \left[\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n} \right] - a_n \\
&= \frac{1}{h} \mathbb{E} \left[a_n h + b_n \Delta W_n + \frac{b_n b'_n}{2} (\Delta W_n^2 - h) \middle| \mathcal{A}_{t_n} \right] - a_n \\
&= \frac{a_n h}{h} + b_n \underbrace{\frac{1}{h} \mathbb{E}[\Delta W_n]}_{=0} + \frac{1}{h} \frac{b_n b'_n}{2} \underbrace{\mathbb{E}[\Delta W_n^2 - h]}_{=0} - a_n \\
&= 0 \quad (4.18)
\end{aligned}$$

Vérifions (W2) :

$$\begin{aligned}
& \mathbb{E} \left[\frac{(Y_{n+1} - Y_n)^2}{h} \middle| \mathcal{A}_{t_n} \right] - b_n^2 \\
&= \frac{1}{h} \mathbb{E} \left[\left(a_n h + b_n \Delta W_n + \frac{b_n b'_n}{2} (\Delta W_n^2 - h) \right)^2 \middle| \mathcal{A}_{t_n} \right] - b_n^2 \\
&= \mathbb{E} \left[\left(\underbrace{a_n \sqrt{h}}_{O(\sqrt{h})} + b_n \frac{\Delta W_n}{\sqrt{h}} + \frac{b_n b'_n}{2} \left(\frac{\Delta W_n^2 - h}{\sqrt{h}} \right) \right)^2 \middle| \mathcal{A}_{t_n} \right] - b_n^2 \\
&= \mathbb{E} \left[a_n^2 h + b_n^2 \frac{\Delta W_n^2}{h} + \frac{b_n^2 b'^2_n}{4} \frac{(\Delta W_n^2 - h)^2}{h} + 2a_n b_n \sqrt{h} \frac{\Delta W_n}{\sqrt{h}} + \right. \\
&\quad \left. 2a_n \sqrt{h} \frac{b_n b'_n}{2} \frac{\Delta W_n^2 - h}{\sqrt{h}} + \frac{b_n^2 b'_n}{2\sqrt{h}} \Delta W_n \frac{\Delta W_n^2 - h}{\sqrt{h}} \middle| \mathcal{A}_{t_n} \right] - b_n^2 \\
&= a_n^2 h + \frac{b_n^2 b'^2_n}{4} \mathbb{E} \left[\frac{(\Delta W_n^2 - h)^2}{h} \right] + \underbrace{\frac{b_n^2 b'_n}{2\sqrt{h}} \mathbb{E} \left[\Delta W_n \frac{\Delta W_n^2 - h}{\sqrt{h}} \right]}_{=0} \\
&= a_n^2 h + \frac{b_n^2 b'^2_n}{4} h \underbrace{\mathbb{E}[(N(0, 1)^2 - 1)^2]}_{\text{borné par rapport à } h} = O(h) \xrightarrow{h \rightarrow 0} 0. \quad (4.19)
\end{aligned}$$

□

Remark 4.14. La solution exacte vérifie (W1) et (W2), voir exo 4.5 page 94.

Remark 4.15. Comme attendu la consistance faible concerne seulement certaines fonctions dépendant de la solution, en particulier les moments.

Definition 4.16 (Consistance forte). Un schéma $(Y_n)_{n \geq 1}$ est dit fortement consistant si :

(F1) la condition (W1) est vérifiée

(F2) : $\lim_{h \rightarrow 0} \mathbb{E} \left[\frac{1}{h} |Y_{n+1} - Y_n - \mathbb{E}[Y_{n+1} - Y_n | \mathcal{A}_{t_n}] - b_n \Delta W_n|^2 \right] = 0$

Theorem 4.17. Les schémas d'Euler-Maruyama (E-M) et

Milshtein (M) (sous hypothèses a, b, b' bornées) sont fortement consistants.

Démonstration. a) Schéma d'Euler-Maruyama (E-M)

(F1) est satisfaite par le théorème précédent.

Vérifions (F2) :

$$Y_{n+1} - Y_n - \mathbb{E}[Y_{n+1} - Y_n | \mathcal{A}_{t_n}] - b_n \Delta W_n = \underbrace{a_n h}_{\mathbb{E}[Y_{n+1} - Y_n | \mathcal{A}_{t_n}]} - b_n \Delta W_n = 0$$

$\mathbb{E}[Y_{n+1} - Y_n | \mathcal{A}_{t_n}]$

b) Schéma de Milshtein (M)

(F1) est satisfaite par le théorème précédent.

Vérifions (F2) :

$Y_{n+1} - Y_n - \mathbb{E}[Y_{n+1} - Y_n | \mathcal{A}_{t_n}] - b_n \Delta W_n = a_n h + b_n \Delta W_n + \frac{b_n b'_n}{2} [\Delta W_n^2 - h] - a_n h - b_n \Delta W_n = \frac{b_n b'_n}{2} [\Delta W_n^2 - h]$. Il faut montrer que $\lim_{h \rightarrow 0} \mathbb{E} \left[\frac{1}{h} \left(\frac{b_n b'_n}{2} [\Delta W_n^2 - h] \right)^2 \right] = 0$. Mais puisque b, b' sont bornées on obtient que

$$\begin{aligned} & \lim_{h \rightarrow 0} \mathbb{E} \left[\frac{1}{h} \left(\frac{b_n b'_n}{2} [\Delta W_n^2 - h] \right)^2 \right] \\ & \leq \lim_{h \rightarrow 0} C_0 h \mathbb{E} \left[\left(\left(\frac{\Delta W_n}{\underbrace{\sqrt{h}}_{\mathcal{N}(0,1)}} \right) - 1 \right)^2 \right] = 0 \quad (4.20) \end{aligned}$$

où C_0 est une constante et on a utilisé le fait que

$\mathbb{E} \left[\left(\left(\frac{\Delta W_n}{\sqrt{h}} \right)^2 - 1 \right)^2 \right]$ est une constante indépendante de h . □

Remark 4.18. La consistance forte implique la consistance faible, voir exo 4.5 page 94.

4.4 Convergence faible et forte

Nous utilisons les mêmes notations, qu'avant, et en particulier dans les deux définitions suivantes le pas de temps h vérifie $h = T/N$, N étant le nombre de pas de temps pour arriver à un T donné (N est entier). On écrira N_h pour figurer mieux cette dépendance.

Definition 4.19 (Convergence forte). *Un schéma $(Y_n)_{n \geq 1}$ est dit fortement convergent à l'ordre $\gamma > 0$ au temps T s'il existe $h_0 > 0$ et $C > 0$ indépendant de h tel que : $\forall h \leq h_0$:*

$$E[|X(hN_h) - Y_{N_h}|] \leq Ch^\gamma \quad (\text{avec } N_h = [T/h] \in \mathbb{N}). \quad (4.21)$$

Definition 4.20 (Convergence faible). *Le schéma $(Y_n)_{n \geq 1}$ est dit faiblement convergent à l'ordre $\beta > 0$ s'il existe $h_0 > 0$ et $C > 0$ indépendant de h tel que : $\forall h \leq h_0, \forall g \in C_p^{2\beta+2}$:*

$$|\mathbb{E}[g(X(hN_h))] - \mathbb{E}[g(Y_{N_h})]| \leq Ch^\beta,$$

où $C_p^{2\beta+2}$ est l'ensemble des fonctions à croissance au plus polynomiale¹ de classe $2\beta + 2$.

Exemple 4.21. *Les fonctions $\log(\cdot)$ et $\sin(\cdot)$ sont à croissance au plus polynomiale. La fonction exponentielle ne l'est pas.*

Exemple 4.22. *Soit $W = (W_t)$ et $B = (B_t)$ deux mouvements Browniens indépendants et X_t la solution exacte de l'équation $dX_t = 0 \cdot dt + 1dW_t$ c'est à dire $X_t = W_t$. Si on propose comme schéma numérique $Y_{n+1} = Y_n + \Delta B_n$ on obtiendra $Y_n = B_{t_n} = B_{nh}$. Bien que les processus W et B soient totalement indépendants, Y_n respecte parfaitement la distribution de la variable W_{t_n} donc en particulier ce schéma est convergent faiblement à tout ordre $\gamma \geq 0$. Il n'est en revanche fortement convergent à aucun ordre.*

1. Une fonction f est dite à croissance au plus polynomiale s'il existe $s \in \mathbb{N}$ et $C_s > 0$ tel que : $|f(x)| \leq C_s(1 + |x|^s), \forall x \in \mathbb{R}$.

Theorem 4.23 (Convergence des schémas d'Euler-Maruyama et Milshtein). *Le schéma E-M converge fortement à l'ordre 1/2 et faiblement à l'ordre 1. Le schéma de Milshtein converge fortement et faiblement à l'ordre 1.*

■ *Démonstration.* Ce théorème est admis. □

4.5 Taylor sous forme intégrale pour ODE

Dans cette partie, on considère une équation différentielle ordinaire, $X'_t = a(t, X_t)$, dont la forme intégrale s'écrit $X_t = X_0 + \int_0^t a(s, X_s) ds$. Nous écrivons t comme indice dans l'équation précédente. Pour toute fonction f assez régulière, en utilisant l'équation de X on obtient :

$$\frac{d}{dt} f(X_t) = a(t, X_t) \frac{\partial}{\partial x} f(X_t) \quad (4.22)$$

L'équation (4.22) peut également s'écrire $f'(X_t) = a \cdot f_x$. Cette définition de f nous permet de l'écrire sous forme intégrale

$$f(X_t) = f(X_0) + \int_0^t Lf(X_s) ds, \quad (4.23)$$

dans laquelle nous avons introduit l'opérateur L qui, pour une fonction f , agit par $L(f) = a \frac{\partial}{\partial x} (f)$. Soit $f(x) = x$; la relation (4.23) nous permet d'écrire $X_t = X_0 + \int_0^t a(X_s) ds$ car ici $L(x) = a \frac{\partial}{\partial x} (x) = a$.

