Reinforcement Learning for the Optimization of Explicit Runge-Kutta Method Parameters

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Abstract

Reinforcement learning is one of the three main paradigms in machine learning, which is increasingly used as a method to approach scientific problems. In this thesis, we introduce and use reinforcement learning to find the optimal parameters of a numerical solver.

We first motivate that solving the linear systems can be done by solving initial value problems. These initial values problems can then be solved with an explicit, two stages Runge-Kutta solver, for which we need to find the optimal parameters for the solver, depending on the parameters of the problem.

Using reinforcement learning, and in particular policy gradient methods, we find that with some care, reinforcement learning can be used to learn the solver parameters as a function of the problem parameters. These results are however tempered by some limitations, as the solver can diverge in certain cases, and convergence speed remains low in general.

Popular abstract

As animals, we learn about the world and how to interact with the world by trial and errors, and are ”rewarded” when it goes well. This idea, applied to computer program is called reinforcement learning, and it does not take long nowadays to find applications of it, be it when interacting with a chat bot or when activating the adaptative cruise control of a car.

In this thesis, we study differential equations, which are equations that, when solved, help us understand physical phenomena, for example the trajectory of a ball when it is kicked, or how the temperature in the room changes when we turn on the AC. While solving these equations on a computer is possible, some parameters need to be chosen judiciously, as the wrong solution can be found otherwise. To mitigate this issue, we use reinforcement learning in this thesis to train a program that find these parameters automatically for some specific equations.

Acknowledgements

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Finally, I would like to thank Paulina Ibek, who worked on a similar thesis at the same time, for the discussions which led to exchanging ideas.

Table of contents

Introduction

Machine learning is everywhere. It has applications in computer vision [1], robotic [2], finance [3], recommender systems [4], playing games at a high level [5] or even discovering new matrix multiplication algorithms [6]. The use of machine learning in scientific problems which has been aptly called *scientific machine learning* is also growing, with the most important example being combining neural network and physic laws to either discover or solve partial differential equations [7].

In this thesis, we focus on studying reinforcement learning, which is one of the three main machine learning paradigm. The three main paradigm are as follow[8, Ch. 1.1]:

- Supervised learning, where we learn using data containing an input, and a desired output. Regression models are an example of a supervised learning.
- Unsupervised learning, where the data only has an input but no desired output. Examples include clustering algorithms.
- Reinforcement learning, in which we have an intelligent agent who learns to do something by interacting with its environment, receiving feedback in the form of rewards which the agent wants to maximize.

What sets apart reinforcement learning from its cousins unsupervised and supervised learning is the introduction of the concept of reward. The agent learns by trial and error, and wants to maximize the rewards it gets over time. This is, in essence, quite similar to how we animals learn to do things, and it is no surprise that reinforcement learning traces its roots from the field of animal learning [9]. Another important root of reinforcement learning comes from the field of optimal control, where the agent and environment of reinforcement learning are respectively the controller and controlled system in control theory [8, Ch. 1.7].

To study reinforcement learning, we need a playground. That playground could be an already established playground (such as the Gymnasium API), but in this thesis we use our own playground, which we find in the realm of numerical differential equation solvers.

Numerical methods for differential equations are amongst the most important methods in numerical analysis. All of these methods have specific strengths and weaknesses. They all have, however, some parameters that need to be chosen, if only for the step size. These parameters have to be chosen to maximize performance, and depend on the problem. In some cases they are taken using some heuristics, but they can also be searched for computationally, which is an issue, as any computation means more time to get to the solution. It would therefore be a great time saver if a computer could *learn* these heuristics, for example using reinforcement learning! This is the playground we use in this thesis, albeit with a reduced scope.

We start by motivating the use of numerical ODE solvers to solve linear systems. As a case study, we have a specific type of linear systems, which appears when discretizing the steady state, one dimensional convection diffusion equation $u_x = bu_{xx} + 1$. Doing so, we end up with two *problem parameters*; b, which is a physical constant, and n, stemming from the discretization. The studied numerical solver is an explicit Runge-Kutta method, and has two parameters, a (pseudo-) time step Δt and another parameter α, which need to be chosen. How to choose these *solver parameters*, as a function of the *problem parameters* is then left to the realm of reinforcement learning.

We then introduce through intuitive examples (and a very cute bunny) the main concepts of reinforcement learning, such as states, actions, state transitions and rewards which are then formalized as a Markov decision process. We then introduce policy gradient methods, and in particular we introduce the classical REINFORCE [10] algorithm, which we use to optimize the solver parameters for the studied linear systems.

The results, while positive, are hampered somewhat by the fact that the method used in this thesis is not a natural fit to what makes reinforcement learning so powerful. A discussion on how to redefine the problem to make better use of the strengths of reinforcement learning will follow.

Chapter 1

Motivation : Pseudo time iterations

Let A be a non singular square matrix of dimension $n \geq 1$ and let $b \in \mathbb{R}^n$. We consider the linear system $Ay = b$, where $b \in \mathbb{R}^n$. The system has the unique solution $y^* = A^{-1}b$. As directly inverting the matrix is a terrible idea, a fundamental problem in numerical analysis is to find numerical methods to solve this. This can be done with the use of direct methods or iterative methods. In this thesis, we consider an iterative method. Consider now the initial value problem(IVP),

$$y'(t) = Ay(t) - b, \;\; y(0) = y_0,$$

where $\boldsymbol{y}_0 \in \mathbb{R}^n$ and $t \in \mathbb{R}$. We adapt the result below from [11, Ch. 9.5].

Multiplying the equation by e^{-At}, where e^{-At} is the usual matrix exponential, and rearranging the terms yields

$$e^{-At}y'(t) - Ae^{-At}y(t) = -e^{-At}b.$$

We recognize on the left hand side the derivative of the product $e^{-At}y(t)$, and thus, by the fundamental theorem of calculus,

$$\left[e^{-Au}y(u)\right]_0^t = \int_0^t -e^{-Au}b \; du.$$

Multiplying by $I = A^{-1}A$ inside the integral above, we get

$$e^{-At}y(t) - y(0) = A^{-1}\int_0^t -Ae^{-Au}b \; du,$$

which can be integrated to get

$$e^{-At}y(t) - y_0 = A^{-1}\left[e^{-At} - b\right].$$

Multiplying each side by e^{At} on the left, and rearranging the terms we get an expression for $y(t)$:

$$y(t) = e^{At}(y_0 - A^{-1}b) + A^{-1}b. \tag{1.1}$$

Here, we also used the fact that $e^{At}A^{-1} = A^{-1}e^{At}$. This gives an expression for the solution of the IVP. Since each of those steps can be taken backward , the solution we get is unique. We have thus proved:

Theorem 1.1. *Let A be a non singular, square matrix of dimension $n \geq 1$, $b \in \mathbb{R}^n$ a vector, and consider the initial value problem*

$$y'(t) = Ay(t) - b,\ y(0) = y_0, \tag{1.2}$$

where $t \to y(t)$ is a function from $\mathbb{R}$ to $\mathbb{R}^n$. Then the problem has a unique solution in the form of

$$y(t) = e^{At}(y_0 - y^*) + y^*,$$

where $y^* = A^{-1}b$, and e^{At} is defined using the usual matrix exponential.

Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the (not necessarily distinct) eigenvalues of A. We write $\lambda_i = a_i + ib_i$, where $a_i, b_i \in \mathbb{R}$ and are respectively the real part and the imaginary parts of the i^{th} eigenvalue. Then, the following results holds[12, Ch. 1]:

Theorem 1.2. *$y(t) \to y^*$ as $t \to +\infty$ for any initial value y_0 if and only if, for all $i = 1, \dots, n$, $a_i < 0$, that is, all the eigenvalues of A have a strictly negative real part.*

We call such matrices *stable* in the rest of this thesis.

Proof. We restrict ourselves to the diagonalizable case. Assume that $A \in \mathbb{R}^{n\times n}$ is diagonalizable and let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A. Then we can write $A = PDP^{-1}$ where D is the diagonal matrix with the eigenvalues of A, and P is the associated eigenvectors matrix:

$$D = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}.$$

Then $e^{At} = \sum_{i=0}^{\infty} \frac{(PDP^{-1}t)^i}{i!} = \sum_{i=0}^{\infty} P\frac{(Dt)^i}{i!}P^{-1}$. The P can be moved outside of the sum to get

$$e^{At} = Pe^{Dt}P^{-1}.$$

Since the matrix exponential of a diagonal matrix is simply the matrix of the exponentiated elements, we have

$$e^{Dt} = \begin{pmatrix} e^{\lambda_1 t} & & & \\ & e^{\lambda_2 t} & & \\ & & \ddots & \\ & & & e^{\lambda_n t} \end{pmatrix}.$$

Let $z(t) = P^{-1}(y(t) - y^*)$, where $y(t)$ is the unique solution to Equation 1.2 for some arbitrary initial value y_0.

Since P is non singular, we can use a continuity argument to state that $y(t) \to y^*$ if and only if $z(t) \to 0$. We have

$$z(t) = P^{-1}e^{At}(y_0 - y^*).$$

We note that $P^{-1}e^{At} = e^{\Delta t}P^{-1}$, thus

$$z(t) = e^{Dt}P^{-1}(y_0 - y^*).$$

Looking at the i^{th} element $z(t)_i$, we have

$$|z(t)_i| = |e^{\lambda_i t}| \left[P^{-1}(y_0 - y^*)\right]_i.$$

The only time dependent term is $|e^{\lambda_i t}| = e^{a_i t}$, with a_i being the real part of λ_i, and $z(t)_i \to 0$ as $t \to +\infty$ if and only if $a_i < 0$.

If this holds for any $i = 1, \dots, n$, then $z(t) \to 0$ as $t \to +\infty$. This proves the sufficient condition.

This is also a necessary condition. Indeed, since y_0 is arbitrary, we can chose it so that $P^{-1}(y_0 - y^*) = (1, \dots, 1)^T$. Then $z(t) = (e^{\lambda_1 t}, e^{\lambda_2 t}, \dots, e^{\lambda_n t})^T$ which converges to 0 only if all the eigenvalues have a strictly negative real part.

□

We now go back to the original problem of solving the linear system $Ay = b$. If all the eigenvalues of A have a strictly negative real part, then, any numerical solver for the initial value problem $y'(t) = Ay(t) - b$ with $y(0) = y_0$, where t is a pseudo-time variable also becomes an iterative solver for the linear system $Ay = b$, as $y(t) \to y^*$.

Remark. The eigenvalues of A are $\lambda_1, \dots, \lambda_n$. If all these eigenvalues have a strictly positive real part, then the eigenvalues of $-A$, which are $-\lambda_1, \dots, -\lambda_n$, have a strictly negative real part. Therefore, $-A$ is stable and to solve the linear problem $Ay = b$, we can simply consider the IVP $y' = (-A)y - (-b) = -Ay + b$ instead, with our best guess of y^* as the initial value.

Chapter 2

A Test Problem, the Convection Diffusion Equation

As a test case, we consider the one dimensional, steady state convection-diffusion equation with fixed boundary conditions

$$u_x = bu_{xx} + 1, \quad u(0) = u(1) = 0. \tag{2.1}$$

Here b is some physical parameter. Moreover, $u(x)$ is defined on the interval $[0, 1]$. This equation has a solution that is given by

$$u(x) = x - \frac{e^{-(1-x)/b} - e^{-1/b}}{1 - e^{-1/b}}. \tag{2.2}$$

We are however interested in solving this numerically, with a finite difference approach. We partition the interval $[0, 1]$ using $n + 2$ equidistant points $x_i, i = 0, ... n + 1$. We denote the distance between each points as $\Delta x = \frac{1}{n+1}$. The approximated value of u at the point x_i is denoted by u^i and we have $u^0 = u(0) = 0$ and $u^{n+1} = u(1) = 0$. We approximate, for $i \geq 1$, the derivative as

$$u^i_x = \frac{u^i - u^{i-1}}{\Delta x},$$

and the second order derivative is approximated by

$$u^i_{xx} = \frac{u^{i+1} - 2u^i + u^{i-1}}{\Delta x^2}.$$

Note that the first derivative is approximated backward in space, which aligns with the convection being in the right direction. For $i = 1, ... , n$, we thus have the approximation

$$\frac{u^i - u^{i-1}}{\Delta x} = b\frac{u^{i+1} - 2u^i + u^{i-1}}{\Delta x^2} + 1.$$

This can be given in a matrix-vector format, by letting $\boldsymbol{u} = (u^1, \dots, u^n)^\top$,

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{B}\boldsymbol{u} + \boldsymbol{d},$$

where $\boldsymbol{d} = (1, 1, \dots, 1)^\top$,

$$\boldsymbol{A} = \frac{1}{\Delta x}\begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix},$$

and

$$\boldsymbol{B} = \frac{b}{\Delta x^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{pmatrix}.$$

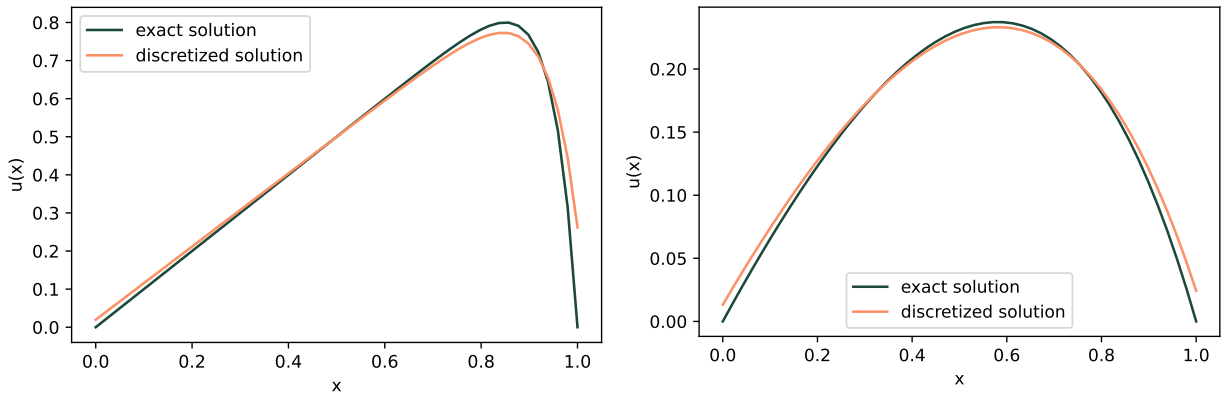
Note that from now on, matrices and vector are denoted in bold italic. With $\boldsymbol{N} = \boldsymbol{A} - \boldsymbol{B}$, the approximate solution of Equation 2.1 is then the solution of the linear system

$$\boldsymbol{N}\boldsymbol{u} = \boldsymbol{d}, \tag{2.3}$$

where $\boldsymbol{N}$ is a square matrix of dimension $n \times n$ and $\boldsymbol{d}$ is the vector of ones of dimension n.