Pour simplifier nos calculs, on pose $a = a(x)$, on considère qu'il n'y a donc pas de dépendance explicite de t . De même, il est important de remarquer que (4.23) est valable pour toute fonction f , en particulier $f = a$. Dans ce cas,

$$a(X_s) = a(X_0) + \int_0^s La(X_{s_2}) ds_2$$

En réintroduisant (4.5) dans la définition de X_t , on obtient

$$\begin{aligned} X_t &= X_0 + \int_0^t \left[a(X_0) + \int_0^s La(X_{s_2}) ds_2 \right] ds \\ &= X_0 + ta(X_0) + \int_0^t \int_0^s La(X_{s_2}) ds_2 ds. \end{aligned}$$

On peut réitérer ce procédé autant de fois que souhaité, ce qui permet donc définir la formule de Taylor sous forme intégrale :

$$\begin{aligned}
 f(X_t) &= f(X_0) + \int_0^t Lf(X_s)ds \\
 &= \dots \\
 &= f(X_0) + \sum_{k=1}^n \frac{t^k}{k!} L^k f(X_0) \\
 &\quad + \int_0^t \int_0^s \int_0^{s_2} \dots \int_0^{s_n} L^{n+1} f(X_{s_n}) ds_n \dots ds. \quad (4.24)
 \end{aligned}$$

En utilisant (4.24) pour $a = 1$, $f(x) = x$, on obtient la formule de Taylor usuelle.

4.6 Formules d'Itô-Taylor

Dans cette partie, on considère une équation différentielle stochastique $dX_t = a(t, X_t)dt + b(t, X_t)dW_t$. La formule d'Itô,

$$\begin{aligned}
 f(X_t) &= f(X_0) \\
 &\quad + \int_0^t \left\{ a(X_s) \frac{\partial}{\partial x} f(X_s) + \frac{1}{2} b(X_s)^2 \frac{\partial^2}{\partial x^2} f(X_s) \right\} ds \\
 &\quad + \int_0^t b(X_s) \frac{\partial}{\partial x} f(X_s) dW_s \quad (4.25)
 \end{aligned}$$

nous conduit à introduire deux opérateurs :

$$L^0 = a(X_s) \frac{\partial}{\partial x} + \frac{1}{2} b(X_s)^2 \frac{\partial^2}{\partial x^2}, \quad L^1 = b(X_s) \frac{\partial}{\partial x}$$

L'équation (4.25) s'écrit alors :

$$f(X_t) = f(X_0) + \int_0^t (L^0 f)(X_s) ds + \int_0^t (L^1 f)(X_s) dW_s \quad (4.26)$$

On souhaite trouver une expression de X_t d'ordre 1. L'équation (4.26) reste vraie pour toute fonction f , en particulier $f(x) =$

x . On a donc l'EDS sous forme intégrale suivante :

$$X_t = X_0 + \int_0^t a(X_s)ds + \int_0^t b(X_s)dW_s$$

En appliquant (4.26) aux fonctions a et b on obtient :

$$\begin{aligned} X_t &= X_0 \\ &+ \int_0^t \left\{ a(X_0) + \int_0^s (L^0 a)(X_\sigma)d\sigma + \int_0^s (L^1 a)(X_\sigma)dW_\sigma \right\} ds + \\ &+ \int_0^t \left\{ b(X_0) + \int_0^s (L^0 b)(X_\sigma)d\sigma + \int_0^s (L^1 b)(X_\sigma)dW_\sigma \right\} dW_s. \end{aligned}$$

Finalement, on a

$$X_t = X_0 + \underbrace{a(X_0) \int_0^t ds}_{O(t)} + \underbrace{b(X_0) \int_0^t dW_s}_{O(t^{1/2})} + R$$

On étudie le reste R , afin d'estimer l'ordre de ses termes.

$$\begin{aligned} R &= \underbrace{\int_0^t \int_0^s (L^0 a)(X_\sigma)d\sigma ds}_{O(t^2)} + \underbrace{\int_0^t \int_0^s (L^1 a)(X_\sigma)dW_\sigma ds}_{O(t^{3/2})} + \\ &+ \underbrace{\int_0^t \int_0^s (L^0 b)(X_\sigma)d\sigma dW_s}_{O(t^{3/2})} + \underbrace{\int_0^t \int_0^s (L^1 b)(X_\sigma)dW_\sigma dW_s}_{O(t)} \end{aligned}$$

On remarque que le dernier terme est d'ordre 1. Pour rappel, on a

$$\begin{aligned} (L^1 b)(X_\sigma) &= (L^1 b)(X_0) + \int_0^\sigma (L^0 L^1 b)(X_u)du \\ &+ \int_0^\sigma (L^1 L^1 b)(X_u)dW_u \quad (4.27) \end{aligned}$$

On va garder dans (4.27) seulement le premier terme, $L^1 b(X_0)$ car on ne s'intéresse qu'aux termes d'ordre 1. Finalement,

on obtient la **formule d'Itô-Taylor à l'ordre 1 de reste** $O(t^{3/2})$:

$$\begin{aligned}
 X_t = X_0 + a(X_0) \int_0^t ds + b(X_0) \int_0^t dW_s \\
 + L^1 b(X_0) \int_0^t \int_0^s dW_\sigma dW_s + R_2 \quad (4.28)
 \end{aligned}$$

Ici R_2 est un terme d'ordre $t^{3/2}$. On peut vérifier que le reste R_2 contient uniquement termes d'ordre supérieurs ou égaux à $3/2$:

$$\begin{aligned}
 R_2 = & \underbrace{\int_0^t \int_0^s L^0 a(X_\sigma) d\sigma ds}_{O(t^2)} + \underbrace{\int_0^t \int_0^s L^1 a(X_\sigma) dW_\sigma ds}_{O(t^{3/2})} + \\
 & + \underbrace{\int_0^t \int_0^s L^0 b(X_\sigma) d\sigma dW_s}_{O(t^{3/2})} \\
 & + \underbrace{\int_0^t \int_0^s \int_0^\sigma L^0 L^1 b(X_u) du dW_\sigma dW_s}_{O(t^2)} + \\
 & + \underbrace{\int_0^t \int_0^s \int_0^\sigma L^1 L^1 b(X_u) dW_u dW_\sigma dW_s}_{O(t^{3/2})}
 \end{aligned}$$

On voit donc bien que tous les termes de R_2 sont d'ordre supérieur à 1, on a donc bien trouvé une expression de X_t d'ordre 1.

4.7 Application de Ito-Taylor à la construction des schémas numériques

Dans cette partie, nous pouvons essayer d'approcher la solution d'une équation différentielle par un calcul numérique avec la méthode d'Euler-Maruyama. Nous allons calculer les

termes apparaissant dans la formule de Ito-Taylor d'ordre 1 en (4.28). $[t_n, t_{n+1}]$:

$$\begin{aligned} X_{t_{n+1}} &= X_{t_n} + a(X_{t_n}) \int_{t_n}^{t_{n+1}} ds + b(X_{t_n}) \int_{t_n}^{t_{n+1}} dW_s \\ &\quad + L^1 b(X_{t_n}) \int_{t_n}^{t_{n+1}} \int_{t_n}^{t_{n+1}} dW_\sigma dW_s + R_2 \end{aligned}$$

En calculant les intégrales on obtient :

$$X_{t_{n+1}} = X_{t_n} + a(X_{t_n})(t_{n+1} - t_n) + b(X_{t_n})(W_{t_{n+1}} - W_{t_n}) + O(h), \quad (4.29)$$

ce qui permet d'obtenir le schéma **d'Euler-Maruyama** qui utilise le développement d'Ito-Taylor avec inclusion de tous les termes d'ordre $\frac{1}{2}$ mais seulement une partie des termes d'ordre 1.

Continuons dans la formule d'Ito-Taylor (4.28) avec le calcul de $L^1 b(X_{t_n})$; par soucis de simplification, on note $b_n = b(X_{t_n})$. Vu la définition de L^1 on obtient alors $L^1 b(X_{t_n}) = b(X_{t_n}) \frac{\partial}{\partial x} b(X_{t_n})$ et donc

$$L^1 b(X_{t_n}) \int_{t_n}^{t_{n+1}} \int_{t_n}^s dW_\sigma dW_s = b_n b'_n \int_{t_n}^{t_{n+1}} (W_s - W_{t_n}) dW_s$$

Remarquons que $\int_0^T W_s dW_s = \frac{W_T^2 - T}{2}$. En intégrant l'expression précédente on obtient :

$$\begin{aligned} L^1 b(X_{t_n}) &= b_n b'_n \left[\frac{(W_s - W_{t_n})^2 - (s - t_n)}{2} \right]_{t_n}^{t_{n+1}} \\ &= \frac{b_n b'_n}{2} \left[(W_{t_{n+1}} - W_{t_n})^2 - (t_{n+1} - t_n) \right] \\ &= \frac{b_n b'_n}{2} (\Delta W_n^2 - h), \end{aligned}$$

avec $\Delta W_n = W_{t_{n+1}} - W_{t_n}$. On a alors l'expression suivante :

$$\begin{aligned} X_{t_{n+1}} &= X_{t_n} + a(X_{t_n})h + b(X_{t_n})(W_{t_{n+1}} - W_{t_n}) \\ &\quad + \frac{1}{2} b_n b'_n (\Delta W_n^2 - h) + O(h^{3/2}), \end{aligned}$$

ce qui justifie l'expression du schéma de Milstein.

4.8 Application à l'évaluation et delta-hedging des produits dérivés options, formules de Black& Scholes

Nous allons brièvement indiquer comment les schémas numériques sont utilisées pour l'évaluation et la couverture (delta-hedging) des produits dérivés. Cette présentation est donnée par souci de complétude, le lecteur intéressé trouvera une discussion beaucoup plus détaillée dans [7].

Nous maintenons les notations précédentes, à savoir le cadre probabiliste usuel, (W_t) un mouvement brownien et S_t un sous-jacent qui vérifie, par hypothèse, l'équation $\frac{dS_t}{S_t} = \mu dt + \sigma dW_t$; on dit qu'on se place dans le cadre d'un modèle Black-Scholes.

To know more 4.23.1. *Nous ne commentons pas ici sur la question si oui ou non en réalité un tel modèle est vérifié; plus précisément la réalité ne vérifie **jamais** aucun modèle exactement, mais certains donnent des erreurs qu'on est prêts à gérer alors que d'autres non. Ceci est une discussion plus générale qui n'entre pas, en ce moment, dans le périmètre de ce cours mais devrait concerner tout praticien.*

Soit C_t le prix à l'instant t d'un produit dérivé dont le payoff à la maturité $T \geq t$ est donné par une variable aléatoire \mathcal{F}_T mesurable. Pour aisance technique nous supposons aussi que $\mathbb{E}[G^2] < \infty$. Par exemple $G = (S_T - K)_+$ pour un call européen alors que $G = \left(\frac{1}{T} \int_0^T S_t dt - K\right)_+$ pour un call asiatique. Alors il est connu qu'il existe une probabilité Q^* dite *risque neutre* et \tilde{W} un Q^* -mouvement brownien tel que

$$\frac{dS_t}{S_t} = r dt + \sigma d\tilde{W}_t, \quad S(0) = S_0 \quad (4.30)$$

et

$$C_t = \mathbb{E}^{Q^*} \left[e^{-r(T-t)} G \mid \mathcal{F}_t \right]. \quad (4.31)$$

Bien sur, ceci s'écrit aussi $e^{-rt}C_t = \mathbb{E}^{Q^*} [e^{-rT}C_T | \mathcal{F}_t]$ qui rappelle une propriété de type martingale pour l'actualisation $\tilde{C}_t = e^{-rt}C_t$ de C_t .

Pour comprendre pourquoi (à nouveau, voir [7] pour une présentation plus rigoureuse) considérons un portefeuille auto-financé Π_t qui **finance** G c'est à dire que $\Pi_T = G$. Il sera composé de Δ_t parts de sous-jacent et le reste en produit sans risque. Bien sur, par absence d'opportunité d'arbitrage il suit que $C_t = \Pi_t$ pour tout t . Par la condition d'auto-financement on peut déduire l'évolution de Π_t : $d\Pi_t = \Delta_t dS_t + (\Pi_t - \Delta_t S_t)rdt$ ou encore, en rappelant la définition de dS_t :

$$d\Pi_t = r\Pi_t dt + \Delta_t dS_t [(\mu - r)dt + \sigma dW_t].$$

Notons maintenant $\tilde{\Pi}_t = e^{-rt}\Pi_t$ (actualisation de Π_t) alors par la formule de Ito appliquée à la fonction $x \mapsto e^{-rt}x$ on peut écrire $d\tilde{\Pi}_t = \Delta_t S_t d[(\mu - r)dt + \sigma dW_t]$. Faisons maintenant un changement de mesure et trouver Q^* équivalente à \mathbb{P} telle que $\tilde{W} = \frac{\mu - r}{\sigma}t + W_t$ soit un Q^* -mouvement Brownien. Alors on obtiendra $d\tilde{\Pi}_t = \Delta_t S_t \sigma d\tilde{W}_t$; ainsi sous la mesure Q^* le processus $\tilde{\Pi}_t$ est un processus d'Ito sans terme en dt donc une martingale, ce qui nous justifie la formule (4.31).

Bien sur, ce raisonnement était sous l'hypothèse qu'on peut trouver un portefeuille Π_t qui finance G c'est à dire tel que $\Pi_t = G$. En fait on peut même montrer ceci, nous allons juste esquisser l'argument. On gardera la même définition de Q^* (qui n'a rien à voir avec le produit dérivé, est juste une transformation impliquant le Brownien (W_t)). Soit donc M_t la martingale définie par $M_t = \mathbb{E}^{Q^*} [e^{-rT}G | \mathcal{F}_t]$ (le fait que (M_t) est une martingale suit des propriétés de l'espérance conditionnelle et du fait que G admet un moment d'ordre 2 fini). Par le théorème de représentation des martingales (qui dit en gros que toute martingale est un processus d'Ito sans terme en dt) il existe donc H_t tel que $M_t = \int_0^t H_s d\tilde{W}_s$ ou encore sous forme intégrale $dM_t = H_t d\tilde{W}_t = H_t \left[\frac{\mu - r}{\sigma} dt + dW_t \right]$. Il suffit maintenant de dérouler les opérations en sens inverse et trouver que portefeuille Π_t contenant $\frac{H_t}{\Delta_t \sigma}$ parts de sous-jacent est auto-financé et finance G .

To know more 4.23.2. *Remarquons que l'existence d'un tel portefeuille nous dit que le risque contenu dans le dérivé S_t peut être compensé (on dit "couvert") en ayant un nombre variable Δ_t de parts de sous-jacents (assez souvent $\Delta_t = \frac{\partial}{\partial S} C_t$). Ou, dit autrement, un portefeuille qui contient -1 dérivé (vendeur) et $+\Delta_t$ parts de sous-jacent S_t sera neutre (on dit "delta neutre") c'est à dire que son évolution au premier ordre est déterministe. En particulier si un tel portefeuille est auto-financé il partira de 0 et arrivera à 0 peu importe le chemin pris par le sous-jacent. On entre ainsi dans le domaine du "delta-hedging", procédure utilisée par les vendeurs d'options qui ne veulent pas faire de paris directionnels sur S_t mais juste empocher leur commission et se couvrir contre tous autres risques.*

Du point de vue numérique pour appliquer (4.31) et calculer le prix d'un produit dérivé (prenons un call européen de strike K comme exemple, c'est à dire $G = (S_T - K)_+$ et $t = 0$) :

1. on simule un nombre M (grand) de réalisations S_t^m , $m = 1, \dots, M$ de S_t (qui suit l'équation (4.30)) : ceci se fait soit par une formule directe après avoir simulé \tilde{W} soit par des schémas numériques tels que Euler-Maruyama ou Milshtein ;
2. calcule la moyenne empirique $\frac{1}{M} e^{-rT} \sum_{m=1}^M (S_T^m - K)_+$ qui sera le prix de l'option à l'instant 0.

4.9 Exercices

Dans tout ce qui suit on considère une EDS

$$dX_t = a(t, X_t)dt + b(t, X_t)dW_t \quad (4.32)$$

Les coefficients a et b qui satisfont, au minimum, les conditions du théorème d'existence d'un processus d'Ito, à savoir :

- a, b sont adaptés à la filtration \mathcal{A}_t du processus X_t
- $\int_0^T |a_s| ds \leq \infty$ ppt , $\int_0^T |b_s|^2 ds \leq \infty$ ppt

Rappel : le pas de temps est ici égal à h et on note $t_n = nh$. Les schémas numériques proposeront des approximations Y_n de X_{t_n} .

Lorsqu'il n'y a pas d'ambiguïté, on note $a_n = a(t_n, Y_n)$, $b_n = b(t_n, Y_n)$.

Exercice 4.1 (Sommes de Riemann, cf. théorème 4.5, page 73).

Soit $\Delta : t_0 = 0 < t_1 < \dots < t_N = T$ une division de $[0, T]$.

1. Calculer la limite en L^2 (si elle existe) de la somme de type Riemann

$$S_1 = \sum_{k=0}^{N-1} B_{t_k} (B_{t_{k+1}} - B_{t_k}); \quad (4.33)$$

lorsque $|\Delta| \rightarrow 0$.

2. Calculer la limite en L^2 (si elle existe) de la somme de type Stratonovich

$$S_2 = \sum_{k=0}^{N-1} B_{\frac{t_k+t_{k+1}}{2}} (B_{t_{k+1}} - B_{t_k}); \quad (4.34)$$

lorsque $|\Delta| \rightarrow 0$.

Exercice 4.2 (formule de Itô). Pour cet exercice $(X_t)_{t \geq 0} \in \mathfrak{J}^2$ et on admettra aussi que $(Y_t)_{t \geq 0}$ (défini ci-dessous) est également dans \mathfrak{J}^2 .

1. Soit $Y_t = \log(X_t)$. Calculer dY_t sachant que $dX_t = \mu X_t dt + \sigma X_t dB_t$.
2. Soit $dX_t = a \cdot dt + b \cdot dB_t$. Calculer dY_t où $Y_t = e^{X_t}$.

Exercice 4.3 (E.D.S. pour quelques modèles financiers). Soit $W = \{W_t, t \geq 0\}$ un mouvement brownien standard.

1. *Modèle de Black-Merton-Scholes* : soit $\mu, \sigma \in \mathbb{R}$. Démontrer, en utilisant un résultat du cours, que l'EDS suivante :

$$dS_t = \mu S_t dt + \sigma S_t dW_t, \quad S(0) = S_0 \in \mathbb{R}, \quad (4.35)$$

admet une solution unique. Montrer que cette solution est

$$S_t = e^{(\mu - \sigma^2/2)t + \sigma W_t} S_0. \quad (4.36)$$

2. *Modèle de Vasicek* : soit $\alpha, \beta, \sigma \in \mathbb{R}$, $\alpha \neq 0$, $\sigma > 0$. Démontrer, en utilisant un résultat du cours, que l'EDS suivante :

$$dr_t = \alpha(\beta - r_t)dt + \sigma dW_t, \quad r(0) = r_0 \in \mathbb{R}, \quad (4.37)$$

admet une solution unique. Montrer que cette solution est

$$r_t = r_0 e^{-\alpha t} + \beta(1 - e^{-\alpha t}) + \sigma e^{-\alpha t} \int_0^t e^{\alpha s} dW_s. \quad (4.38)$$

3. *Modèle de Cox-Ingersoll-Ross (CIR)* : soit $\alpha, \beta, \sigma \in \mathbb{R}$, $\alpha \neq 0$, $\sigma > 0$. Dire si le résultat du cours peut être utilisé pour démontrer que l'EDS suivante admet une solution unique :

$$dr_t = \alpha(\beta - r_t)dt + \sigma \sqrt{|r_t|} dW_t, \quad r(0) = r_0 \geq 0. \quad (4.39)$$

Exercice 4.4. (*consistance faible*) On suppose a bornée : $|a(t, x)| \leq M \quad \forall t, x$.

1/ Montrer que le schéma suivant, dit "Euler Maruyama faible"

$$Y_{n+1} = Y_n + a(t_n, Y_n)h + b(t_n, Y_n)\xi_n \sqrt{h} \quad (4.40)$$

est faiblement consistant. Ici ξ_n sont des variables aléatoires indépendantes entre elles et indépendantes de \mathcal{A}_{t_n} telles que $P(\xi_n = \pm 1) = \frac{1}{2}$.

2/ Généraliser pour d'autres variables ξ_n .

3/ Le schéma est-il fortement consistant ?

Exercice 4.5. (*consistance forte et faible*)

1. Montrer que pour tout schéma la consistance forte implique la consistance faible.
2. Montrer que la solution exacte vérifie les conditions de consistance forte (donc faible aussi).