Remark. $\boldsymbol{N}$ is diagonally dominant. Since all elements of the diagonal are positive, we can use Gershgorin circle theorem to prove that all the eigenvalues of $\boldsymbol{N}$ have a positive real part. We thus only need to assume $\boldsymbol{N}$ is non singular to prove that $-\boldsymbol{N}$ is stable.

We plot two examples of what the exact solution (Equation 2.2) and the discretized solution (Equation 2.3) look like for different values of b in Figure 2.1



(a) $b = 0.05$, $n = 50$.

(b) $b = 0.5$, $n = 50$.

Figure 2.1: Exact and discretized solution of the convection diffusion equation, for different parameters.

To solve this linear system, we use the method highlighted before. To make it easier for later, we choose to scale N so that its diagonal elements are 1. This allows us to have all eigenvalues in the circle centered around 1 with radius 1 independently of the parametrization. Setting $\eta = \frac{1}{\Delta x} + \frac{2b}{\Delta x^2}$, solving Equation 2.3 is equivalent to solving the system

$$\boldsymbol{M}\boldsymbol{u} = \boldsymbol{e}, \tag{2.4}$$

where with $\boldsymbol{M} = \frac{\boldsymbol{N}}{\eta}$, $\boldsymbol{e} = \frac{\boldsymbol{d}}{\eta}$. The eigenvalues of $\boldsymbol{N}$ are also scaled by $\frac{1}{\eta}$, and therefore $-\boldsymbol{M}$ is stable, assuming it is non singular. We are now ready to solve the system iteratively using an ODE solver. To do that, we introduce a (pseudo) time variable t and we consider the ODE

$$\boldsymbol{u}'(\boldsymbol{t}) = \boldsymbol{e} - \boldsymbol{M}\boldsymbol{u}(\boldsymbol{t}). \tag{2.5}$$

where $\boldsymbol{M}$ and $\boldsymbol{e}$ depends on both n and b. From now on, we call b and n the problem parameters. We can use Theorem 1.2 with the non singularity assumption to guarantee that $\boldsymbol{u}(\boldsymbol{t})$ converges to a steady state independently of its chosen initial value. In the next chapter, we introduce a numerical method to solve this differential equation, which we will use in this thesis.

Remark. The convection diffusion equation is derived in [13] , chap. 3 from the continuity equation for a scalar quantity u and is

$$\frac{\partial u}{\partial t} + \Delta.(\vec{v}u - \nabla(Du)) = R.$$

We will assume that the quantity u, is the temperature in Kelvin, and has the S.I unit K. The physical quantities are:

- $\vec{v}$, which is the velocity of the medium the quantity is in, in ms^{-1}. (the advection/convection).
- D is the diffusion coefficient, in $\mathrm{m}^2\mathrm{s}^{-1}$.
- R is governing whether the quantity is created when $R > 0$, or destructed when $R < 0$. The unit is $K\mathrm{s}^{-1}$.

We can now simplify the equation by considering it in a single dimension x

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}.(vu - \frac{\partial}{\partial x}(Du)) = R.$$

This further simplifies to $u_t + vu_x - Du_{xx} = R$.

Then, in the steady state, $u_t = 0$ so we get

$$u_x = \frac{D}{v}u_{xx} + \frac{R}{v},$$

and we recognize Equation 2.1, with $b = \frac{D}{v}$, and $1 = \frac{R}{v}$. This also means that we "lose" two parameters in the studied test problem for simplification purposes. Nevertheless, this can be used to give some degree of intuition behind Figure 2.1. When the diffusion is high compared to the convection, the quantity is more centered, but on the other hand, when the convection speed is high compared to the diffusion, the quantity u is "flushed" to the right (assuming $v > 0$).

Chapter 3

Explicit Runge-Kutta Method

3.1 A small introduction to explicit Runge-Kutta methods

This section aims to introduce explicit Runge-Kutta methods, [14, Ch. 3], which we use in this paper. We consider solving a generic initial value problem of the form

$$y'(t) = f(t, y(t)), \quad y(0) = y_0.$$

If we know, for an instant t_n, the value for $y(t_n)$, we can compute the value of y at instant $t_{n+1} = t_n + \Delta t$ by integrating

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(u, y(u))\, du,$$

and with the change of variable $u = t_n + \Delta t\tau$, we have

$$y(t_{n+1}) = y(t_n) + \Delta t \int_0^1 f(t_n + \Delta t\tau, y(t_n + \Delta t\tau))\, d\tau.$$

The problem is finding a suitable way to compute the integral above. An elementary approach is to use the current value of $f(t_n, y(t_n))$ and to treat f as constant, thus defining the sequence

$$y_{n+1} = y_n + \Delta t f(t_n, y_n),$$

where $y_n \approx y(t_n)$, $y_0 = y(0)$. This is the explicit Euler's method. We now want to exploit quadrature formulas for numerical integration. Let $c_j \in [0, 1], j = 1, 2, \dots, \nu$, where ν is an integer, be the nodes in the quadrature formula, with their associated weight $b_j, j = 1, 2, \dots, \nu$. A quadrature formula for the integral is then of the form

$$\int_0^1 f(t_n + \Delta t\tau, y(t_n + \Delta t\tau))\, d\tau \approx \sum_{j=1}^{\nu} b_j f(t_n + \Delta t c_j, y(t_n + \Delta t c_j)).$$

This is all well and good, except that we have to know the values $y(t_n + \Delta c_j)$, which we do not possess. We can however, play pretend and compute an approximation of these values $\xi_j \approx y(t_n + \Delta t c_j), j = 1, \dots, \nu$.

The ξ_j are called *stage values*. [15]. The main idea to use the ξ_i's to compute ξ_j, using a linear combination of the terms $f(t_n + \Delta t c_j, \xi_i)$. That is

$$\xi_i = y_n + \Delta t \sum_{j=1}^{\nu} a_{ij} f(t_n + \Delta t c_j, \xi_j),$$

for $i = 1, \dots, \nu$, where the a_{ij} are some well chosen values, which is not in scope of this thesis. To simplify notation, we note A as the square array containing the a_{ij} parameters, that is $A_{ij} = a_{ij}$, $c = (c_1, \dots, c_\nu)^\top$ the vector of nodes, and $b = (b_1, \dots, b_\nu)^\top$ the vector of weights. An RK method is then written in the form of the following array, also called a Butcher tableau:

$$\begin{array}{c|c} c & A \\ \hline & b^\top \end{array}.$$

We remark that if, for any $j \geq i$, $a_{ij} \neq 0$, then we will need to know ξ_j to compute ξ_i, which involves solving an equation, making the method *implicit*. We consider here *explicit* methods, where we can compute ξ_{i+1} if we know $\xi_j, j = 1, \dots, i-1$. Since we know $f(t_n, y_n)$, we choose $a_{11} = 0$ and $c_1 = 0$. An explicit RK method is then of the form

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j f(t_n + \Delta t c_j, \xi_j),$$

where the stage values ξ_j are computed sequentially as follow

$$\begin{aligned}
&\xi_1 = y_n, \\
&\xi_2 = y_n + \Delta t a_{2,1} f(t_n, \xi_1), \\
&\xi_3 = y_n + \Delta t a_{3,1} f(t_n, \xi_1) + \Delta t a_{3,2} f(t_n + \Delta t c_2, \xi_2), \\
&\quad \vdots \\
&\xi_\nu = y_n + \Delta t \sum_{j=1}^{\nu-1} a_{\nu,j} f(t_n + \Delta t c_j, \xi_j).
\end{aligned}$$

3.2 Application to the test problem

We now have to solve the ODE $u'(t) = e - Mu(t)$ where M depends on the problem parameters b and $\Delta x = 1/(n+1)$, and n is the chosen number of subdivisions of $[0, 1]$. We consider in this thesis the following RK method with two stages [15];

$$\begin{array}{c|cc} 0 & & \\ \alpha & \alpha & \\ \hline & 0 & 1 \end{array}.$$

Remark. This RK method can be extended to more stages. We only need the last stage value to compute the time step update, and we only need to compute the stage values sequentially using only the last stage value calculated. This makes it possible, when programming the method, to simply to do the update of the variable ξ in place inside the computer memory. Such methods are thus memory efficient.

This solver has two parameters, namely the (pseudo) time step Δt and α, where $\alpha \in [0, 1]$.

The goal is for the solver to converge to a steady state solution in as few iterations as possible.

3.2.1 A note on stability

Using the same notation as before for the stage values and the studied RK method, for the equation $u'(t) = f(t, u(t))$, we have $\xi_1 = u_n$,

$$\xi_2 = u_n + \Delta t \alpha f(t_n, \xi_1) = u_n + \Delta t \alpha f(t_n, u_n).$$

The update is thus;

$$u_{n+1} = u_n + \Delta t f(t_n + \alpha \Delta t, \xi_2).$$

In the test problem case, $f(t_n, \boldsymbol{u}_n) = \boldsymbol{e} - \boldsymbol{M}\boldsymbol{u}_n$, and we get the update

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \Delta t \left[\boldsymbol{e} - \boldsymbol{M}(\boldsymbol{u}_n + \alpha \Delta t(\boldsymbol{e} - \boldsymbol{M}\boldsymbol{u_n}))\right].$$

After a few lines of computation, we get the following iteration,

$$\boldsymbol{u}_{n+1} = \left[\boldsymbol{I} - \Delta t(\boldsymbol{I} - \alpha \Delta t \boldsymbol{M})\boldsymbol{M}\right] \boldsymbol{u}_n + \left[\Delta t(\boldsymbol{I} - \alpha \Delta t \boldsymbol{M})\right] \boldsymbol{e}. \tag{3.1}$$

This iteration is of the form $\boldsymbol{u}_{n+1} = \boldsymbol{K}\boldsymbol{u}_n + \boldsymbol{L}\boldsymbol{e}$, where

$$\boldsymbol{L} = \Delta t \left[\boldsymbol{I} - \alpha \Delta t \boldsymbol{M}\right] \tag{3.2}$$

and

$$\boldsymbol{K} = \boldsymbol{I} - \boldsymbol{L}\boldsymbol{M} = \left[\boldsymbol{I} - \Delta t(\boldsymbol{I} - \alpha \Delta t \boldsymbol{M})\boldsymbol{M}\right]. \tag{3.3}$$

We recognize this iteration as a linear stationary iteration, which converges to a unique fixed point for any starting value $\boldsymbol{u}_0$ if and only if $\rho(K) < 1$, [16, Ch. 2.2], where $\rho(\boldsymbol{K})$ is the spectral radius of $\boldsymbol{K}$. Furthermore, this iteration satisfies the consistency requirement $\boldsymbol{K} = \boldsymbol{I} - \boldsymbol{L}\boldsymbol{M}$, so the fixed point, when it exists, is $\boldsymbol{u}^* = \boldsymbol{M}^{-1}\boldsymbol{e}$.

Remark. One may remark that $\boldsymbol{K} = p(\Delta t \boldsymbol{M})$ with $p(z) = 1 - z + \alpha z^2$ a polynomial. This polynomial is also the stability polynomial of the RK method [15].

3.2.2 Residual ratios

We have shown in the last section the sufficient and necessary condition for the solver to converge to the desired solution $\boldsymbol{u}^* = \boldsymbol{M}^{-1}\boldsymbol{e}$. This condition is that $\rho(\boldsymbol{K}) < 1$. The spectral radius can be computed with power iterations [17, Pt. V], but this is an expensive task that we may not be able to do in practice. Furthermore, the derivation of $\boldsymbol{K}$ is specific to this method, and may not be as accessible with other methods. We instead turn our attention to another method.

We set $\boldsymbol{u}_0 = \boldsymbol{e}$ as an initial value. We define the relative residual after k steps as

$$r_k = \frac{||\boldsymbol{M}\boldsymbol{u}_k - \boldsymbol{e}||}{||\boldsymbol{e}||}, \tag{3.4}$$

where $||.||$ is the 2-norm.

If the solver we chose is stable, then $||r_k|| \to 0$ as $k \to \infty$. We define now the residual ratio at step k to be the ratio of the residuals at step k and $k-1$. That is

$$\rho_k = \frac{r_k}{r_{k-1}} = \frac{||\boldsymbol{M}\boldsymbol{u}_k - \boldsymbol{e}||}{||\boldsymbol{M}\boldsymbol{u}_{k-1} - \boldsymbol{e}||}. \tag{3.5}$$

Note that the residual ratio depends on both the problem parameters and the solver parameters. It will be useful in future sections to make that relation evident by using the notation $\rho_{k,b,n}(\alpha, \Delta t)$. Figure 3.1 shows the evolution of the relative residual, as well as the residual ratio for specific parameters. After a certain number of iterations, the residual ratio stabilizes. This can be however be after a large amount of iterations, so the rate of convergence can be costly to compute.

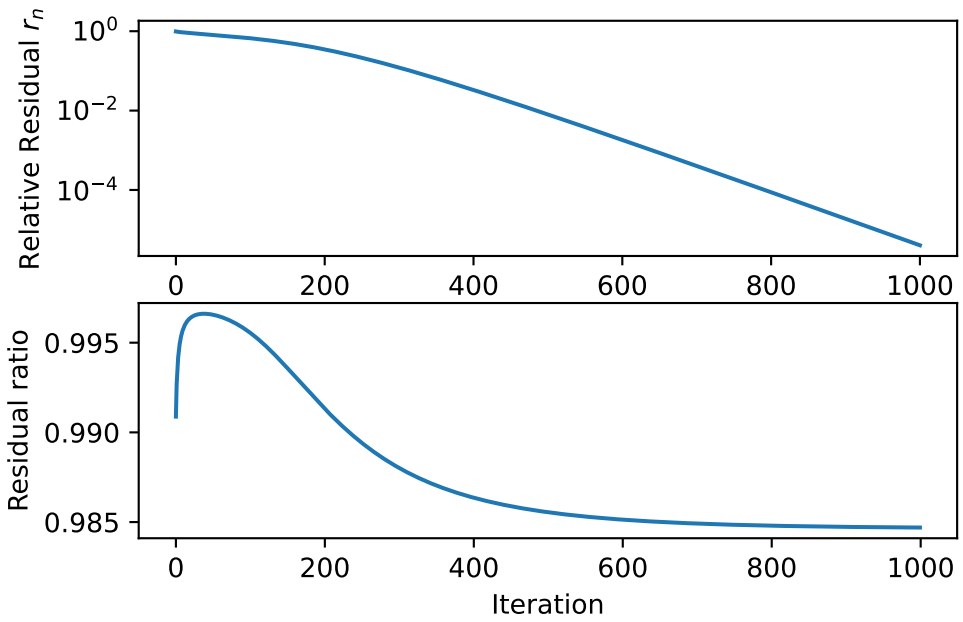


Figure 3.1: Evolution of the residual norm over iteration, with problem parameters $n = 50$ and $b = 0.05$, and RK parameters $\Delta t = 1$ and $\alpha = 0.2$.