Exercice 4.6. (*schéma de Heun pour EDS*) Dans cet exercice on considère que dans (4.32) les coefficients a et b sont indépendants du temps, de classe C^2 et a, b et les dérivées d'ordre 1 et 2 (a', a'', b', b'') également bornées. On étudie une généralisation formelle du schéma de Heun

$$Y_{n+1} = Y_n + \frac{1}{2} \left\{ a(Y_n) + a\left(Y_n + a(Y_n)h + b(Y_n)\Delta W_n\right) \right\} h \\ + \frac{1}{2} \left\{ b(Y_n) + b\left(Y_n + a(Y_n)h + b(Y_n)\Delta W_n\right) \right\} \Delta W_n \quad (4.41)$$

Montrer que ce schéma n'est pas fortement consistant pour tout choix de a et b et trouver pour quels types de coefficients le schéma l'est (conditions suffisantes).

Exercice 4.7 (*consistance : définitions*). Montrer que pour l'équation (4.32) les définitions de la consistance comme EDS et comme EDO coïncident si $b = 0$ (a et b seront supposés aussi régulières que nécessaire).

Exercice 4.8 (*ordre fort EM limité à 1/2*). Donner un exemple de coefficients a et b tels que le schéma d'Euler Maruyama appliqué à l'équation (4.32) ait un ordre de convergence forte strictement inférieur à 1.0.

Exercice 4.9. Dans l'équation (4.32) on supposera a, b Lipschitz, de croissance au plus quadratique en X . Montrer qu'un schéma fortement consistant partant de $X(0)$ converge fortement. Appliquer au schémas Euler-Maruyama et Milstein et montrer que dans ces cas l'ordre de convergence γ est supérieur à 0.5.

Exercice 4.10 (*Calcul Ito-Taylor pour Milstein*). Expliquer en quoi le terme supplémentaire, dans Milstein par rapport à Euler-Maruyama, est lié au développement de Ito-Taylor.

Exercice 4.11 (Schéma EDS multi-step). Avec les notations du cours, soit le schéma EDS défini par $Y_{n+1} = Y_n + \frac{3}{2}a_n h - \frac{1}{2}a_{n-1}h + b_n\sqrt{h}\xi_n$ ou ξ_n sont des variables i.i.d de moyenne m et variance σ^2 finie, et chaque ξ_n indépendante de la filtration \mathcal{A}_{t_n} . On suppose que a, b sont des fonctions indépendantes du temps, et a, b, a', b', a'', b'' bornées.

1. Trouver m et σ^2 tel que le schéma soit faiblement consistant.
2. Le schéma est-il fortement consistant ? Justifier.

Exercice 4.12 ((Schéma EDS)). Avec les notations du cours, soit le schéma EDS défini par $Y_{n+1} = Y_n + ha(Y_{n+1}) + b_n\Delta W_n$. On suppose que a, b sont des fonctions indépendantes du temps, et a, b, a', b', a'', b'' bornées.

1. Montrer que le schéma est bien posé en montrant que l'équation $Z = Y_n + ha(Z) + b_n\Delta W_n$ admet une solution unique pour h suffisamment petit.
2. Calculer $\mathbb{E}[Y_{n+1} - Y_n | \mathcal{A}_{t_n}]$.
3. Le schéma satisfait-il la première condition de consistance forte ? Justifier.
4. Le schéma est-il fortement consistant ? Justifier.

4.10 TP Python EDS

- Exercice 4.13** (Mouvement Brownien). 1. Écrire un programme qui calcule une réalisation d'un mouvement Brownien W_t , sur un horizon $T = 1$ avec $N = 500$, $h = T/N$. Dessiner cette réalisation.
2. En modifiant le programme précédent, sans ajout de boucle "for", calculer M réalisations du mouvement Brownien W_t (mêmes paramètres). Dessiner $M = 50$ telles réalisations sur le même plot.
 3. En utilisant les sommes de Riemann-Itô (4.3) calculer $\int_0^T W_t dW_t$ et comparer avec la formule exacte pour divers valeurs de h et en faisant une moyenne sur les réalisations.

Exercice 4.14 (Schémas EM et M). *Dans cet exercice nous allons considérer l'EDS $dX_t = \theta(\mu - X_t)dt + \sigma dW_t$; X_t porte le nom de processus d'Ornstein-Uhlenbeck. Nous choisirons $\theta = 1.0$, $\mu = 10.0$, $\sigma = 3.0$, $X_0 = 0$, $T = 1$, $N = 100$.*

1. *Écrire un programme qui simule X_t avec un schéma d'Euler-Maruyama faible (voir exo 4.4), dessiner le résultat pour $M = 100$ scénarios.*
2. *En modifiant le programme précédent, implémenter le schéma de Milshtein (+ dessin).*
3. *Montrer numériquement, en faisant varier h et en adaptant M , que EM converge fortement à l'ordre 0.5, M à l'ordre 1 et EM faiblement à l'ordre 1 (on prendra une fonction test à préciser).*

Exercice 4.15 (Calcul de prix d'option européenne). *Dans cet exercice nous allons considérer l'EDS $dS_t = \mu S_t dt + \sigma S_t dW_t$ (modèle de Black-Scholes). Ici $T = 1.0$, $N = 255$, $M = 100$ (nombre de réalisations à faire varier), $S_0 = 100.$, $\mu = 0.1$, $\sigma = 0.25$, $r = 0.05$ (taux d'intérêt sans risque), $K = 110$ (strike).*

1. *Écrire un programme qui simule W_t , S_t (avec une formule exacte); dessiner S_t . Calculer le prix de l'option et un intervalle de confiance autour.*
2. *Pareil mais avec un schéma d'Euler Maruyama pour le calcul de S_t .*

Dans tous les cas dessiner les résultats.

Indication : pour l'intervalle de confiance on pourra utiliser la fonction suivante :

```
import numpy as np

def bootstrap_mean_confidence_interval(data, num_iterations=10000,
    alpha=0.05):
    """
    A function to compute the average and a confidence interval
    around it.

    Use example
    data = np.array([0.2, 0.5, 0.7, 0.8, 1.1, 1.3, 1.5, 1.8, 2.0,
    2.2])
    print(bootstrap_mean_confidence_interval(data))

    Parameters
```

```

data : 1D array of data
num.iterations : number of bootstrap iterations, default is
                10000.
alpha : confidence level, the default is 0.05.

Returns : the average and a confidence interval around it as a
          tuple

```

```

"""
n = len(data)
means = np.zeros(num.iterations)

for i in range(num.iterations):
    means[i] = np.mean(np.random.choice(data, size=n, replace=
                                        True))

means.sort()
lower_bound = means[int(num.iterations * (alpha / 2))]
upper_bound = means[int(num.iterations * (1 - alpha / 2))]
mean_estimate = np.mean(means)

return mean_estimate, (lower_bound, upper_bound)

```


Chapitre 5

Quelques corrections

5.1 Correction exercices section 2.10

Exercice 5.1. *Correction de l'exercice 2.12.*

Après UN seul pas de temps : schéma EE donne [1.1, 2.23, 2.94] (calculs directs). Pour info (calculs pas possible à faire facilement) le schéma EI donne [1.114, 2.256, 2.946] et le schéma CN donne [1.107, 2.242, 2.943].

Après DEUX PAS DE TEMPS le schéma EE donne [1.213, 2.483, 2.886] (calculs directs); ceci permet d'identifier un des schémas. Pour info le schéma EI donne [1.244, 2.543, 2.9] et le schéma CN donne [1.228, 2.511, 2.893]. Pour identifier il faut utiliser la EI, en allant en arrière!!

5.2 Correction TP Python, section 2.11

Exercice 5.2. *Correction de l'exercice 2.16.*

```
# -*- coding: utf-8 -*-
"""
Created on Mon Mar  8 12:12:15 2021

@author: turinici
"""

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
%matplotlib auto

# np.sqrt(2.)*np.sqrt(2.) == 2.
# False !!!!
```

```

#parameters
T=10.0 # final time
N=100 # number of time steps
h = T/N #
U0 = 0.0

def ftxt(t,x):
# define the function entering the ODE  $x'(t) = f(t,x(t))$ 
    return (2.0*np.sqrt(np.abs(x)))

def Explicit_Euler(h,N,ode_function,initial_value):
    """
    Parameters
    -----
    h : time step
    N : number of time steps (integer)
    input_function : function to integrate
    initial_value : initial value of the ODE

    Returns
    -----
    List of approximate solution obtained by Explicit Euler scheme
    of step h.

    """
    U= [0.0]*(N+1) # creates a list on N+1 elements, filled with
                    value 0
    U[0]=initial_value

    for ii in range(N):
        U[ii+1]=U[ii]+h*ode_function(ii*h,U[ii])
    return(U)

# define the time grid
trange = np.linspace(0,T,num=N+1,endpoint=True)
# solve by EE the ODE : use EE at any time step and put in a numpy
array : solution
solution = Explicit_Euler(h,N,ftxt,U0)
solution2 = Explicit_Euler(h,N,ftxt,np.sqrt(2.)*np.sqrt(2.)-2.)

# plot the results
plt.figure(1)
#plt.plot(solution)
plt.plot(trange,solution,'*r',trange,solution2,'ob')
plt.xlabel('time_(t)')
plt.ylabel('x(t)')
plt.legend(['infinite_precision_solution_x(t)', 'finite_precision_
solution_x(t)'])

```

Exercise 5.3. Correction de l'exercice 2.17.

```

# -*- coding: utf-8 -*-
"""
Created on Mon Mar  8 14:30:03 2021

@author: turinici
"""

import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint

%matplotlib inline
%%matplotlib auto

#parameters
T=100 # final time
N=250 # number of time steps

```

```

h = T/N #
S0 = 20000
I0=10.
R0=0.

y0 = [S0, I0, R0]
####

beta=1.15
gamma=1./1.
print('reproduction_number=', beta/gamma)

def sir_list(y, t, betaSIR, gammaSIR):
    """
    define the SIR function
    Parameters
    -----
    t : time
    x : list of components of dimension d

    Returns
    -----
    a list, value of the function
    """
    S, I, R=y
    ntotal=S+I+R
    return [-betaSIR*S*I/ntotal, betaSIR*S*I/ntotal-gammaSIR*I,
            gammaSIR*I]

def sir_array(y, t, betaSIR, gammaSIR):
    """ like sir_list but return an array """
    return np.array(sir(y, t, betaSIR, gammaSIR))

#sir=sir_array
sir=sir_list

# define the time grid
trange = np.linspace(0, T, num=N+1, endpoint=True)
solution = odeint(sir, y0, trange, args=(beta, gamma))

Ssol=solution[:, 0]
Isol=solution[:, 1]
Rsol=solution[:, 2]

plt.figure(2, figsize=(4,2))
plt.xlabel('temps')
plt.plot(trange, Ssol, '-b', trange, Isol, ':r', trange, Rsol, '--g')
plt.legend(['S', 'I', 'R'])
plt.tight_layout()
plt.savefig('sir.pdf')

plt.figure(4, figsize=(7.5,2.5))
plt.subplot(1,3,1)
plt.xlabel('temps')
plt.plot(trange, Ssol, '-b', linewidth=4)
plt.legend(['S', 'I', 'R'])
plt.subplot(1,3,2)
plt.xlabel('temps')
plt.plot(trange, Isol, ':r', linewidth=4)
plt.legend(['I'], loc='upper_right')
plt.subplot(1,3,3)
plt.xlabel('temps')
plt.plot(trange, Rsol, '--g', linewidth=4)
plt.legend(['R'])
plt.savefig('sir3.pdf')

```

```

%%%
#in this second part we explore the order of error of several
  schemes

# TODO

# 1/ obtain the precise values of X(t) for t1=T0=52 and t2=60
# if times values are already in the trange just use:
#X52=[Ssol[52],Isol[52],Rsol[52]]

#otherwise compute again with odeint
t1=52.0
T0=t1
t2=60.0
new_trange = [0.0, t1, t2]
new_solution = odeint(sir, y0, new_trange, args=(beta, gamma), rtol
  =1.e-10)

Xinit=new_solution[1]
Xend=new_solution[2]

def ftxt(t, y):
    """ define the function used by the ODE"""
    return sir_array(y, t, beta, gamma)

#this is the function appearing in the formula U_{n+1}= U_n + h \
  phi(Un, ...)
#Explicit Euler
def phi_function_EE_scheme(Un, ftxt, h, tn):
    return ftxt(tn, Un)
#Heun
def phi_function_Heun_scheme(Un, ftxt, h, tn):
    return 0.5*( ftxt(tn, Un) +ftxt(tn+h, Un + h*ftxt(tn, Un)) )
#RK4
def phi_function_RK4_scheme(Un, ftxt, h, tn):
    K1 = ftxt(tn, Un)
    K2 = ftxt(tn+h/2., Un+h/2.*K1)
    K3 = ftxt(tn+h/2., Un+h/2.*K2)
    K4 = ftxt(tn+h, Un+h*K3)
    return (K1+2.*K2+2.*K3+K4)/6.

# starting from value at t1 solve numerically with EE, Heun,
  compare at time T2
# the numerical and the precise values for different values of h

error_list_RK4=[]
error_list_Heun=[]
error_list_EE=[]
hlist=[0.05, 0.01, 0.1, 0.5, 1., 2., 4.]

for h in hlist:
    current_N=np.int64((t2-t1)/h)
    #test if t2-t1 is really a multiple of h: assert()
    #assert(current_N*h == t2-t1)
    #use Xinit as initial values
    current_X_RK4=Xinit
    current_X_EE=Xinit
    current_X_Heun=Xinit
    for jj in range(current_N):
        current_X_RK4=current_X_RK4 + \
            h*phi_function_RK4_scheme(current_X_RK4, ftxt, h, t1+jj*
            h)
        current_X_Heun=current_X_Heun + \
            h*phi_function_Heun_scheme(current_X_Heun, ftxt, h, t1+
            jj*h)
        current_X_EE=current_X_EE + \
            h*phi_function_EE_scheme(current_X_EE, ftxt, h, t1+jj*h)

    #error_list_Heun.append(np.abs(current_X[0]-Xend[0]))

```

```

error_list_Heun.append(np.sum(np.abs(current_X_Heun-Xend)))
error_list_EE.append(np.sum(np.abs(current_X_EE-Xend)))
error_list_RK4.append(np.sum(np.abs(current_X_RK4-Xend)))

plt.figure(3, figsize=(16,8))
plt.loglog(hlist, error_list_EE, 'o-', hlist, error_list_Heun, 'o-',
           hlist, error_list_RK4, 'o-',)
plt.legend(['error_EE', 'error_Heun', 'error_RK4'])

```

Exercise 5.4. Correction de l'exercice 2.18

```

# -*- coding: utf-8 -*-
"""
Created on Mon Mar  8 12:12:15 2021

@author: turinici : TP no. 1 :ex 2.17: stability of Explicit Euler

for  $z'(t) = L * z(t)$  with  $L = i = \text{sqrt}(-1)$ 
With notation  $z = x+iy$  :
 $x, y = z$ 
 $x' = \text{Re}(z') = \text{Re}(i * z) = \text{Re}(i*(x+iy)) = -y$ 
 $y' = \text{Im}(z') = \text{Im}(i*z) = \text{Im}(i*(x+iy)) = x$ 
ODE equation is :  $[x, y]' = [-y, x]$ 
"""

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
%matplotlib auto

#parameters
T=100.*2*np.pi # final time = 100*2*pi
N=5000 # number of time steps
h = T/N #
U0 = [1.,0.]

def ftxt(t, z):
    """
    define the function entering the ODE  $x'(t) = f(t, x(t))$ 
    Parameters
    -----
    t : time
    z : list of components of dimension d

    Returns
    -----
    a list, value of the function
    """
    x, y = z
    return [-y, x]

def Explicit_Euler(h, N, ode_function, initial_value):
    """
    Parameters
    -----
    h : time step
    N : number of time steps (integer)
    input_function : function to integrate
    initial_value : initial value of the ODE

    Returns
    -----
    List of approximate solution obtained by Explicit Euler scheme
    of step h.
    """
    U = [initial_value]*(N+1) # creates a list on N+1 elements,
    # filled with value 0

```

```

    for ii in range(N):
        U[ii+1]=[uik+h*xk for xk,uik in zip(ode_function(ii*h,U
            [ii]), U[ii])]
#         U[ii+1]=list(np.array(U[ii])+h*np.array(ode_function(ii*h
            ,U[ii])))
        return(U)

# define the time grid
trange = np.linspace(0,T,num=N+1,endpoint=True)
# solve by EE the ODE : use EE at any time step and put in a numpy
array : solution
solution = Explicit_Euler(h,N,ftxt,U0)

solutionx = [z[0] for z in solution]
solutiony = [z[1] for z in solution]

# plot the results
plt.figure(1)
plt.subplot(2,1,1)
plt.plot(trange,solutionx,'-r')
plt.xlabel('time_(t)')
plt.ylabel('z')
plt.legend(['Real(z(t))'])
plt.subplot(2,1,2)
#plt.plot(solution)
plt.plot(trange,solutiony,'-b')
plt.xlabel('time_(t)')
plt.ylabel('z')
plt.legend(['Im(z(t))'])

```

5.3 Correction des exercices 'backward' TP section 3.8

Exercise 5.5. Correction de l'exercice 3.9

```

# -*- coding: utf-8 -*-
"""
Created on Mon Mar  8 14:30:03 2021

@author: turinici
"""

import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint
from scipy.interpolate import interp1d

%matplotlib inline
#%matplotlib auto

#parameters
T=150 # final time
N=150 # number of time steps
h = T/N #
S0 = 1.e+6
I0=10.
R0=0.
ntotal0=S0+I0+R0

# constant appearing in function c(beta) = c0/beta
c0=1.0

```



```

def cost(t, beta_function):
    """implements the cost function:  $c(\beta(t)) = c_0/\beta(t)$ 

    Inputs: beta is a function, t is a number

    """
    return c0/beta_function(t)

def dcost(t, beta_function):
    """implements the derivative of the cost function:  $c'(\beta(t)) = -c_0/\beta(t)**2$ 

    Inputs: beta is a function, t is a number

    """
    return -c0/beta_function(t)**2

# test: dcost(1., lambda t : 3.)
y0 = [S0, I0, R0]

beta=0.5
gamma=1./3.
print('reproduction_number=', beta/gamma)

def sir_list(y, t, betaSIR, gammaSIR):
    """
    define the SIR function
    Parameters
    -----
    t : time
    x : list of components of dimension d

    Returns
    -----
    a list, value of the function

    """
    S, I, R=y
    ntotal=S+I+R
    return [-betaSIR*S*I/ntotal, betaSIR*S*I/ntotal-gammaSIR*I,
            gammaSIR*I]

def sir_array(y, t, betaSIR, gammaSIR):
    """ like sir_list but return an array """
    return np.array(sir(y, t, betaSIR, gammaSIR))

#sir=sir_array
sir=sir_list

# define the time grid
trange = np.linspace(0, T, num=N+1, endpoint=True)
solution = odeint(sir, y0, trange, args=(beta, gamma))

Ssol=solution[:,0]
Isol=solution[:,1]
Rsol=solution[:,2]

#construct functions S,I,R
Sfun = interp1d(trange, Ssol, fill_value="extrapolate")
Ifun = interp1d(trange, Isol, fill_value="extrapolate")
Rfun = interp1d(trange, Rsol, fill_value="extrapolate")

plt.figure(2)
plt.plot(trange, Ssol, trange, Isol, trange, Rsol)
plt.legend(['S', 'I', 'R'])

```

```

def sir_list_beta_function(y,t,beta_function,gammaSIR):
    """
    define the SIR function
    Parameters
    -----
    t : time
    x : list of components of dimension d

    Returns
    -----
    a list, value of the function
    """
    S,I,R=y
    ntotal=S+I+R
    betat=beta_function(t)
    return [-betat*S*I/ntotal,betat*S*I/ntotal-gammaSIR*I,gammaSIR
            *I]

def adjoint_list_beta_function(lambdamu,t,beta_function,gammaSIR,
    Sfunction,Ifunction,Rfunction):
    """
    define the SIR function
    Parameters
    -----
    t : time
    x : list of components of dimension d

    Returns
    -----
    a list, value of the function
    """
    lambda_t,mu_t=lambdamu
    betat=beta_function(t)
    It=Ifunction(t)
    St=Sfunction(t)
    Rt=Rfunction(t)
    ntotal=St+It+Rt
    return [betat*It*(lambda_t-mu_t)/ntotal,betat*St*(lambda_t-
            mu_t)/ntotal+gammaSIR*mu_t]

#see how can we use ODEINT to solve backwards:
# example exp(2*t) : x' = 2*x
# tmp=odeint(lambda x,t : 2.*x, 10.0, [0, 0.5, 1., 1.5, 2.])
# tmp = array([[ 10.],[ 27.18281891],[ 73.89056376],[200.85537821],[545.98153731]])
# we want to solve backward: give value at time 2 =
545.9815003314424
# tmp2=odeint(lambda x,t : 2.*x, 545.98153731, [0, 0.5, 1., 1.5,
2.][::-1])

betafunction =lambda t : beta

adjoint_solution = odeint(adjoint_list_beta_function, [-1.,0.],
    trange[::-1],
    args=(betafunction,gamma,Sfun,Ifun,Rfun)
)

lambdasol=adjoint_solution[:,0][::-1]#in order to correspond to
    trange not to trange[::-1]
musol=adjoint_solution[:,1][::-1]

#compute the gradient
gradientST = Ssol*Isol*(lambdasol-musol)