3.3 A small experiment

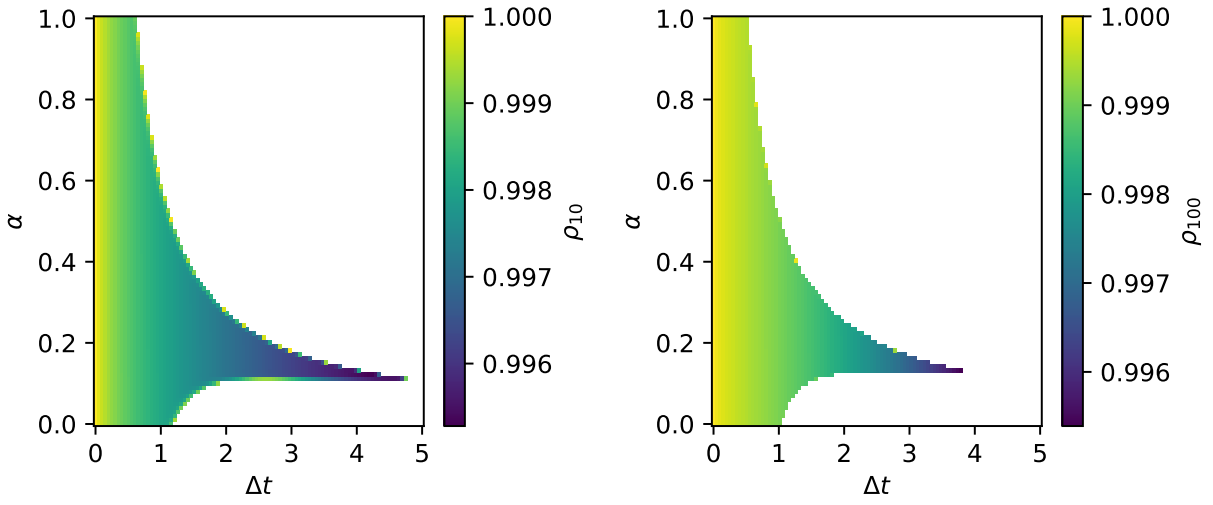
We are interested in finding the best parameters $(\Delta t, \alpha)$ to use for some specific problem parameters (b, n). Ideally, we should minimize the asymptotic residual ratio ρ_∞, but this is computationally intensive, so we restrict ourselves to minimizing the residual ratio ρ_k after a fixed amount of iterations.

As we've seen in Figure 3.1, ρ_k can vary quite a bit depending on k, so we decide to investigate the residual ratio after 10 iterations and 100 iterations. We set the problem parameters $b = 0.05$, and $n = 100$, and we plot $\rho_{k,0.05,100}(\Delta t, \alpha)$ for different values of k. This is achieved by making a linear grid for parameters Δt and α of size 100×100, where α varies between 0 and 1, and Δt varies between 0 and 5, then computing the residual ratios on that grid.

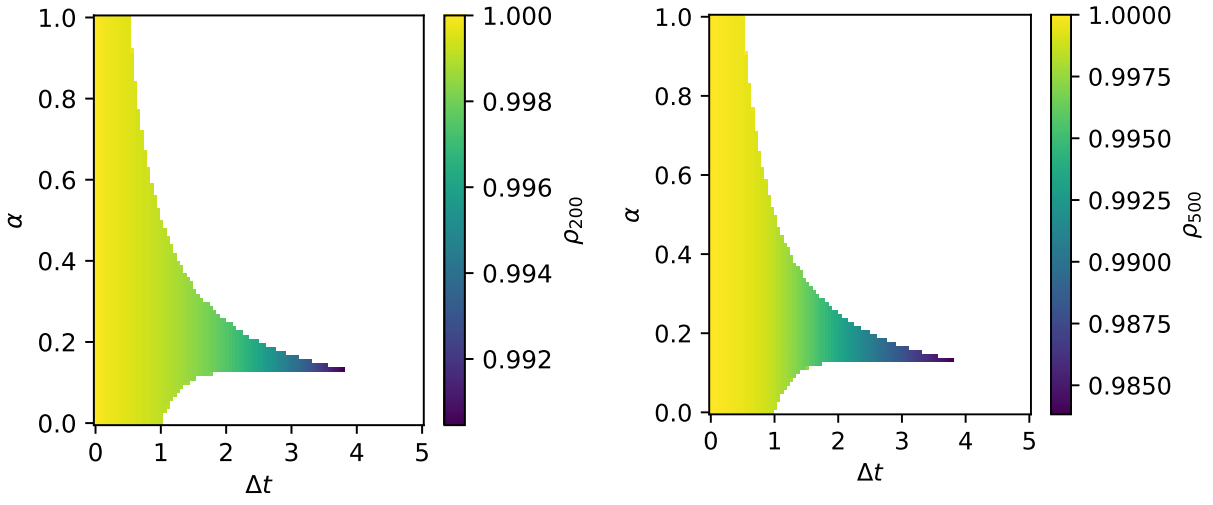
We wish to find the optimal parameters for this specific problem, that is, the ones that minimize ρ_k, for different values of k. We are also interested in seeing how much the optimal parameters depend on k.

After 100 iterations, we see that we need to choose the parameters in more narrow region than after 10 iterations to get $\rho_{100} < 1$, suggesting that convergence of the solver may not hold even if it seems to hold for the first few iterations. However, this doesn't seem to be the case when we consider higher values of k. Nevertheless, we can see how the solver parameters interact with the residual ratio.

By doing this experiment, we motivate the following method: using a grid search, look for the solver parameters that minimize ρ_k, where k has to be chosen as low as possible to minimize computing time, but also high enough to ensure that the solver won't diverge after more iterations. This method however need to be repeated for each individual problem parameters. We therefore explore a possible solution to this problem by using a reinforcement learning algorithm to "learn" the optimal solver parameters α and Δt, as a function of the problem parameters b and n.



(a) ρ_{10} (b) ρ_{100}



(c) ρ_{200} (d) ρ_{500}

Figure 3.2: Contour plot of some residual ratios ρ_k, for different k after different number of iterations, for the specific problem parameters $n = 100$ and $b = 0.05$. Note that the area in white is where $\rho_k > 1$.

Chapter 4

Basics of Reinforcement Learning (RL)

In this section, we outline the main ideas behind reinforcement learning and how they can be applied in the context of this thesis. The reader familiar with the material may skip this section.

4.1 A non mathematical, yet delicious example!

In Reinforcement Learning tasks, we are training an *agent* that interacts with its *environment* by taking decisions. In this example, we are the agent, and the environment is the kitchen. Suppose we want to cook a delicious meal. At any point in time, we are making decisions such as;

- Which ingredients we use. Do we use tofu or seitan? Do we add spice or more chili pepper? When do we incorporate the sauce?
- Which cookware we use? Cast iron, or non-stick pan?
- Whether to put the oven to $200°C$ or $220°C$.
- Or simply do nothing!

All of these decisions, which we will call *actions* from now on, are taken based on the current *state* of the environment, that is the cooking process. How we decide which *action* to take given a current *state* will be called the *policy* from now on.

After each action, the cooking process gets to a new *state* and we taste the meal. By tasting it, we get a *reward* that depend on how well we did. Maybe the food started to burn in which case we get a negative reward, or maybe we made the food tastier, in which case we get a positive reward. In this example, there is a *starting state*, where we decide to cook something, and a *terminal state*, in which we finished cooking and get to enjoy the meal.

But how do we learn how to cook, how do we know what *action* to take at a specific *state*? That is, how do we learn the *policy*? We learn it by getting feedback, which is defined by the *reward* we get after each action. Some of those rewards are immediate, for example, if we add some spices to our food and it tastes better. We want to have a *policy* that maximizes the total *rewards* we get over a entire cooking session. This also mean that we have to balance how we prefer the immediate rewards against the future rewards. For example, adding a spice may make the meal taste better in the short term, for which we get a reward, but it may clash later when we add other ingredients, leading to a worse meal and worse *rewards* down the line.

Each time we cook, we learn what works and what doesn't, and remember that for any future time we cook. But, if we want to get better at cooking, we must not just repeat the *actions* that worked! We also have to take some risks, and *explore* the potential actions we can take at each state! On the other hand, we still need to rely and *exploit* what we know. There is a balance to find between *exploitation* and *exploration* so as to learn as fast as possible.

4.2 Another example: Leonardo the rabbit

The last example is an intuitive way of thinking of reinforcement learning as similar to the way we animals learn about the world and its processes. The ideas behind reinforcement learning borrow a lot from the fields of psychology and neuroscience[18], and modelling how we learn is a gargantuan task that is, for this very reason, outside of the scope of this thesis!

We turn our attention to a more modest example that is much easier to model, and is an example that one can find in a lot of reinforcement learning books[8], [19]. We consider the case of Leonardo the rabbit. Leonardo, the agent, is situated in the outside world, which is represented as a 3×3 grid (the environment). He wants to get to the carrot at the bottom right as fast as possible. To help Leonardo get to his meal, we will use reinforcement learning.

4.2.1 States

The first thing we do is give a number to each box in the grid, from 1 to 9. We call the set of all boxes number as the state set, which we denote by $\mathcal{S}$. In this example, $\mathcal{S} = \{1, 2, \dots, 9\}$ (see Figure 4.1). A state is defined as any element in the state set, which we denote by $s \in \mathcal{S}$. The state is the box Leonardo is in.

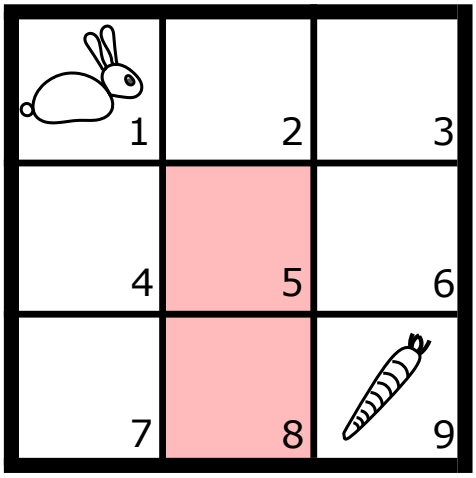


Figure 4.1: Can you help special agent Leonardo get to his carrot? The grid environment, where our fluffy friend is situated in. His state is $s = 1$.

4.2.2 Actions

Leonardo, in this grid, can move in any 4 directions, that is left, right, up or down. We call this the action set $\mathcal{A}$, and in this example $\mathcal{A} = \{\text{left,right,up,down}\}$. An action is defined as any element in the action set, which we denote by $a \in \mathcal{A}$.

4.2.3 State transitions

At this point, we can introduce a time variable t. The initial time is set to $t = 0$, and, after Leonardo takes an action t moves forward by 1, and he finds himself in a new state. This is what we call a state transition(see Figure 4.2).

We want to keep track of Leonardo positions and actions over time, which is why we denote the state Leonardo is in at time t by S_t, and the action he takes by A_t. In this example, there is the initial state $S_0 = 1$.

Remark. S_t and A_t are random variables, which is we note in uppercase. Specific observations of S_t and A_t will be in lowercase, that is respectively s_t and a_t.

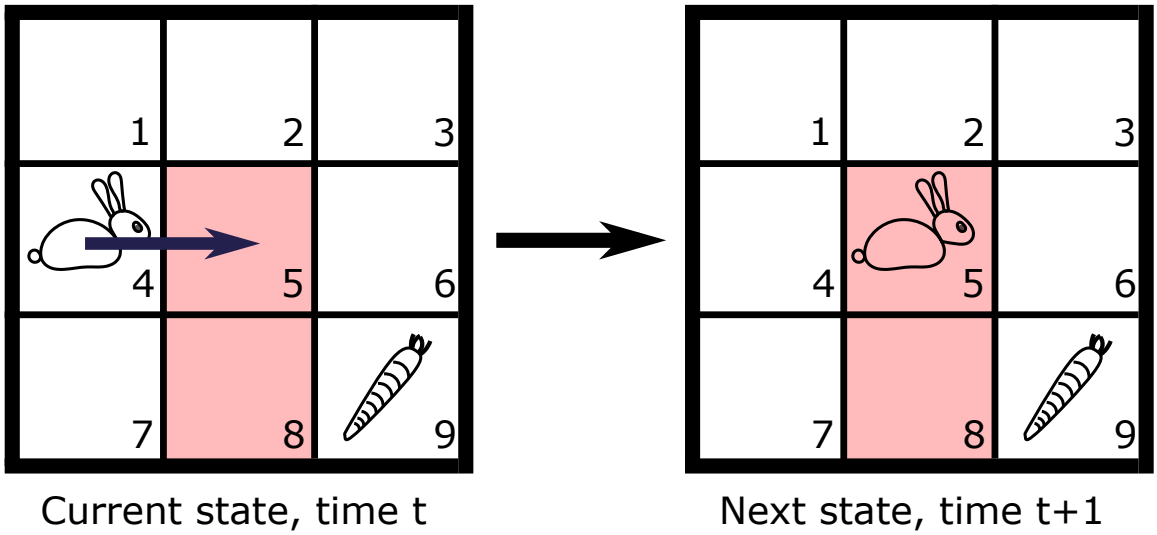


Figure 4.2: An example of state transition. Leonardo, being at the state $s_t = 4$, takes the action $a_t = \text{right}$. After this action, he is at the state $s_{t+1} = 5$. Leonardo gets the reward $r_{t+1} = -5$.