```

```

dcostarray=[dcost(t,betafunction) for t in trange]
gradient = dcostarray-gradientST/ntotal0
plt.figure(6)
plt.subplot(3,1,1)
plt.plot(trange,gradientST)
plt.subplot(3,1,2)
plt.plot(trange,gradient)
plt.subplot(3,1,3)
plt.plot(trange,dcostarray)

plt.figure(7)
plt.plot(trange,gradient)
plt.figure(8)
plt.plot(trange,-gradientST)

```

5.4 Correction des exercices EDS section 4.9

Rappel dans le calcul des espérances conditionnelles les propriétés suivantes sont utiles (\mathcal{A} est une tribu) :

a/ $E(XZ|\mathcal{A}) = ZE(X|\mathcal{A})$ si Z est mesurable par rapport à \mathcal{A}

b/ $E(X|\mathcal{A}) = EX$ si X est indépendante de \mathcal{A}

c/ majoration : $E(X|\mathcal{A}) \leq E(|X||\mathcal{A})$

Les exercices 4.1 à 4.3 concernent le calcul stochastique. Ils sont corrigés dans le livre [7, Chapitre 2] dont une version pdf est disponible en ligne (adresse du pdf : voir rubrique "Bibliographie" page 122).

Exo. 4.4 Nous vérifions les deux propriétés dans la définition de la consistance faible.

$$\begin{aligned}
 E\left(\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n}\right) - a_n &= \mathbb{E}\left(\frac{a_n h + b_n \sqrt{h} \xi_n}{h} \middle| \mathcal{A}_{t_n}\right) - a_n \\
 &= a_n + \frac{b_n}{\sqrt{h}} \mathbb{E} \xi_n - a_n = 0
 \end{aligned} \tag{5.1}$$

où nous avons utilisé le fait que a_n et b_n sont mesurable p/r à \mathcal{A}_{t_n} et aussi le fait que ξ_n est indépendante de \mathcal{A}_{t_n} , et $\mathbb{E} \xi_n = 0$. Donc

$$\mathbb{E} \left| E \left(\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n} \right) - a_n \right|^2 = \mathbb{E} 0 = 0 \quad (5.2)$$

ce qui donne la première majoration dans la définition de la consistance, avec $c(h) = 0$.

La deuxième condition :

$$\begin{aligned} \mathbb{E} \left(\frac{(Y_{n+1} - Y_n)^2}{h} \middle| \mathcal{A}_{t_n} \right) &= \mathbb{E} \left(\frac{(a_n h + b_n \sqrt{h} \xi_n)^2}{h} \middle| \mathcal{A}_{t_n} \right) \\ &= h a_n^2 + 2 a_n b_n \sqrt{h} \mathbb{E} \xi_n + b_n^2 \mathbb{E} \xi_n^2 = h a_n^2 + b_n^2. \end{aligned} \quad (5.3)$$

Nous avons à nouveau utilisé $\mathbb{E} \xi_n = 0$ mais aussi $\mathbb{E} \xi_n^2 = 1$ (et bien sur l'indépendance de ξ_n et la mesurabilité de a et b p/r à \mathcal{A}_{t_n}). On conclut

$$\mathbb{E} \left| \mathbb{E} \left(\frac{(Y_{n+1} - Y_n)^2}{h} \middle| \mathcal{A}_{t_n} \right) - b_n^2 \right|^2 = \mathbb{E} (h a_n^2)^2 \leq h^2 M. \quad (5.4)$$

Mais $M h^2 \rightarrow 0$ pour $h \rightarrow 0$, ce qui achève la démonstration de la consistance faible (avec $c(h) = M h^2$ dans les deux estimations).

2/ On remarque que toute suite de variables aléatoires ξ_n indépendantes entre elles et indépendantes de \mathcal{A}_{t_n} de moyenne 0 et variance 1 donnent les même résultat.

3/ Il ne peut pas l'être, car la deuxième condition de la définition de la consistance forte ne serait pas satisfaite (en effet, les variables ξ_n n'ont aucune relation avec les ΔW_n , donc en particulier ne peuvent pas les compenser lors du calcul, et on reste avec un terme qui ne tend pas vers zéro pour $h \rightarrow 0$).

Exo. 4.6

Les calculs de cet exo ne sont pas tout à fait similaires à ceux de l'application précédente pour la raison suivante : $a(Y_n + a_n h + b_n \Delta W_n)$ n'est ni indépendante de \mathcal{A}_{t_n} ni mesurable par rapport à \mathcal{A}_{t_n} ; effectivement, la fonction a mélange

ΔW_n d'une part et Y_n, a_n et b_n d'autre part donc, $a(Y_n + a_n h + b_n \Delta W_n)$ n'est pas indépendante de \mathcal{A}_{t_n} à cause de la présence des Y_n, a_n et b_n et n'est pas mesurable p/r à \mathcal{A}_{t_n} à cause de la présence de ΔW_n . Il nous faut alors remplacer le calcul exacte de l'espérance conditionnelle, qu'on pouvait faire avant, par un calcul approché par des formules de Taylor.

On remarque tout d'abord que, avec les notations $a_n = a(Y_n)$, $b_n = b(Y_n)$, $a'_n = a'(Y_n)$, $b'_n = b'(Y_n)$, une formule de Taylor à l'ordre 2 nous donne :

$$a(Y_n + a_n h + b_n \Delta W_n) = a_n + a'_n \cdot (a_n h + b_n \Delta W_n) + \frac{a''(\alpha_y^n)}{2} \cdot (a_n h + b_n \Delta W_n)^2 \text{ pour un certain point } \alpha_y^n.$$

De même :

$$b(Y_n + a_n h + b_n \Delta W_n) = b_n + b'_n \cdot (a_n h + b_n \Delta W_n) + \frac{b''(\beta_y^n)}{2} \cdot (a_n h + b_n \Delta W_n)^2 \text{ pour un certain point } \beta_y^n.$$

Remarque : e.g., a'_n est mesurable p/p à \mathcal{A}_{t_n} car il s'agit d'une fonction i.e. $a'(\cdot)$ appliquée à une variable Y_n qui elle est mesurable p/r à \mathcal{A}_{t_n} .

Il ne reste plus qu'à faire les calculs de la même façon qu'avant. Nous omettons **seulement** le calcul immédiat initial qui utilise l'indépendance et la mesurabilité p/r à \mathcal{A}_{t_n} ; le lecteur est par contre invité à refaire si besoin.

$$\begin{aligned} & E \left(\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n} \right) - a_n \\ &= a_n + \frac{a_n a'_n h + \mathbb{E} \left(\frac{a''(\alpha_y^n)}{2} (a_n h + b_n \Delta W_n)^2 \middle| \mathcal{A}_{t_n} \right)}{2} \\ &+ \frac{b_n b'_n}{2h} \mathbb{E} \Delta_n^2 + \frac{\mathbb{E} \left(\frac{b''(\beta_y^n)}{2} \cdot (a_n h + b_n \Delta W_n)^2 \Delta W_n \middle| \mathcal{A}_{t_n} \right)}{2h} - a_n. \end{aligned} \tag{5.5}$$

A ce point, sous les hypothèses de l'exo, nous pouvons donc

estimer que

$$E \left(\frac{Y_{n+1} - Y_n}{h} \middle| \mathcal{A}_{t_n} \right) - a_n = \frac{b'_n b_n}{2} + O(\sqrt{h}) \quad (5.6)$$

A titre d'exemple, détaillons le traitement du terme

$$\frac{\mathbb{E} \left(b''(\beta_y^n) \cdot (a_n h + b_n \Delta W_n)^2 \Delta W_n \middle| \mathcal{A}_{t_n} \right)}{4h}.$$

Tout d'abord il faut se rappeler que β_y^n dépend de ΔW_n aussi, donc $b''(\beta_y^n)$ n'est pas forcément mesurable par rapport à \mathcal{A}_{t_n} (ni forcément indépendant de \mathcal{A}_{t_n}). Donc on aura seulement des majorations :

$$\begin{aligned} & \frac{\mathbb{E} \left(b''(\beta_y^n) \cdot (a_n h + b_n \Delta W_n)^2 \Delta W_n \middle| \mathcal{A}_{t_n} \right)}{2h} \\ & \leq M_2 \frac{\mathbb{E} \left((a_n h + b_n \Delta W_n)^2 |\Delta W_n| \middle| \mathcal{A}_{t_n} \right)}{2h} \end{aligned}$$

où $M_2 = \sup_x |b''(x)|$. On continue les majorations :

$$\begin{aligned} & M_2 \frac{\mathbb{E} \left((a_n h + b_n \Delta W_n)^2 |\Delta W_n| \middle| \mathcal{A}_{t_n} \right)}{2h} \\ & \leq M_2 \left\{ \mathbb{E} a_n^2 h |\Delta W_n| + 2 \mathbb{E} a_n b_n |\Delta W_n|^2 + \mathbb{E} \frac{b_n^2 |\Delta W_n|^3}{h} \right\} \\ & \leq C(h\sqrt{h} + \sqrt{h}^2 + \sqrt{h}^3) \leq C'h^{1/2} \end{aligned}$$

avec des constantes C, C' indépendantes de h .

Revenant à (5.6), comme $b_n b'_n$ n'a aucune raison d'être petit pour $h \rightarrow 0$ (en fait il ne dépend même pas de h), le schéma n'est pas consistant en général.

Un calcul similaire nous montre que

$$\mathbb{E} \left(\frac{1}{h} \left| Y_{n+1} - Y_n - \mathbb{E}(Y_{n+1} - Y_n | \mathcal{A}_{t_n}) - b_n \Delta W_n \right|^2 \right) = O(h). \quad (5.7)$$

En conclusion, le schéma est fortement (donc faiblement) consistant si et seulement si $bb' = 0$ c'est à dire $b = \text{constant}$.

Exo. 4.7 On suppose a aussi régulière que voulu, par exemple de classe C^∞ bornée avec toutes ses dérivées bornées. Dans le cas où $b = 0$, (4.32) est complètement déterministe et devient une EDO. Le processus d'Ito X_t solution de (4.32) ne dépend plus de l'aléa ω . Il est donc pertinent de comparer la notion de consistance pour les EDO avec les deux notions de consistance pour les EDS. Ainsi, si on prend un schéma $(Y_n)_{n \in \mathbb{N}}$ qui approche la solution à (4.32) et part d'une condition initiale déterministe $Y_0 = X_0 \in \mathbb{R}$, il n'est pas nécessaire de le faire dépendre de ΔW_n et on peut l'écrire sous la forme $Y_{n+1} = Y_n + h\Phi(t_n, Y_n, a_n, h)$, $a_n = a(t_n, Y_n)$, $\Delta W_n = W_{t_{n+1}} - W_{t_n}$, avec Φ aussi régulière que voulu (par exemple de classe C^∞ bornée avec toutes ses dérivées bornées). Comme tout est déterministe ici, la quantité $\Phi(t_n, Y_n, a_n, h)$ est indépendante de \mathcal{A}_{t_n} et on obtient donc

$$\begin{aligned} \mathbb{E}(Y_{n+1} - Y_n | \mathcal{A}_{t_n}) &= h\mathbb{E}(\Phi(t_n, Y_n, a_n, h) | \mathcal{A}_{t_n}) \\ &= h\mathbb{E}(\Phi(t_n, Y_n, a_n, h)) \\ &= h\Phi(t_n, Y_n, a_n, h). \end{aligned}$$

La condition première condition de consistance faible devient donc

$$\lim_{h \rightarrow 0^+} \mathbb{E} \left(\left| \frac{h\Phi(t_n, Y_n, a_n, h)}{h} - a_n \right|^2 \right) = 0,$$

i.e., comme tout est déterministe,

$$\lim_{h \rightarrow 0^+} |\Phi(t_n, Y_n, a_n, h) - a_n|^2 = 0,$$

i.e.

$$\lim_{h \rightarrow 0^+} a_n - \Phi(t_n, Y_n, a_n, h) = 0.$$

Or

$$a_n = a(t_n, Y_n) = \tilde{X}'(t_n),$$

où \tilde{X}' est l'unique solution à (4.32) vérifiant $\tilde{X}(t_n) = Y_n$. De plus, comme \tilde{X}' est de classe C^∞ et $\tilde{X}(t_n) = Y_n$, on a notamment que

$$\frac{\tilde{X}(t_{n+1}) - Y_n}{h} \rightarrow \tilde{X}'(t_n) = a_n \text{ quand } h \rightarrow 0^+.$$

Ainsi,

$$\begin{aligned} \lim_{h \rightarrow 0^+} a_n - \Phi(t_n, Y_n, a_n, h) &= 0 \\ \Leftrightarrow \lim_{h \rightarrow 0^+} \left(a_n - \frac{\tilde{X}(t_{n+1}) - Y_n}{h} \right) \\ &+ \left(\frac{\tilde{X}(t_{n+1}) - Y_n}{h} - \Phi(t_n, Y_n, a_n, h) \right) = 0 \\ \Leftrightarrow \lim_{h \rightarrow 0^+} \frac{\tilde{X}(t_{n+1}) - Y_n}{h} - \Phi(t_n, Y_n, a_n, h) &= 0, \end{aligned}$$

ce qui est bien dire que l'erreur de troncature locale donnée en (2.9) tend vers 0 quand $h \rightarrow 0^+$, compte tenu de la Remarque 2.7. De même,

$$\begin{aligned} \mathbb{E} \left(\frac{(Y_{n+1} - Y_n)^2}{h} \middle| \mathcal{A}_{t_n} \right) &= h^2 \mathbb{E} \left((\Phi(t_n, Y_n, a_n, h))^2 \middle| \mathcal{A}_{t_n} \right) \\ &= h^2 \mathbb{E}(\Phi(t_n, Y_n, a_n, h)^2) \\ &= h^2 \Phi(t_n, Y_n, a_n, h)^2. \end{aligned}$$

De plus, $b_n = 0$ ici. Ainsi la condition (W_2) de consistance faible devient donc

$$\lim_{h \rightarrow 0^+} \mathbb{E} \left(\left| \frac{h^2 \Phi(t_n, Y_n, a_n, h)^2}{h} \right|^2 \right) = 0,$$

i.e., comme tout est déterministe,

$$\lim_{h \rightarrow 0^+} |h \Phi(t_n, Y_n, a_n, h)^2|^2 = 0,$$

i.e.

$$\lim_{h \rightarrow 0^+} h^2 \Phi(t_n, Y_n, a_n, h)^4 = 0,$$

ce qui est automatiquement vérifié puisque l'on a supposé Φ bornée.

Pour la consistance forte, la première condition est identique à la première condition de consistance faible. Quant à la deuxième condition de consistance forte, on remarque qu'ici, par un calcul déjà fait

$$Y_{n+1} - Y_n - \mathbb{E}(Y_{n+1} - Y_n | \mathcal{A}_{t_n}) = h\mathbb{E}(\Phi(t_n, Y_n, a_n, h)).$$

Ainsi, comme $b_n = 0$, la condition F_2 se réécrit ici comme

$$\lim_{h \rightarrow 0^+} \mathbb{E} \left(\frac{1}{h} |h\Phi(t_n, Y_n, a_n, h)|^2 \right) = 0,$$

i.e., comme tout est déterministe,

$$\lim_{h \rightarrow 0^+} \frac{1}{h} |h\Phi(t_n, Y_n, a_n, h)|^2 = 0,$$

i.e.

$$\lim_{h \rightarrow 0^+} h\Phi(t_n, Y_n, a_n, h)^2 = 0,$$

ce qui est automatiquement vérifié puisque l'on a supposé Φ bornée.

Ainsi, dans ce cas, les conditions de consistance faible et forte sont identiques entre elles et identiques à la condition de consistance pour les EDO qui est que l'erreur de troncature locale donnée en (2.9) tende vers 0.

Exo. 4.8 Si on était dans le cas d'une EDO (*i.e.* $b = 0$), on sait que le schéma d'Euler-Maruyama est équivalent au schéma d'Euler explicite usuel et que l'ordre de convergence est forcément 1. Ainsi, pour trouver un exemple adéquat, il est nécessaire de prendre $b \neq 0$. Le cas le plus simple serait de prendre $b = 1$ et $a = 0$, mais dans ce cas, la solution approchée serait malheureusement égale à la solution exacte (le vérifier). Il faut donc chercher quelque chose d'un peu plus compliqué. Prenons un autre cas simple (il y en a sûrement une infinité d'autres qui marchent, peut-être de manière plus

élémentaire). Posons $f(t, x) = tx$. f est de classe C^∞ en (t, x) . Alors, par la formule d'Ito,

$$\begin{aligned} df(t, W_t) &= \frac{\partial f}{\partial t}(t, W_t)dt + \frac{\partial f}{\partial x}(t, W_t)dW_t \\ &+ \frac{1}{2} \frac{\partial^2 f}{\partial x^2}(t, W_t)dt = W_t dt + tdW_t, \end{aligned}$$

ce que l'on peut réécrire comme

$$d(tW_t - \int_0^s W_s ds) = tdW_t.$$

Ainsi, si l'on pose $X_t = tW_t - \int_0^s W_s ds$, W_t est solution de

$$dX_t = tdW_t, X_0 = 0.$$

Regardons donc ce que donne l'application du schéma d'Euler-Maruyama à cette EDS, en partant de $Y_0 = 0$, sur l'intervalle de temps $[0, 1]$ (*i.e.* $T = 1$ ici, et donc $N = \frac{1}{h}$) :

$$Y_{n+1} = Y_n + t_n (W_{t_{n+1}} - W_{t_n}) = Y_n + nh (W_{t_{n+1}} - W_{t_n}).$$

Il est très facile de résoudre cette récurrence est d'en déduire que

$$Y_n = Y_0 + h \sum_{i=1}^n i (W_{t_i} - W_{t_{i-1}}) = h \sum_{i=1}^n i (W_{t_i} - W_{t_{i-1}}).$$

Notamment,

$$Y_N = h \sum_{i=1}^N i (W_{t_i} - W_{t_{i-1}}) = h \sum_{i=1}^{N-1} i (W_{t_i} - W_{t_{i-1}}) + W_1 - W_{1-h}.$$

Comme on s'intéresse à de la convergence forte, on regarde l'erreur en N donnée par la formule

$$\begin{aligned} e_N(h) &= \mathbb{E}(|Y_N - X_1|) \\ &= \mathbb{E}(|W_{1-h} - \int_0^1 W_s ds - h \sum_{i=1}^{N-1} i (W_{t_i} - W_{t_{i-1}})|). \end{aligned}$$

Reste donc à estimer cette quantité. On sait que les $W_{t_i} - W_{t_{i-1}}$ sont toutes indépendantes deux à deux et suivent une loi gaussienne centrée de variance h . Les variables aléatoires $i(W_{t_i} - W_{t_{i-1}})$ sont donc aussi toutes indépendantes deux à deux et suivent une loi gaussienne centrée de variance $i^2 h$. Leur somme

$$\sum_{i=1}^{N-1} i(W_{t_i} - W_{t_{i-1}})$$

est donc encore une gaussienne centrée de variance

$$\sigma^2 = h \sum_{i=1}^{N-1} i^2 = h \frac{(N-1)(N+1)(2N-1)}{6} = \frac{(1-h)(2-h)}{6h^2}.$$

Ainsi, la variable aléatoire

$$\left| \sum_{i=1}^{N-1} i(W_{t_i} - W_{t_{i-1}}) \right|$$

est une “loi normale repliée” dont l’espérance est donnée par

$$\sigma \sqrt{\frac{2}{\pi}} = \sqrt{\frac{(1-h)(2-h)}{3\pi h^2}}.$$

On en déduit par inégalité triangulaire que

$$e_N(h) \geq \mathbb{E}(|W_{1-h} - \int_0^1 W_s ds|) - \sqrt{\frac{(1+h)(2+h)}{3}} \pi h^2.$$

Un développement limité donne que

$$\sqrt{\frac{(1-h)(2-h)}{3\pi h^2}} = \frac{\sqrt{\frac{2}{3\pi}}}{h} - \frac{1}{2} \sqrt{\frac{3}{2\pi}} + O(h).$$

Il reste à estimer $\mathbb{E}(|W_{1-h} - \int_0^1 W_s ds|)$.