4.2.4 Policy

Leonardo, as the agent, only has access to his current state S_t. He has to take an action A_t, but how does he know which action to take? To do that, he uses a policy, which we denote by a function π. More formally, π is a function that defines the probability of taking the action $A_t = a$ if the state is $S_t = s$. We denote this by $\pi(a|s)$.

Suppose for example that $S_t = 3$. Leonardo has no idea of where the carrot is, but he knows that he can not go up nor to the right, so his policy is to go down, or right at random. Then:

- The probability to go right is $\pi(\text{right}, 3) = 0.5$.
- The probability to go down is $\pi(\text{down}, 3) = 0.5$.

More specifically, for any state s, we define the conditional probability mass function $\pi(a|s) = \Pr(A_t = a|S_t = s)$, where Pr denote a probability. Hence, for any fixed state s, $\sum_{a \in \mathcal{A}} \pi(a|s) = 1$.

Remark. We will assume that Leonardo only cares about what his current state is to take an action, and not for how long he has been in the grid. This makes the policy independent of the time t.

4.2.5 Rewards

While Leonardo only takes actions by looking at his current state, he still wants to get to the carrot as fast as possible. He knows his current state s_t and takes the action a_t. Doing so, he ends up in the state s_{t+1} and he gets a reward.

- The red colored box are difficult to get in, so if he ends up on one of the red colored box, he gets a reward of -5. This is for example the case in Figure 4.2.
- If he ends up on the carrot, he gets a reward of $+5$.
- If he ends up in any other state, he gets a reward of -1, as he does not want to lose time.

More formally, we denote the reward Leonardo gets after taking the action A_t from the state S_t by R_{t+1}. The set of all possible rewards is denoted by $\mathcal{R}$. Here $\mathcal{R} = \{-1, 5, -5\}$. R_t is again a random variable and we denote an observation of the reward at time t by r_t.

4.2.6 State transitions and rewards probabilities

Suppose now that there is a teleporter in the 4th box. This teleporter is however unreliable. Half the time, it teleports whoever steps in the box to the 9^{th} box, meaning Leonardo could potentially get directly to his prize! The other half of the time, however, it teleports the user to the 7^{th} box.

Suppose now that Leonardo is at state $s_t = 1$, he takes the action $a_t =$ down to the teleporter(see Figure 4.3). Then:

- The next state is $s_{t+1} = 9$ with probability 0.5.
- The next state is $s_{t+1} = 7$ with probability 0.5.

But now, the reward he gets is random too!

- If he end up in the 9^{th} box, $r_{t+1} = 5$.
- If the teleporter does not work and he ends up in the 7^{th} box, $r_{t+1} = -1$.

More specifically, this means that state transitions and rewards need to be modelled by a probability, more specifically, the probability of getting a reward $r \in \mathcal{R}$, and that the next state is $s' \in \mathcal{S}$ given that the agent takes the action $a \in \mathcal{A}$ at the state $s \in \mathcal{S}$. We formalize a state transition probability as the conditional probability defined in the sample space $\mathcal{S} \times \mathcal{R}$

$$p(s', r|s, a) = \Pr(S_{t+1} = s', R_{t+1} = r|S_t = s, A_t = a).$$

4.3 Finite Markov decision process

We formalize the above example by defining a Markov decision process (MDP). This definition and the ones up until the end of this chapter are adapted from [19].

Definition 4.1. (Markov decision process). A finite Markov decision process (MDP) is defined as a discrete time process, where we have:

- A finite set of all states $\mathcal{S}$.
- A finite set of all possible actions $\mathcal{A}$.
- A reward set $\mathcal{R}(s, a)$, which contains the potential rewards received after taking any action $a \in \mathcal{A}$ from any state $s \in \mathcal{S}$.

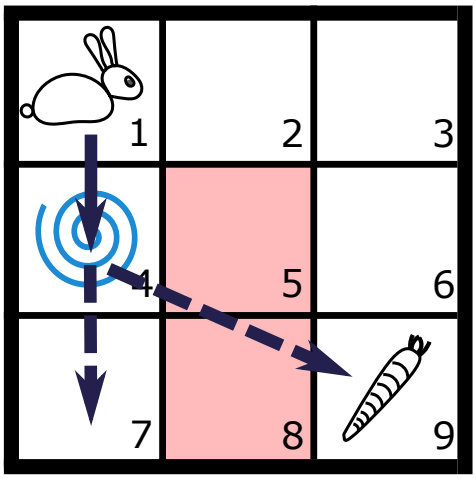


Figure 4.3: Will it be worth the risk? Leonardo has taken the action a = down at the state $s = 1$. There is a 50% chance he ends up right on his prize! The state transition and reward probability is $p(s' = 9, r = 5|s = 1, a = down) = 0.5$. Similarly, $p(s' = 7, r = -1|s = 1, a = down) = 0.5$.

We use the notation S_t, A_t as the state and action of the process at time t. The reward R_t is the reward received at time t. S_t, A_t and R_t are random variables.

A Markov decision process also has a model, which consists of the state and reward transition probabilities:

- The probability, given that the current state is s, and that the action taken is a, that the next state is s' and the next reward is r. That is $p(s', r|s, a) = \Pr(S_{t+1} = s', R_{t+1} = r|S_t = s, A_t = a)$.

Furthermore, a Markov decision process has a policy that governs, for any state $s \in \mathcal{S}$, the probability of taking action $a \in \mathcal{A}$, that probability is $\pi(a|s) = \Pr(A_t = a|S_t = s)$. We assume that the policy is not dependent on time.

Finally, a Markov decision process has the Markov property, or lack of memory. The state transition and rewards probabilities are only dependent on the current state S_t and action A_t, and not the states and actions that preceeded. Mathematically, $\Pr(S_{t+1} = s', R_{t+1} = r|S_t, A_t, S_{t-1}, A_{t-1}, \dots, S_0, A_0) = \Pr(S_{t+1} = s', R_{t+1} = r|S_t, A_t)$.

An example of Markov decision process with two states can be seen in Figure 4.4.

Remark. The state space $\mathcal{S}$ and the action space $\mathcal{A}$ can be finite or not. We only consider the case of finite Markov decision process to make matters easier.

Remark. The model in a Markov decision process is often impossible to define in advance. This problem is remedied by using *model free* algorithms.

4.4 State Value and Bellman Equation

We have a Markov decision process, which serves as a nice mathematical formalization of an agent and its environment [8]. Now we want to train the agent to make the best possible decisions? Answering this question is the goal of the next sections.

We first define a trajectory. We denote by S_t the state of an agent at instant t. Then, according to the policy, this agent takes the action A_t. After taking this action, the agent is now at the state S_{t+1}, and it gets the rewards R_{t+1}. Then the agent takes action A_{t+1}, and gets to a new state S_{t+2} with reward R_{t+2}.

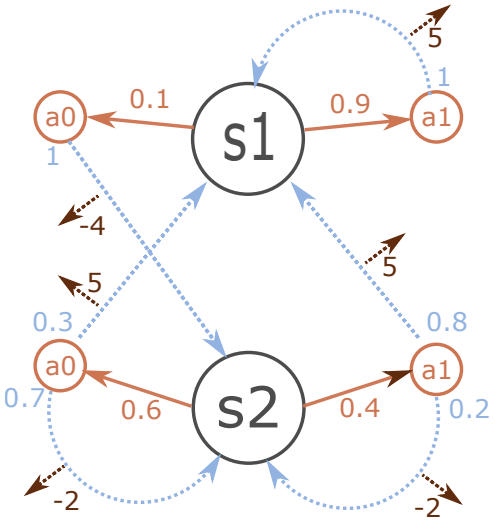


Figure 4.4: An example of a Markov decision process with two states s_1 and s_2 and two possible actions a_0 and a_1 for each states. The dashed lines represent the model transitions. After each action, the process get to a new state and a reward is given, here in dark red.

This continues indefinitely. We define the trajectory of an agent with starting state $S_t = s_t$ as the chain of states, actions and rewards from time t onward:

$$S_t = s_t, A_t \to R_{t+1}, S_{t+1}, A_{t+1} \to R_{t+2}, S_{t+2}, A_{t+2} \to \cdots,$$

Note that, due to the Markov property and the fact that we assume the policy is time independent, the starting value of t is not important.

Remark. In some environments, it is natural for the agent to have a task that has a starting state and a finishing states (for example, beginning a cooking session and finishing it, or starting a game and winning/losing at it.) We call these tasks *episodic tasks* and in these cases, a finite trajectory $S_0, A_0 \to ... \to S_T$ is also called an *episode*. In the cases where the task is such that no such state can be defined, a trajectory is not finite and we call these tasks *continuing tasks*, which will be the case in this thesis.

In reinforcement learning setting, we assume that we have no control of the environment model (for example, one can not change the rules of a game), but that we have control over the agent decisions (i.e the policy) and how we reward that agent. The goal of any reinforcement learning algorithm is thus to define the rewards properly and then to find a policy that maximizes the rewards the agent gets. We now define the discounted return along a trajectory,

Definition 4.2. Let $t = 0, 1, ...$ The (discounted) return along the trajectory $S_t, A_t \to S_{t+1}, A_{t+1}, R_{t+1} \to S_{t+2}, A_{t+2}, R_{t+2} \to ...$ is the random variable given by

$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \cdots = \sum_{k=0}^{+\infty} \gamma^k R_{t+1+k},$$

where $\gamma \in [0, 1)$ is called the discount rate.

Remark. By setting a discount rate that is less than 1 in continuing tasks, we make sure that the discounted return is well defined in the case of bounded rewards. Indeed, if, for any t, $|R_t| \leq M$, then $\sum_{k=0}^{+\infty} |\gamma^k R_{t+1+k}| \leq \sum_{k=0}^{+\infty} \gamma^k M = \frac{M}{1-\gamma}$, so the series is absolutely convergent.

The *discounted return* is thus the sum of rewards along a trajectory, with a penalty for rewards far in the future, controlled by the *discount rate*. The discount rate is chosen depending on whether we want the agent to favor short term rewards, in which case a discount rate closer to 0 can be chosen, or long term rewards, with a discount rate closer to 1.

Since the discounted return is a random variable, we can look at its expectation, in particular, we are interested in its conditional expectation, given a starting state $S_t = s$. This expectation is called the state value [8].

Definition 4.3. State value The state value of a state s is the function, defined for any $s \in \mathcal{S}$ as the conditional expectation of the discounted return, given $S_t = s$,

$$v_\pi(s) = E[G_t|S_t = s] = E[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + ... |S_t = s],$$

where π is a given policy.

Remark. Once again, the Markov property and the time independence of the policy mean that the state value does not depend on time.

We remark that

$$\begin{aligned} G_t &= R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + ... \\ &= R_{t+1} + \gamma \left(R_{t+2} + \gamma R_{t+3} + ... \right) \\ &= R_{t+1} + \gamma G_{t+1}. \end{aligned} \tag{4.1}$$

This expression of the return can be used in conjunction with the definition of the state value above to get

$$v_\pi(s) = E[G_t|S_t = s] = E[R_{t+1}|S_t = s] + \gamma E[G_{t+1}|S_t = s]. \tag{4.2}$$

The first term is the expectation of immediate reward, following a certain policy π, the second is the expectation of future rewards. Let us expand on that formula a bit more. We now make use of the "law of total expectation":

Theorem 4.1. *Let X and Y be random variables, and suppose $E[|Y|] < \infty$. Then*

$$E[Y] = E\left[E[Y|X]\right]$$

Using this, the expectation of immediate reward is

$$E[R_{t+1}|S_t = s] = E[E[R_{t+1}|S_t = s, A_t]] = \sum_{a \in \mathcal{A}} \pi(a|s) \sum_{r \in \mathcal{R}} \sum_{s' \in \mathcal{S}} rp(s', r|s, a).$$

We now develop the second part in the RHS of Equation 4.2, and use the law of total expectation again to get

$$E[G_{t+1}|S_t = s] = E[E[G_{t+1}|S_t = s, S_{t+1}]] = \sum_{s' \in \mathcal{S}} p(s'|s) E[G_{t+1}|S_t = s, S_{t+1} = s'],$$

where $p(s'|s) = \sum_{a \in \mathcal{A}} \sum_{r \in \mathcal{R}} p(s', r|s, a)\pi(a|s)$ is the probability of the next state being s' if the current state is s. Because of the Markov property of the MDP, we can remove the conditioning $S_t = s$ and thus, $E[G_{t+1}|S_t = s, S_{t+1} = s'] = E[G_{t+1}|S_{t+1} = s] = v_\pi(s')$. Then

$$E[G_{t+1}|S_t = s] = \sum_{s' \in \mathcal{S}} \sum_{a \in \mathcal{A}} \sum_{r \in \mathcal{R}} v_\pi(s')\pi(a|s)p(s', r|s, a). \tag{4.3}$$

Putting Equation 4.2 and Equation 4.3 together, we get Bellman's equation:

$$v_\pi(s) = \sum_{a \in \mathcal{A}} \sum_{r \in \mathcal{R}} \sum_{s' \in \mathcal{S}} \pi(a|s)p(s', r|s, a) \left[r + \gamma v_\pi(s')\right]. \tag{4.4}$$

Remark. The Bellman equation depends on the given policy and gives a recursive relation for the state values. Solving this equation is called policy evaluation which involves fixed point iterations (see example below).

Example 4.1. We can directly derive the state values in the MDP in Figure 4.4. We remark that in this example, given a specific state transition, the reward we get is deterministic, which simplifies the computations.