On en déduit que

$$e_N(h) \geq C'(T) \sqrt{h},$$

pour une constante $C'(T) > 0$ dépendant de T dont la valeur nous importe peu. Évidemment, ceci interdit que l'on puisse avoir $e_N(h) \leq C''h$ pour un certain $C'' > 0$ (tout simplement car $C'(t)\sqrt{h} \leq C''h$ est forcément faux pour h suffisamment petit en divisant chaque côté par \sqrt{h}), et donc le schéma n'est pas d'ordre 1 dans ce cas. De fait, le schéma est au mieux d'ordre $1/2$. Comme il a été admis en cours que le schéma d'Euler-Maruyama était d'ordre de convergence fort au moins $1/2$, on ne peut pas améliorer le \sqrt{h} dans l'inégalité précédente.

Exo. 4.10

Avec les notations du cours, on s'intéresse donc au terme

$$I = L^1 b(X_n) \int_{t_n}^{t_n+h} \int_{t_n}^s dW_\sigma dW_s$$

du développement d'Ito-Taylor, qui domine tous les termes de reste placés dans R_2 comme montré en cours. On rappelle que dans le cas où b ne dépend pas de t , L^1 est donné par

$$L^1 : b \mapsto bb'.$$

De plus, le terme additionnel du schéma de Milstein par rapport au schéma d'Euler-Maruyama est donné par

$$J = \frac{1}{2} b(X_n) b'(X_n) ((\Delta W_n)^2 - h).$$

Ainsi, si on veut démontrer que $I = J$, il suffit de démontrer que

$$\int_{t_n}^{t_n+h} \int_{t_n}^s dW_\sigma dW_s = \frac{1}{2} ((\Delta W_n)^2 - h).$$

Pour ce faire, on commence par remarquer que

$$\int_{t_n}^s dW_\sigma = W_s - W_{t_n},$$

de telle sorte que

$$\begin{aligned} \int_{t_n}^{t_n+h} \int_{t_n}^s dW_\sigma dW_s &= \int_{t_n}^{t_n+h} W_s dW_s - W_{t_n} \int_{t_n}^{t_n+h} dW_s \\ &= \int_{t_n}^{t_n+h} W_s dW_s - W_{t_n} (W_{t_n+h} - W_{t_n}). \end{aligned}$$

Maintenant, on utilise la formule d'Ito pour calculer la quantité $d(W_t^2)$. On pose $g(t, x) = x^2$, de telle sorte que $d(W_t^2) = d(g(t, B_t))$. g est de classe C^∞ et

$$\frac{\partial g}{\partial t}(t, x) = 0, \quad \frac{\partial g}{\partial x}(t, x) = 2x, \quad \frac{\partial^2 g}{\partial x^2}(t, x) = 2.$$

On obtient alors

$$d(W_t^2) = \frac{\partial g}{\partial t}(W_t)dt + \frac{\partial g}{\partial x}(W_t)dW_t + \frac{1}{2} \frac{\partial^2 g}{\partial x^2}(W_t)dt = 2W_t dW_t + dt.$$

En intégrant entre t_n et $t_n + h$, on obtient

$$W_{t_n+h}^2 - W_{t_n}^2 = 2 \int_{t_n}^{t_n+h} W_s dW_s + (t_n + h - t_n).$$

En prenant en compte que $t_n + h - t_n = h$, on en déduit que

$$\int_{t_n}^{t_n+h} W_s dW_s = \frac{1}{2} (-h + W_{t_n+h}^2 - W_{t_n}^2).$$

Ainsi, en mettant bout à bout les calculs précédents, on en déduit que

$$\begin{aligned} \int_{t_n}^{t_n+h} \int_{t_n}^s dW_\sigma dW_s &= \frac{1}{2} (-h + W_{t_n+h}^2 - W_{t_n}^2) - W_{t_n} (W_{t_n+h} - W_{t_n}) \\ &= \frac{1}{2} (h + W_{t_n+h}^2 - W_{t_n}^2 - 2W_{t_n} W_{t_n+h} + 2W_{t_n}^2) \\ &= \frac{1}{2} (-h + W_{t_n+h}^2 + W_{t_n}^2 - 2W_{t_n} W_{t_n+h}) \\ &= \frac{1}{2} (-h + (W_{t_n+h} - W_{t_n})^2), \end{aligned}$$

ce qui était le résultat voulu puisque par définition, $\Delta W_n = W_{t_n+h} - W_{t_n}$.

5.5 Correction des exercices EDS TP section 4.10

Exercice 5.6. *Correction de l'exercice 4.13*

```

# -*- coding: utf-8 -*-
"""
Created on Mon Apr 12 14:51:49 2021

@author: turinici
"""
import numpy as np
import matplotlib.pyplot as plt

#TODO implement a brownian motion

#first idea: use the properties of the Wt:
T=1.0
N=255
M=10#number of scenarios
dt= T/N
W0=0#standard brownian motion
trange=np.linspace(0,T,N+1,endpoint=True)
# We know that Wt is a normal value of variance t
Wl=np.sqrt(trange)*np.random.randn(N,1)
plt.figure(1)
plt.subplot(1,2,1)
plt.plot(trange[:,Wl])
#not working because the covariance is always zero ... and not min
(s,t)
#good implementation: with increments

#another idea: use the cummulative increments property of B.M.
dW=np.sqrt(dt)*np.random.randn(N,M)
W=np.zeros((N+1,M))
W[0,:]=W0
W[1,:]=W0+np.cumsum(dW,0)

plt.figure(2)
plt.plot(trange,W)

#compute \int_0^T W_t d W_t : using the Riemann-Ito sums
# in fact we compute sum_n W(t_n) * (increment between $t_n$ and
# $t_{n+h}$)
# also compute integral minus W_T^2/2 and plot for all
scenarios

int_WdW=np.zeros_like(W)
int_WdW[0,:]=0.0

for ii in range(N):
    int_WdW[ii+1,:]=int_WdW[ii,:]+ W[ii,:]*dW[ii,:]

plt.figure(3,figsize=(15,5))
plt.subplot(1,3,1)
plt.plot(trange,int_WdW)
plt.title('$t_{mapsto}\int_0^t W_u d W_u$')
plt.xlabel('t')
plt.subplot(1,3,2)
plt.plot(trange,W**2/2-int_WdW)
plt.title('$t_{mapsto}W_t^2/2-\int_0^t W_u d W_u$')
plt.xlabel('t')
plt.subplot(1,3,3)
plt.plot(trange,W**2/2-int_WdW- trange[:,None]**2/2)
plt.title('$t_{mapsto}W_t^2/2-t/2-\int_0^t W_u d W_u$')
plt.xlabel('t')
plt.tight_layout()
plt.show()

```

Exercise 5.7. Correction de l'exercice 4.14 and 4.15

```

"""
@author: Gabrel Turinici
"""

```

```

import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm

#implementation of the Black-Scholes formula
def blsprice(Price, Strike, Rate, TimeToMaturity, Volatility,
            DividendRate=0):
    """
    Computes price of option with analytic formula.
    input:
        S: Price - Current price of the underlying asset.

        Strike: Strike - Strike (i.e., exercise) price of the option
        .

        Rate: Rate - Annualized continuously compounded risk-free
              rate of return over
              the life of the option, expressed as a positive decimal
              number.

        TimeToMaturity: Time - Time to expiration of the option,
                       expressed in years.

        Volatility: volatility
        DividendRate = continuous dividend rate

    output: price of a call and of a put (tuple)
    """

    if TimeToMaturity <= 1e-6: # the option already expired
        call = np.max(Price-Strike,0)
        put = np.max(Strike-Price,0)
        return call, put

    d1 = np.log(Price/Strike)+(Rate-DividendRate + Volatility
        **2/2.0)*TimeToMaturity;
    d1 = d1/(Volatility * np.sqrt(TimeToMaturity))
    d2 = d1-(Volatility*np.sqrt(TimeToMaturity))

    call = Price * np.exp(-DividendRate*TimeToMaturity) * \
        norm.cdf(d1)-Strike * np.exp(-Rate*TimeToMaturity) * norm.
        cdf(d2)
    put = Strike * np.exp(-Rate*TimeToMaturity) * norm.cdf(-d2)\
        -Price * np.exp(-DividendRate*TimeToMaturity) * norm.cdf(-
        d1)
    return call, put

T=1.0
N=255
M=300#number of scenarios
dt= T/N
W0=0#standard brownian motion
trange=np.linspace(0,T,N+1,endpoint=True)

dW=np.sqrt(dt)*np.random.randn(N,M)
W=np.zeros((N+1,M))
W[0,:]=W0
W[1:,:]=W0+np.cumsum(dW,0)

plt.figure(2)
plt.plot(trange,W)

S0=100.
mu=0.1
sigma=0.25

```

```

tau_x_r=0.05

#compute S_t with dS_t = mu S_t dt + sigma S_t d W_t
St=np.zeros_like(W)
St[0,:]=S0

for ii in range(N):
    St[ii+1,:]=St[ii,:]+ mu*St[ii,:]* dt + sigma*St[ii,:]*dW[ii,:]

plt.figure(3)
plt.plot(trange , St)
plt.title(' $S_t$')

#compute the Monte Carlo price of an option
# solve St in risk-neutral probability, denote rn_St

#compute rn_St with
# d rn_St = r rn_St dt + sigma rn_St d W_t
rn_St=np.zeros_like(W)
rn_St[0,:]=S0

for ii in range(N):
    rn_St[ii+1,:]=rn_St[ii,:]+ tau_x_r*rn_St[ii,:]* dt \
        + sigma*rn_St[ii,:]*dW[ii,:]

#compute the price of the call
K=110
prixcall , _ = blsprice(S0,K,tau_x_r,T,sigma)
prixMC=np.exp(-tau_x_r*T)*np.mean(np.maximum(rn_St[-1,:]-K,0))

print(" prix_Monte_Carlo=",prixMC)

plt.subplot(2,2,4)
plt.hist(np.exp(-tau_x_r*T) * 
    np.maximum(rn_St[-1,:]-K,0)-prixcall ,50)
plt.title(' hist_du_prix_Monte_Carlo')

erreur_MC =prixMC-prixcall
#plt.savefig("euler-maruyama-monte_carlo.jpg")

```


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