In particular, for the state s_2, There are two possible actions a_0 and a_1 we can take. The policy is to take action a_0 with a probability 0.6, and action a_1 with a probability 0.4. When we take for example action a_0, the probability of the next state being s_1 is 0.3, in which case the reward is 5. Proceeding similarly for all the possible actions and rewards, we get

$$\begin{aligned}
v_\pi(s_2) &= \sum_{a=0}^{1} \sum_{r \in \mathcal{R}} \sum_{s'=1}^{2} \pi(a|s)p(s', r|s_2, a) \left[r + \gamma v_\pi(s')\right] \\
&= 0.6 \sum_{r \in \mathcal{R}} \sum_{s'=1}^{2} p(s', r|s_2, a = 0) \left[r + \gamma v_\pi(s')\right] + 0.4 \sum_{r \in \mathcal{R}} \sum_{s'=1}^{2} p(s', r|s_2, a = 1) \left[r + \gamma v_\pi(s')\right] \\
&= 0.6 \left[0.3(5 + \gamma v_\pi(s_1)) + 0.7(-2 + \gamma v_\pi(s_2))\right] + 0.4 \left[0.2(-2 + \gamma v_\pi(s_2)) + 0.8(5 + \gamma v_\pi(s_1)\right].
\end{aligned}$$

After some computations, we end up with

$$v_\pi(s_2) = 1.5 + \gamma(0.5, 0.5) \begin{pmatrix} v_\pi(s_1) \\ v_\pi(s_2) \end{pmatrix}.$$

Similarly $v_\pi(s_1) = 4.1 + \gamma(0.9, 0.1)(v_\pi(s_1), v_\pi(s_2))^\top$. This leads to the system:

$$\begin{pmatrix} v_\pi(s_1) \\ v_\pi(s_2) \end{pmatrix} = \begin{pmatrix} 4.1 \\ 1.5 \end{pmatrix} + \gamma \begin{pmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{pmatrix} \begin{pmatrix} v_\pi(s_1) \\ v_\pi(s_2) \end{pmatrix}.$$

We stop here to remark that this equation is of the form $v_\pi = r_\pi + \gamma \boldsymbol{P}_\pi v_\pi$. $\boldsymbol{P}_\pi$ can be related to a state transition matrix in a markov chain and is row stochastic. Furthermore, since $\gamma < 1$, we motivate solving the equation by using fixed point iterations. This is the main idea behind *dynamic programming* [20]. In this case, we can simply solve the system directly. For example, with $\gamma = 0.5$, we get the state values $v_\pi(s_1) = 7.875$, $v_\pi(s_2) = 4.625$.

4.5 Action Value

The state value gives information about a specific state, however, we are also often interested in knowing how much we stand to gain by taking a particular action at a particular state. This lead to the definition of the action value.

Definition 4.4. Action value The action value is defined as the expectation of discounted return G_t, given a specific action a, taken at the current state s:

$$q_\pi(a|s) = E\left[G_t|A_t = a, S_t = s\right] = E\left[\sum_{|} A_t = a, S_t = s\right],$$

where $G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + ...$

We also have, from Definition 4.3, and the law of total expectation,

$$v_\pi(s) = E[G_t|S_t = s] = E\left[E[G_t|S_t = s, A_t = a]\right].$$

Then,

$$v_\pi(s) = \sum_{a\in\mathcal{A}} \pi(a|s) E\left[G_t|S_t = s, A_t = a\right],$$

and we can get the relation between state value and action value:

$$v_\pi(s) = \sum_{a\in\mathcal{A}} \pi(a|s) q_\pi(a|s). \tag{4.5}$$

We remark that by viewing $\pi(a|s)$ as a probability mass function, we can express the state values as another expectation:

$$v_\pi(s) = E[q_\pi(a|s)],$$

where A is random variable with p.m.f $\pi(a|s)$. Actions values are important in the sense that they tell us of the "value of taking an action over another", and they appear naturally in almost all reinforcement learning algorithms. One important thing to note is that, by "comparing" Equation 4.5 and Equation 4.4, we get an equivalent definitions of the action values as

$$q_\pi(a|s) = \sum_{r\in\mathcal{R}} \sum_{s'\in\mathcal{S}} p(s', r|s, a)\left[r + \gamma v_\pi(s')\right]. \tag{4.6}$$

Equation 4.6 means that if we have access to the state values, we can compute the action values, while Equation 4.5 works in the opposite way, deriving state values from the action values.

Remark. A more rigorous approach to derive Equation 4.6 would be similar to how we derive Bellman's equation.

4.6 Optimal policy and value iteration

Now that we have defined the state values, we want to find a policy that maximizes them, that is, find a policy which we denote by $\pi^*(a, s)$ such that, for any state s and for any policy $\pi(a|s)$, $v_{\pi^*}(s) \geq v_\pi(s)$. It turns out that not only this optimal policy exist, but that we can find it by repeating the following steps, starting from any policy π_0:

- Test the current policy, that is evaluate the state values.
- From these state values, compute the action values.
- Using these action values, set a new and better policy that aim to choose the best actions.

More specifically, we present the pseudo code for the value iteration algorithm.

Value iteration pseudocode
INPUT:
- An initial policy π_0.
- Discount rate γ.
- A stopping criterion.

OUTPUT: An approximation of the optimal policy π^*, at an arbitrary precision;

i <- 0;
DO:
    Compute the state values $v_{\pi_i}(s)$, using fixed point iterations;
    FOR all state s:
        Compute, for all $a \in \mathcal{A}$,the action values $q_{\pi_i}(a, s)$ using Equation 4.6 and the computed state values;
        Denote by a^* the action with the best action value $q_{\pi_i}(a^*, s)$;
        Set the new policy $\pi_{i+1}(a^*, s) = 1$, and set for all the other actions $\pi_{i+1}(a, s) = 0$;
    END FOR
    i <- i + 1
UNTIL Stopping criterion is met.

This algorithm is important in the sense that we can prove that it converges to an optimal policy, that maximizes all state values! Unfortunately, this algorithm scales poorly. In Example 4.1, we found that computing the state values is equivalent to solving a 2×2 linear system. In the general case, this system as the same dimensions as the number of states. Depending on the problem, solving this linear system can become prohibitively expensive (for example, there are several orders of magnitude more legal board states in a game of go than atoms in the observable universe [21]), and yet we can design a program that can beat the best human players handily [5]! Nevertheless, the main idea of starting with an initial policy, then getting a better and better policy over time is a fundamental idea in reinforcement learning.

Chapter 5

Policy Gradient Method

Now that we have access to the main definitions used in RL, we can study the problem we had at the end of chapter 3 through the lens of RL.

The last chapter has been quite long as we introduced reinforcement learning, so as a reminder, we summarize the work we've done so far. We have a test problem, the convection diffusion equation Equation 2.1, which we discretize, and with the following **problem parameters**:

- A parameter $b \in [0, 1]$ in the steady-state convection diffusion equation , and
- a discretization parameter $n \in \mathbb{N}$ defining the number of interior points in the linear grid used to discretize this equation.

We end up with a linear system of the form $\boldsymbol{Mu} = \boldsymbol{e}$ (Equation 2.4). To solve this system, we solve the ODE $\boldsymbol{u}'(t) = \boldsymbol{e} - \boldsymbol{Mu}(t)$ using an explicit Runge-Kutta method with two **solver parameters** (see Section 3.2):

- Δt, the (pseudo) time step, and
- α, a parameter specific to the Runge Kutta method used.

We relate this solver to a stationary iterative method of the form $\boldsymbol{u}_{n+1} = \boldsymbol{K}\boldsymbol{u}_n + \boldsymbol{Le}$, where $\boldsymbol{K} = \boldsymbol{I} - \boldsymbol{LM}$. This method is convergent if and only if the spectral radius of $\boldsymbol{K}$ is strictly less than one. We could compute this spectral radius, but this is an computationally intensive task, so we use an approximation. This approximation is the residual ratio after 10 iterations of the Runge-Kutta solver, starting with $\boldsymbol{u}_0 = \boldsymbol{e}$.

We define this ratio as $\rho_{10,b,n}(\Delta t, \alpha)$, a function parametrized by b and n, with arguments Δt and α. We are faced with the following optimization problem:

For any problem parameters b, n, find the optimal solver parameters

$$(\Delta t^*, \alpha^*) = \arg\min_{\Delta t, \alpha} \rho_{10,b,n}(\Delta t, \alpha). \tag{5.1}$$

Remark. We've already seen in Section 3.3 that the optimal parameters can lead to divergence of the solver once more iterations are computed, which is problematic, so we are perfectly happy to find "good enough, but not optimal" solver parameters where this issue will not happen, hopefully. This issue can be mitigated by computing the residual ratio after more iterations, at the cost of it being more computationally expensive.

5.1 Modelling the problem as a reinforcement learning problem

We are interested in using reinforcement learning to solve the above problem. The last chapter provided an overview of the elements of reinforcement learning, and we can now translate our problem in a RL setting.

Modelling the states

We start by modelling the states. The most natural way of defining the states is to use the problem parameters b and n. We thus define a specific state as a pair of problem parameters $s = (b, n) \in [0, 1] \times \mathbb{N}^*$.

Modelling the actions and the policy

Once we know a specific state, that is the problem parameters, we need to choose the two solver parameters Δt and α. A specific action is then a pair $a = (\Delta t, \alpha) \in \mathbb{R}^+ \times [0, 1]$. The policy is then denoted by $\pi(a = (\Delta t, \alpha)|s = (b, n))$. We will discuss the policy more in depth in the next chapter.

Modelling the rewards

Once a state-action pair is chosen, the residual ratio $\rho_{10,b,n}(\Delta t, \alpha)$ is computed. The reward can then be defined as a function of the computed residual ratio,

$$r = 1 - \rho_{10,b,n}(\Delta t, \alpha).$$

This reward is positive when the residual ratio is less than one, and negative otherwise. This mean that a reinforcement learning agent, which seek to maximize the reward it gets, will aim to minimize the residual ratio.

State transitions

In the definition of a Markov decision process (Definition 4.1), we also have a probabilistic model of the state and rewards transition $p(s', r|s, a)$. Right away, we can see that this model is difficult to define, as we can not now, for a specific state and action, what reward we will get.

On the other hand, we can still control the state transitions. In this regard, we choose a new state, at random, after an action and reward is computed. More precisely, we choose a new parameter b, uniformly between 0 and 1, and a new parameter n, between 5 and 200, following a discrete uniform distribution as well. These values for n are arbitrary, with a maximum of 200 to spare us of long computational time when computing the rewards. We also cap the minimum value of n to an arbitrary minimum of 5 as those values are simply too low to get a acceptable discretization error, and we do not want to train an agent to solve for these states.

Other challenges

There are still several challenges that need to be addressed:

- In our problem, the State-Action space is continuous. We previously assumed finite spaces.
- In the definition of a MDP, we have a model: if we know a specific state and action, we have a probabilistic model of the reward the agent get and the next state of the environment. In our case, we know the model the state transitions, but we have no way of knowing the rewards.

5.2 Dealing with a large state-action space.

In the last chapter, we made the assumption that every space, be it state, action, or reward is finite. This assumption, while practical to derive theoretical results from, is in practice not always followed, as some states may be continuously defined for example.

We take our problem as formulated before. The state is defined as the problem parameters, that is $b \in [0, 1]$ and $n = 1, 2, ...$ Without any adjustment, the state space is of the form $[0, 1] \times \mathbb{N}$, and is not finite.

Similarly, the policy is defined by choosing the values $(\alpha, \Delta t) \in [0, 1] \times \mathbb{R}^+$, depending on the state. Once again, the action space is continuous.

One approach would be to discretize the entire state $\times$ action space, and then to apply classical dynamic programming algorithms to get some results. Then, after an optimal policy is found, do some form of interpolation for problem parameters outside of the discretized space. This approach has its own merit, as there are 3 dimensions that need to be discretized, and n can be chosen within a finite range.

Another approach is to use an approximation function. One way to do that is to approximate the value function $v(s)$ by some parametrization $v(s) \approx \hat{v}(s, \omega)$ where $\omega \in \mathbb{R}^d$ are d parameters. Such methods are called *value based*. The method we use in this thesis, on the other hand, use an approximation of the policy function defined as $\pi(a|s, \boldsymbol{\theta})$, where $\boldsymbol{\theta} \in \mathbb{R}^d$ is a parameter vector. Such methods are called *policy based*. The reason to chose from this class of algorithm is two-fold.

- When thinking about the test problem, a straightforward approach is to choose the solver parameters as a linear function of the problem parameters. A policy based approach allow us to do exactly this.
- By doing so, we automatically take care of the need to interpolate between discrete states and action, which would be another headache we would have to deal with.

Remark. Approximation is usually done using neural networks. In the case of this thesis, a linear approximation is used.

5.3 Model-based, model-free

One problem we are faced with is the issue of the model of the state and rewards transition, that is

$$p(s', r|s, a) = \Pr(S_{t+1} = s', R_{t+1} = a|S_t = s, A_t = a).$$

Thankfully, we are dealing with random variables, and with random variables, Monte-Carlo methods follow.

In particular, we often only need to compute the expectations of functions of random variables. This can be done is the following way. Let X be a random variable and $x_1, x_2, ..., x_n$ be independent samples of X. Then, we can estimate $E[X]$ as the empirical mean of our samples, that is:

$$\hat{X}_n = \frac{x_1 + \cdots + x_n}{n}.$$

5.4 Policy gradient methods

5.4.1 Objective function

Let $\boldsymbol{\theta} \in \mathbb{R}^d$ be a parameter vector and $\pi(a|s, \boldsymbol{\theta}) = p(A_t = a|S_t = s, \boldsymbol{\theta})$ an approximate policy that is derivable w.r.t θ. We want to define an objective function $J(\boldsymbol{\theta})$ that we want to maximize in order to find the best value of $\boldsymbol{\theta}$.

To this end, we make the following assumption, the first one being for simplicity, and the second one being specific to the problem we modelled in the former sections in this chapter.

- The states and action set are finite.
- The states are uniformly distributed, and so are the state transitions. That is, for any $s, s' \in \mathcal{S}, \Pr(S_t = s) = 1/|\mathcal{S}| = \Pr(S_t = s|S_{t-1} = s')$, where $|\mathcal{S}|$ is the number of element of S. This correspond to the idea of taking a new state at random in our problem.

We define the objective function

$$J(\boldsymbol{\theta}) = \overline{v_\pi(S)} = \frac{1}{|\mathcal{S}|} \sum_{s \in S} v_\pi(s). \tag{5.2}$$

That is, $J(\boldsymbol{\theta})$ is the average, (non weighted, as per assumption) state value.

We want to maximize this objective function by changing the policy parameter θ. To this end, we use a gradient ascent algorithm of the form

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}), \tag{5.3}$$

where $\nabla_{\boldsymbol{\theta}}$ represents the gradient operator, w.r.t $\boldsymbol{\theta}$. This gradient is

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{|\mathcal{S}|} \sum_{s \in S} \nabla_{\boldsymbol{\theta}} v_\pi(s). \tag{5.4}$$

We are faced with the immediate issue that the algorithm requires knowing this gradient.

5.4.2 Policy gradient theorem

We prove, using the aforementioned assumptions a specific case of the policy gradient theorem. This proof is adapted from [8],chap 13.2. We also remind the reader that both the state values and the action values depend on the policy π and thus depend on $\boldsymbol{\theta}$.

From the last chapter, we have the expression of the state values

$$v_\pi(s) = \sum_{a \in \mathcal{A}} \pi(a|s, \boldsymbol{\theta}) q_\pi(a, s).$$

We take the gradient of $v_\pi(s)$ w.r.t θ to get

$$\nabla_{\boldsymbol{\theta}} v_\pi(s) = \sum_{a \in \mathcal{A}} \nabla_{\boldsymbol{\theta}} \pi(a|s, \boldsymbol{\theta}) q_\pi(a, s) + \pi(a|s, \boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} q_\pi(a, s). \tag{5.5}$$

We now turn our attention to the $\nabla q_\pi(a, s)$ term above. We use the expression of the actions value in Equation 4.6,

$$\nabla_{\boldsymbol{\theta}} q_\pi(a, s) = \nabla_{\boldsymbol{\theta}} \left[\sum_r \sum_{s'} p(s', r|s, a)(r + \gamma v_\pi(s')) \right].$$

Both $p(s', r|s, a)$ and the reward r do not depend on the policy, and therefore not on $\boldsymbol{\theta}$. The gradient is thus

$$\nabla_{\boldsymbol{\theta}} q_\pi(a,s) = \gamma \sum_{s'} \left[\sum_r p(s', r|a, s) \right] \nabla_{\boldsymbol{\theta}} v_\pi(s').$$

By the assumption of the state transition probabilities and the law of total probabilities $\sum_r p(s', r|a, s) = 1/|\mathcal{S}|$, and thus

$$\nabla q_\pi(a,s) = \gamma \sum_{s'} \frac{1}{|\mathcal{S}|} \nabla v_\pi(s').$$

We recognize the expression of the objective function's gradient $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ to get $\nabla_{\boldsymbol{\theta}} q_\pi(a,s) = \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$. We insert this in Equation 5.5 and we get

$$\nabla_{\boldsymbol{\theta}} v_\pi(s) = \sum_{a \in \mathcal{A}} \nabla_{\boldsymbol{\theta}} \pi(a|s, \boldsymbol{\theta}) q_\pi(a,s) + \gamma \pi(a|s, \boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}).$$

Since the policy $\pi(a|s)$ is a probability over the action space, it sums to 1 and we can get the second part of the RHS out of the sum

$$\nabla_{\boldsymbol{\theta}} v_\pi(s) = \gamma J(\boldsymbol{\theta}) + \sum_{a \in \mathcal{A}} \nabla_{\boldsymbol{\theta}} \pi(a|s, \boldsymbol{\theta}) q_\pi(a,s).$$

Using $\nabla J(\boldsymbol{\theta}) = \frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \nabla_{\boldsymbol{\theta}} v_\pi(s)$, we get

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \left[\gamma J(\boldsymbol{\theta}) + \sum_{a \in \mathcal{A}} \nabla_{\boldsymbol{\theta}} \pi(a|s, \boldsymbol{\theta}) q_\pi(a,s) \right], \tag{5.6}$$

$$= \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) + \sum_{s \in \mathcal{S}} \frac{1}{|\mathcal{S}|} \sum_{a \in \mathcal{A}} \nabla_{\boldsymbol{\theta}} \pi(a|s, \boldsymbol{\theta}) q_\pi(a,s). \tag{5.7}$$

And after a small rearrangement of the terms,

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{1-\gamma} \sum_{s \in \mathcal{S}} \frac{1}{|\mathcal{S}|} \sum_{a \in \mathcal{A}} \nabla \pi(a|s, \boldsymbol{\theta}) q_\pi(a,s, \boldsymbol{\theta}).$$

This is a special case of the policy gradient theorem. The reason to put the fraction $1/|\mathcal{S}|$ inside the first sum is to get a parallel with the more general expression, where in general, we have a weighted sum with different weight depending on the state. Depending on the objective function used, this can be for example the stationary distribution of the states for a given policy.

We state the policy gradient theorem in a more general form.

Theorem 5.1. ***Policy gradient theorem*** *(For continuing cases, with discount factor $\gamma < 1$.)*

Let $\pi(a|s, \boldsymbol{\theta})$ be a stochastic policy that is derivable w.r.t $\boldsymbol{\theta}$.

Let $\mu(s)$ be the probability mass function of the stationary distribution of the states, following the policy π.

Define the objective function $J(\boldsymbol{\theta}) = \overline{v_\pi(S)} = \sum_{s \in \mathcal{S}} \mu(s) v_\pi(s)$. The gradient of J w.r.t $\boldsymbol{\theta}$ is then proportional to the weighted sum

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \propto \sum_s \mu(s) \sum_a q_\pi(a, s, \boldsymbol{\theta}) \nabla \pi(a|s, \boldsymbol{\theta}).$$

Remark. With our assumptions $\mu(s) = \frac{1}{|S|}$. A proper treatment of the problem would involve properly defining Markov chains and stationary distributions, which is out of the scope of this thesis. We've seen in example Example 4.1 that the state transition matrix P_π appears. This relation between Markov chains and MDP is explored in [19], as well as the policy gradient theorem. For more information on Markov chains, see [22].

The policy gradient theorem is powerful in the sense that we can derive the gradient of the objective function, something that is tied to the environment, to establishing the gradient of the parametrized policy function, which we have more control over.

5.4.3 REINFORCE algorithm

Here, we introduce reinforce the classic REINFORCE algorithm [10]. Even with the policy gradient theorem, we are still faced with the problem of estimating the action values q_π. We remark that the formula in the policy gradient is an expectation,

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \propto E\left[\sum_a q_\pi(a, S) \nabla \pi(a|S, \boldsymbol{\theta})\right],$$

where S is the random variable given by the probability mass function $\mu(s)$. By using the identity $\frac{\nabla f}{f} = \nabla \ln f$, we can also rewrite the inner term as

$$\sum_a q_\pi(a, S) \nabla_{\boldsymbol{\theta}} \pi(a|S, \boldsymbol{\theta}) = \sum_a \pi(a|S) q_\pi(a, S) \nabla_{\boldsymbol{\theta}} \ln \pi(a|S, \boldsymbol{\theta}),$$

which is also an expectation, and thus

$$\nabla J(\theta) \propto E\left[q_\pi(A, S) \nabla_{\boldsymbol{\theta}} \ln \pi(A|S, \boldsymbol{\theta})\right].$$

We also know from before that the action value is also the conditional expectation of the return $q_\pi(s, a) = E[G_t | S_t = s, A_t = a]$. Thus,

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \propto E\left[G_t \nabla \ln \pi(A_t|S_t, \boldsymbol{\theta})\right]. \tag{5.8}$$

Note that the variable t has been introduced Since this is an expectation, we can estimate it by using samples. Retracing our steps, the k'th sample, which we note as e_k have to be chosen as follow.

- Chose a state $S_0 = s$ at random, following its stationary distribution.
- Chose an action $A_0 = a$ according to the policy $\pi(A_0 = a|S_0 = s, \boldsymbol{\theta})$.
- Compute the log policy gradient. Then, get the return $G_0 = g$ for the state-action pair (s, a). The sample is then $e_k = g \nabla_{\boldsymbol{\theta}} \ln \pi(a|s, \boldsymbol{\theta})$.

Then, the estimator for the RHS in Equation 5.8 is given by

$$\hat{E}_n = \frac{1}{n} \sum_{k=1}^{n} e_k,$$

where n is the number of samples we have. Using a gradient ascent algorithm, we can update the parameters $\boldsymbol{\theta}$,

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \alpha \frac{1}{n} \sum_{k=1}^{n} e_k.$$

This method has three problems:

- The states need to be chosen according to the stationary distribution $\mu(s)$, which is not trivial. Thankfully, with our assumption of random state transitions, $\mu(s) = \frac{1}{|\mathcal{S}|}$.
- To get each sample e_k, we need to compute a return. Doing so, we end up visiting a lot of different states and gathering a lot of information that we end up discarding. This issue is an issue of low sample efficiency and is usually best handled via temporal difference based methods, where one estimate the returns after a finite number of steps. These methods are out of scope of the thesis.
- For continuing cases(where the are no final states), the return is an infinite sum of random variable, which we can not sample. We will have to stop after τ transitions and use the estimate $G_t \approx \sum_{t=0}^{\tau} \gamma^t R_{t+1}$. This introduces some bias, in particular when $\gamma \approx 1$ and τ is small. Once again, this can be resolved by temporal difference based methods.

Let us forget about the truncations issues for now. When we sample the expectation in Equation 5.8, we get a trajectory

$$s_0, a_0 \to s_1, a_1 \to s_2, a_2 \dots .$$

Then, we can estimate, via Monte Carlo estimation, the return G_0. Doing this, we also have access to the trajectory

$$s_1, a_1 \to s_2, a_2 \dots ,$$

and thus we can also estimate the return G_1! Therefore, we can use a single episode to estimate multiple samples! Using this idea, we can generate an episode of length $\tau + 1$:

$$s_0, a_0 \to s_1, a_1, r_1 \to s_2, a_2, r_2 \to \dots \to s_{\tau+1}, r_{\tau+1}.$$

For any $t = 0, \dots, T$, the estimated return is then defined as

$$\hat{G}_t = \sum_{k=t}^{\tau} \gamma^{t-k} r_{k+1}.$$

Remark. Because the initial state is chosen following a stationary distribution, we also ensure that the subsequent states are chosen following this same distribution.

We can now state the REINFORCE algorithm [10], also called policy gradient Monte-Carlo in pseudo code format:

REINFORCE algorithm pseudocode
INPUT:
- A parameter vector $\boldsymbol{\theta} \in \mathbb{R}^d$, and a parametrized policy $\pi(a|s, \boldsymbol{\theta})$ with computable gradient $\nabla_{\boldsymbol{\theta}} \pi(a|s, \boldsymbol{\theta})$;
- Learning rate α;

- Discount rate γ;
- Episode length $\tau + 1$;
- Number of episode to iterate for n;

OUTPUT: The updated parameter $\boldsymbol{\theta}$;

FOR n episodes:

Generate an episode, following $\pi(a|s, \boldsymbol{\theta})$, of length T+2 the form $s_0, a_0 \to s_1, a_1, r_1 \to s_2, a_2, r_2 \to ... \to s_{\tau+1}, r_{\tau+1}$;

FOR t=0 ... :

Compute the estimated return $\hat{G}_t = \sum_{k=t}^{\tau} \gamma^{t-k} r_{k+1}$;

Compute the log gradient $\nabla \ln \pi(a_t|s_t, \theta)$;

Update $\theta \leftarrow \theta + \alpha \hat{G}_t \nabla \ln \pi(a_t|s_t, \boldsymbol{\theta})$;

Remark. Because of the finite episode length, the REINFORCE algorithm is more suited for episodic tasks, but it is also usable for continuing tasks, if we accept some bias. Another alternative to reduce bias would be to discard the last few estimated returns $\hat{G}_\tau, \hat{G}_{\tau-1}, ...$ as they are the most biased.

The REINFORCE update can be interpreted as updating the parameters to make it more likely to take an action if the estimated sample return is good, and the opposite otherwise. Furthermore, by looking at the term $\nabla \ln \pi = \frac{\nabla \pi}{\pi}$, we can see that if the probability of taking the action is low, then the gradient becomes bigger! That way, this gradient act as a balance between exploration and exploitation. Otherwise we would update the parameters as much for a rare action than a common one, and the common action is taken more often which lead to the common action having much more sway in the process.

Chapter 6

Implementation

6.1 A linear approximation of the policy

We have now defined policy gradient methods as a way to address two issues that happened when we translated the problem as defined in the beginning of the last chapter. These issues being the need for a model free method, and dealing with large, and even infinite state and action set.

We need to define a policy of the form $\pi(a|s,\boldsymbol{\theta})$, where $a = (\Delta t, \alpha)$ is the action of choosing the solver parameters, given a pair of problem parameters, that is some state, $s = (b, n)$. We choose to have a policy of the form $(\Delta t, \alpha) \approx A(b,n)^\top + c$, where A is a two by two matrix and c a 2-vector. Furthermore, this policy need to be stochastic for the REINFORCE algorithm to work.

We remark that the action space is, in our case, continuous, so the policy has to be over a continuous action space. In the discrete case, the policy is $\pi(a|s,\boldsymbol{\theta})$ is a probability mass function, so that $\sum_a \pi(a|s,\boldsymbol{\theta}) = 1$. We extend it to continuous action space by considering π as a probability density function instead, and replacing the sum by an integral, that is $\int_{a\in\mathcal{A}} \pi(a|s,\boldsymbol{\theta}) = 1$[23].

Let s be a given state, $s = (b, n)$. We first define the values μ_α and $\mu_{\Delta t}$,

$$\begin{pmatrix} \mu_\alpha \\ \mu_{\Delta t} \end{pmatrix} = \begin{pmatrix} \theta_0 & \theta_1 \\ \theta_2 & \theta_3 \end{pmatrix} \begin{pmatrix} b \\ n \end{pmatrix} + \begin{pmatrix} \theta_4 \\ \theta_5 \end{pmatrix}. \tag{6.1}$$

where $\boldsymbol{\theta} = (\theta_0, \theta_1, \dots, \theta_5)^\top \in \mathbb{R}^6$. μ_α and μ_{Δ_t} can be regarded as "the deterministic policy". Around this deterministic policy, we add some noise, specifically Gaussian noise to get the stochastic policy

$$\alpha \sim \mathcal{N}(\mu_\alpha, \sigma^2),$$

and independently,

$$\Delta t \sim \mathcal{N}(\mu_{\Delta t}, \sigma^2).$$

Here $\mathcal{N}(\mu, \sigma^2)$ is the normal distribution, with mean μ and standard deviation σ, and we choose σ fixed in this thesis. We thus have a policy of the Since α and Δt are chosen independently, the joint probability density of both parameters is the product of both marginal probability density function, that is

$$\pi(a = (\Delta t, \alpha)|s, \boldsymbol{\theta}) = f_1(\alpha) \cdot f_2(\Delta t),$$

where

$$f_1(\alpha) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\alpha - \theta_0 b - \theta_1 n - \theta_4)^2}{2\sigma^2}\right),$$

and similarly,

$$f_2(\Delta t) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\Delta t - \theta_2 b - \theta_3 n - \theta_5)^2}{2\sigma^2}\right).$$

Taking the logarithm, we get $\ln(f(\alpha, \Delta t)) = \ln(f_1(\alpha)) + \ln(f_2(\Delta t))$. Thus,

$$\ln(f_1(\alpha)) = \ln(\frac{1}{\sqrt{2\pi}\sigma}) - \frac{(\alpha - \theta_0 b - \theta_1 n - \theta_4)^2}{2\sigma^2}.$$

We now take the gradient w.r.t $\boldsymbol{\theta}$ to get

$$\nabla_{\boldsymbol{\theta}} \ln(f_1(\alpha)) = \xi_\alpha (b\theta_0, n\theta_1, 0, 0, \theta_4, 0)^\top, \tag{6.2}$$

where $\xi_\alpha = \frac{(\alpha - \theta_0 b - \theta_1 n - \theta_4)}{\sigma^2}$.

Doing a similar thing with Δt, we get the gradient,

$$\nabla_{\boldsymbol{\theta}} \ln(f_2(\Delta t)) = \xi_{\Delta t} (0, 0, b\theta_2, n\theta_3, 0, \theta_5)^\top, \tag{6.3}$$

where $\xi_{\Delta t} = \frac{(\Delta t - \theta_2 b - \theta_3 n - \theta_5)}{\sigma^2}$. We now add both gradients together to get the gradient of the policy, for a specific action $a = (\alpha, \Delta t)$ and state $s = (b, n)$:

$$\nabla_{\boldsymbol{\theta}} \ln \pi(a|s, \boldsymbol{\theta}) = \xi_\alpha (b\theta_0, n\theta_1, 0, 0, \theta_4, 0)^T + \xi_{\Delta t} (0, 0, b\theta_2, n\theta_3, 0, \theta_5)^\top. \tag{6.4}$$

6.2 Implementation of the REINFORCE algorithm

Now that everything has been defined, the REINFORCE algorithm can be applied to find an optimal policy.

6.2.1 Algorithm code

We present in this section the full training in a pseudo code format. The full code is written in a more modular way, and is available on the appendix, as well as on GitHub.

```
##Doesn't run, as it needs other functions
##but is a good bridge between pseudocode and the
##full code
learning_rate = 1e-8
gamma = 0 #Discount factor
initial_theta = [0,0,0,0,0.3,2] #Good enough theta
sigma = 0.1 #Standard dev for the policy
number_of_episodes = 1000
episode_length = 20
```

```
for i in range(number_of_episodes):
    #Generate an episode
    #Choose an initial starting state, at random(uniformly)
    b , n = state_transition()
    #Create an episode object, which will have
    #The history of the trajectory
    episode = Episode(length = episode_length)
    for j in range(episode_length):
        #Get the action, according to the policy we defined before
        delta_t, alpha = get_action(b,n,sigma,theta) #pi(a|s,theta)
        #Then compute the residual ratio, after n_iter of the RK2 solver.
        res_ratio = compute_res_ratio(b,n,delta_t,alpha,n_iter = 10)
        reward = 1 - res_ratio #The lower the res ratio, the better the reward
        #Save the state action and rewards inside the episode object
        #so that we can access it later
        episode.save(b,n,alpha,delta_t,reward, position = j)
        #Then get to a new state, at random
        b , n = state_transition()
    #Now that we have an episode, we can apply REINFORCE
    #and update our policy accordingly
    for k in range(episode_length):
        #Get access to s_k, a_k, r_{k+1}
        b , n , delta_t, alpha , reward = episode.get(k)
        #Get the log likelihood of the action a_k, as in Eq 6.4
        log_lik_gradient = get_log_lik_gradient(b,n,alpha,delta_t,sigma)
        #Estimage the return Eq 5.9
        estimated_return = 0
        for l in range(k, episode_length):
            #episode.reward_hist[l] is R_{l+1}
            estimated_return += episode.reward_hist[l] * (gamma**(l-t))
        ##Update the policy
        theta = theta + learning_rate * log_lik_gradient * estimated_return
#We end up with an updated theta, that is a better policy.
```

6.2.2 A first experiment

We implement the REINFORCE algorithm to the test problem. There are a few hyperparameters to set.

- The learning rate is set to $\alpha = 1 \times 10^{-8}$.
- The discount rate is set to $\gamma = 0$, as the state transitions have no relationship with the actions taken, there is no reason to prefer long term rewards.
- Because the discount rate is so low, there is no bias added by estimating the returns at the end of the episodes. The episodes length is set to 20 as we want to use the updated policy as often as possible.
- The standard deviation of the policy parameters is set to $\sigma = 0.1$.

This leaves the choice of the initial value for $\boldsymbol{\theta}$. While it is possible for the parameters to be random, or all set to 0, we use the experiment done in chapter 4 to use. In Figure 3.2a, it seems that a policy of $\alpha = 0.3$ and $\Delta t = 2$ is a reasonable choice. Since this was done only for a single set of problem parameters, we have no idea of the relationship between problem parameters and optimal solver parameters. Therefore, we only set the parameter $\theta_4 = 0.3$, and $\theta_5 = 2$, the other parameters are set to 0.

The algorithm is run for 50000 episodes, and we observe the evolution of the parameters theta(Figure 6.1).

Since the discount rate is set to 0, in any state, the return is the instant reward received by the agent over a single episode. So, for an episode of length l, we have the rewards $r_1, r_2, \dots, r_l$. Then, we can plot the average reward $r_{av} = \frac{r_1+r_2+\cdots+r_l}{l}$ over each episode. Because the variance of r_{av} is still high, we use the rolling average of r_{av} over the last $k = 50$ episodes as a smoother.

The average reward is the no scaling reward in Figure 6.2 and is trending upward with successive episodes, which is the intended behavior of the algorithm. However, there are certain problems that have been made apparent by the two plots:

- Despite running the algorithm for a long time, some of the elements of $\boldsymbol{\theta}$ have barely changed, and it is clear that we are far from any convergence of the reward function.
- Even with smoothing, it is apparent that the method has a high variance.
- It seems that θ_1 and θ_3 vary quite a bit over time whereas the other parameters have a steady rate of change.

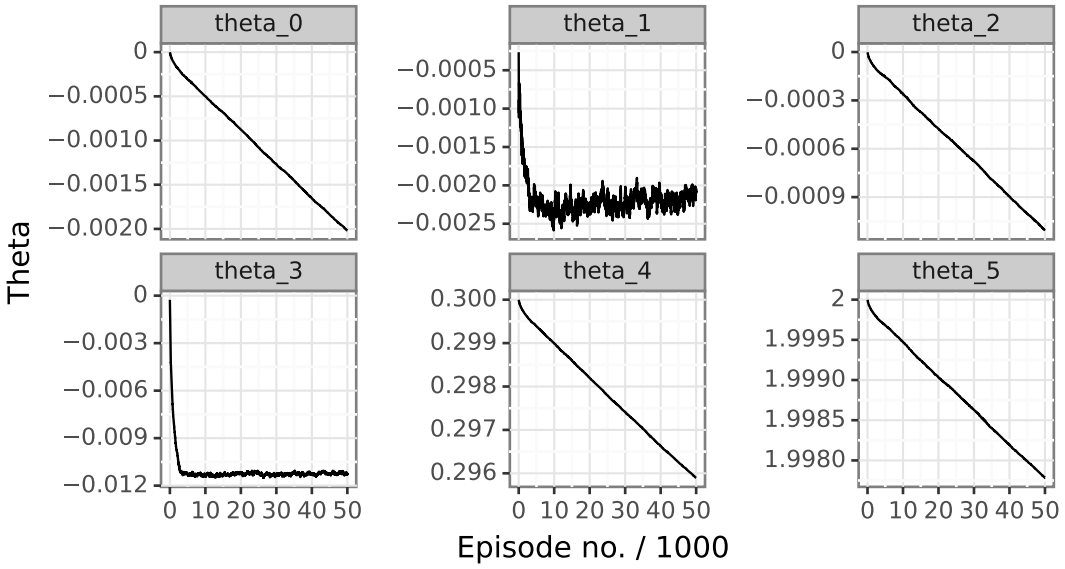


Figure 6.1: Evolution of the θ parameters in a first experiment.

The slow apparent convergence rate can not be mitigated by a higher learning rate, as this empirically leads to divergence issues.

The high variance is typical of reinforcement learning tasks, and in particular Monte Carlo based methods, which REINFORCE is a part of. That being said, there exists much better methods that can reduce this variance, at the expense of introducing some bias, such as for example actor-critics methods [8, Ch. 13.5], or proximal policy optimization (PPO) [24]. Both of these methods are not explored in this thesis.

6.3 Scaling the parameters

To address the slow convergence problem, we start with a motivating example.

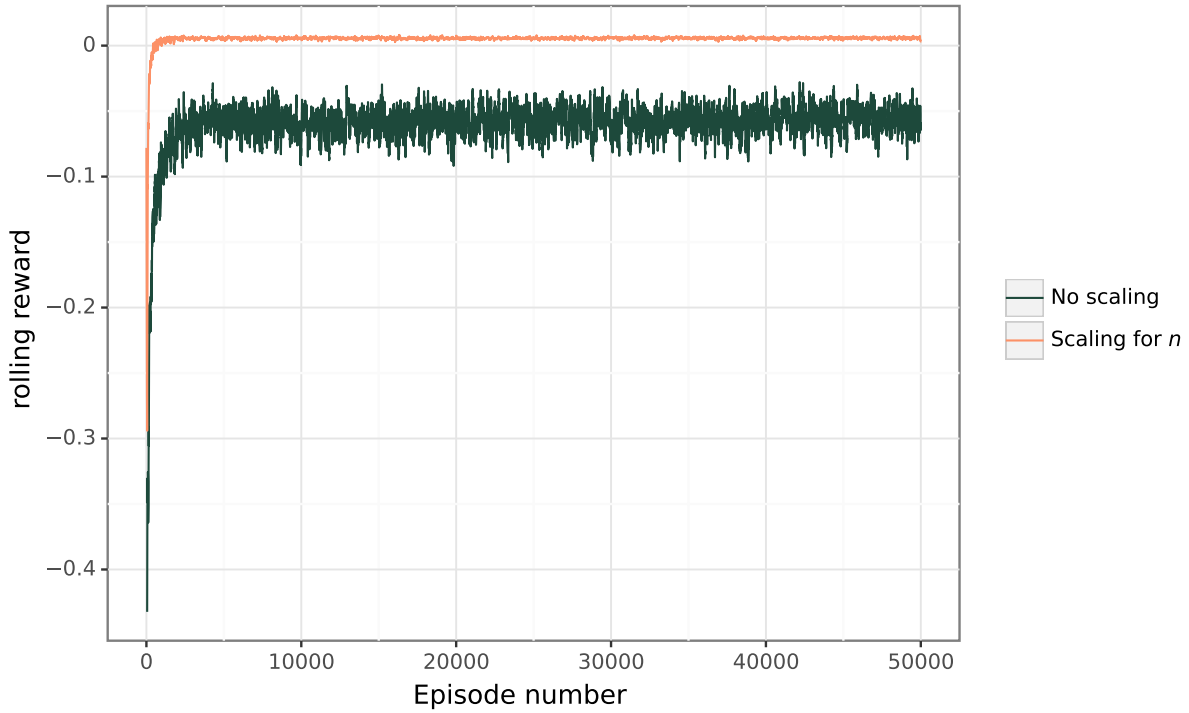


Figure 6.2: Evolution of the rolling average (k=50) of the average episode reward, with or without scaling.

6.3.1 A motivating example of gradient descent

Consider the loss function $f(x, y) = x^2 + 9y^2$. The function admits a global minimum at $x = y = 0$, and its gradient given by

$$\nabla f(x, y) = (2x, 18y)^\top.$$

Therefore, the gradient descent iteration, with learning rate $\alpha > 0$, is the iteration

$$\begin{pmatrix} x_{t+1} \\ y_{t+1} \end{pmatrix} = \begin{pmatrix} x_t \\ y_t \end{pmatrix} - \alpha \begin{pmatrix} 2x_t \\ 18y_t \end{pmatrix}.$$

That is $x_{t+1} = (1 - 2\alpha)x_t$ and $y_{t+1} = (1 - 18\alpha)y_t$. The iterates converge to $x = y = 0$ if and only if $\alpha < 1/9$. If however, $\frac{1}{9} < \alpha < 1$, we will have convergence for x, but not for y.

The reason for this is that the gradient is steeper in the y direction than the x direction, which leads to comparatively bigger change in y than x in the gradient descent iterations.

To remedy this, we can use a change of variable $z = 3y$. Then $f(x, z) = x^2 + z^2$. The gradient descent iteration is then given by

$$\begin{pmatrix} x_{t+1} \\ y_{t+1} \end{pmatrix} = \begin{pmatrix} x_t \\ y_t \end{pmatrix} - \alpha \begin{pmatrix} 2x_t \\ 2y_t \end{pmatrix}.$$

That is, $x_{t+1} = (1 - 2\alpha_x)x_t$ and $z_{t+1} = (1 - 2\alpha_y)y_t$. This converges to 0 if and only if $0 < \alpha < \frac{1}{2}$, which means we can afford a much bigger learning rate. With $\alpha = \frac{1}{2}$, the gradient descent algorithm can now converge to 0 in a single iteration!

6.3.2 Changing the variable

This section is born from an intuitive idea and is for this reason less formal than the rest. Looking at the equation for the gradient of the log policy (Equation 6.4), we notice that the gradient has a similar expression in each direction. More particularly, the gradient in the direction i is given by the partial derivative

$$\frac{\partial \ln \pi(a|s, \boldsymbol{\theta})}{\partial \theta_i} = \xi_{\alpha,\Delta t}(\_)\theta_i$$

where $\xi_{\alpha,\Delta t}$ is either ξ_α (Equation 6.2) or $\xi_{\Delta t}$ (Equation 6.3), and $(\_)$ is either:

- b in the directions θ_0 and θ_2.
- n in the directions θ_1 and θ_3.
- 1 in the directions θ_4 and θ_5.

Using the motivating example above, we've seen that it can be a good idea to rescale some variables so that the gradient is as "steep" in all directions. However, in this case, n can vary between 5 and 200, while b only varies between 0 and 1. This motivate the idea that, in order to make a gradient "as steep" in all directions.

Instead of using n directly, we now use the scaled variable

$$n' = \frac{n - 5}{200}.$$

Since n can vary between 5 and 200, n' can have values between 0 and 1, just like the values of b. Everything then follows by simply replacing n by n' in Section 6.1. The new deterministic policy is

$$\begin{pmatrix} \mu_\alpha \\ \mu_{\Delta t} \end{pmatrix} = \begin{pmatrix} \theta_0 & \theta_1 \\ \theta_2 & \theta_3 \end{pmatrix} \begin{pmatrix} b \\ n' \end{pmatrix} + \begin{pmatrix} \theta_4 \\ \theta_5 \end{pmatrix}, \tag{6.5}$$

and the equation of the gradient is unchanged, with the exception of replacing n by n' everywhere.

With this change implemented, we rerun the first experiment. All the parameters are the same, except that the learning rate can is now set to $\alpha = 2 \times 10^{-4}$ without divergence. Compared to the first experiment, the average episode reward is much better, as seen in Figure 6.2.

6.4 Impact of initial conditions

Gradient based iterations use the local information about an objective (or loss) function $J(\theta)$ to compute the update $\boldsymbol{\theta} \to \boldsymbol{\theta} \pm \alpha \nabla J(\boldsymbol{\theta})$. This local behavior also means that any convergence of gradient descent is to a local minimum, and we can't be certain that this mimimum is a global minimum.

Let us test whether the algorithm converges to the same values regardless of initial conditions. The third experiment is then to run the algorithm with the same parameters, but with varied initial conditions, and to visualize the results, both in the average rewards and the evolution of $\boldsymbol{\theta}$ over 200000 episodes.

The evolution of $\boldsymbol{\theta}$ is in Figure 6.3, and the rolling average of the average episode reward is plotted in Figure 6.4 for different initial value for $\boldsymbol{\theta}$. It turns out that while convergence in reward is to the same values, the parameter θ_3 does not seem to converge to the same value. Furthermore, even with such a large amount of episodes, it is not clear if the other parameters converged.

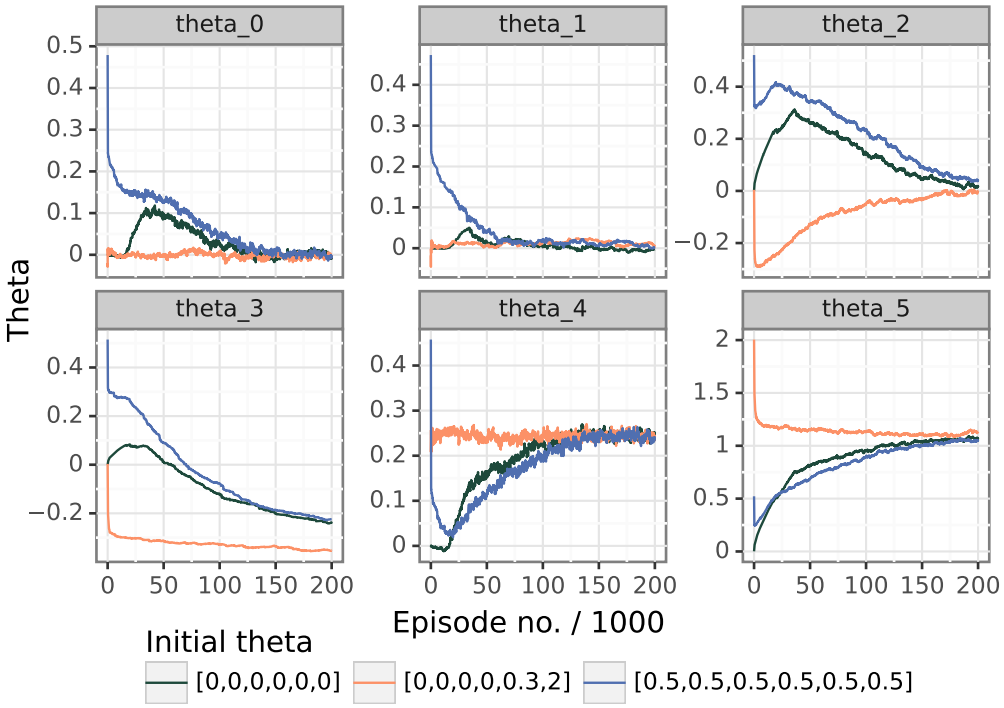


Figure 6.3: Evolution of the theta parameters with different initial parameters.

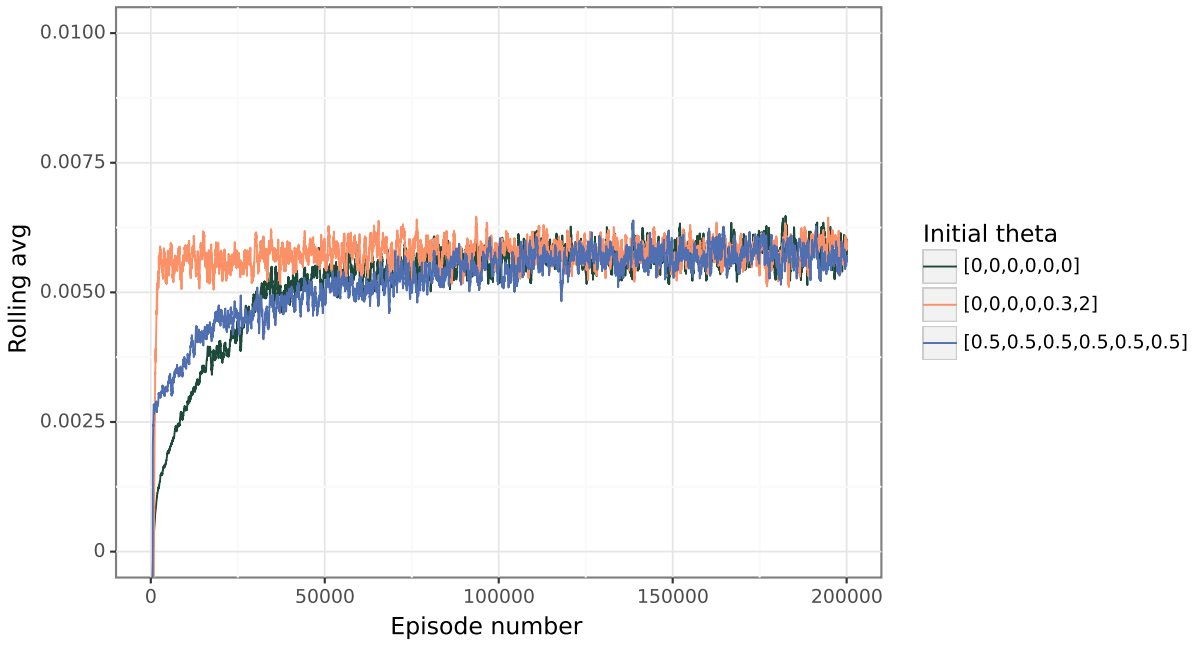


Figure 6.4: Evolution of the rolling average($k = 500$) of the average episode reward for different initial parameters.

6.5 Further results

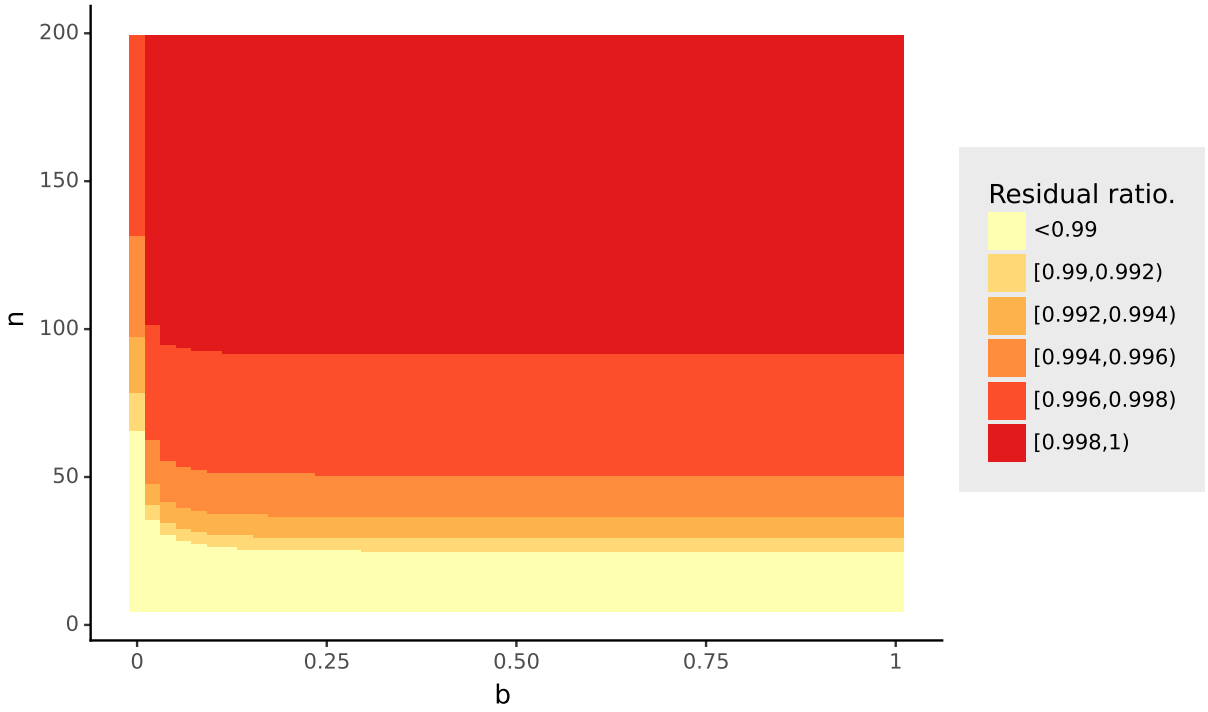
The average reward of the episode is a nice way to report on the performance of the method. However, it is difficult to interpret how the model performs once we have found some optimal parameters $\boldsymbol{\theta}^*$. In particular, by using the REINFORCE algorithm, the policy function has to be stochastic during training. The actual policy we choose can, however, be deterministic. So, at the risk of adding some bias, we remove the noise σ in the policy and choose to use the "deterministic policy" $\alpha = \mu_\alpha$, $\Delta t = \mu_{\Delta t}$, as in Equation 6.1, and we denote this policy by $\pi_d(a|s, \boldsymbol{\theta}^*)$. For the value of $\boldsymbol{\theta}^*$, we use its last value in the second experiment, which is (with some rounding off)

$$\boldsymbol{\theta}^* = (-3.606 \times 10^{-3}, 4.476 \times 10^{-3}, -3.598 \times 10^{-4}, -0.3542, 0.2435, 1.1305)^\top.$$

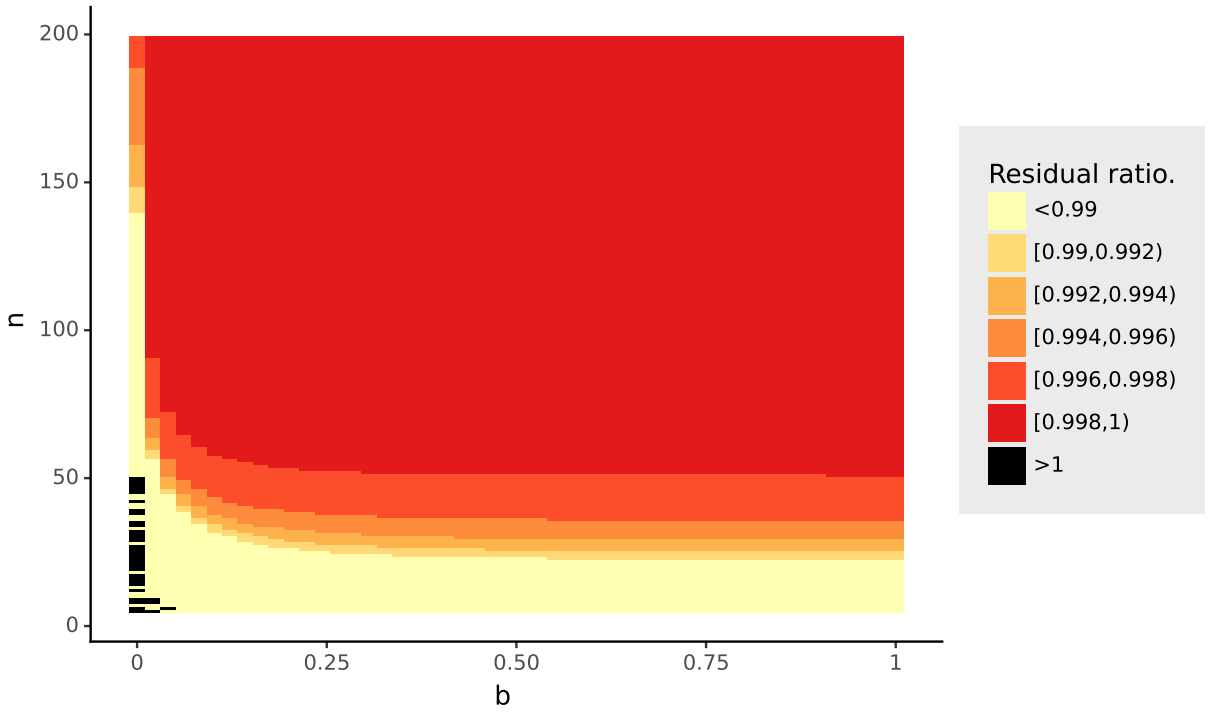
Then, we compute the value of $\rho_{10,b,n}$ using this policy and for different values of n and b, the results are as below in Figure 6.5. While we have convergence at any point, the convergence is slow, and the maximum value for ρ_{10} is 0.99917. Referring back to the grid search experiment(see Figure 3.2), this slow convergence is also partly an issue with the solver itself.

Since we trained the policy on ρ_{10}, it may be a good idea to check if the solver still converges when we compute more iterations. The result are in Figure 6.5. There are some points where the solver diverges, which is a problem in particular because the point where it diverges are for small values of b, which is often the case physically.

This divergence indicates that it may be a good idea to further train the learned policy by computing ρ_{100}, and having a reward of $1 - \rho_{100}$ instead of $1 - \rho_{10}$. This of course means that the training time will have to be longer. In that case, we can set $\boldsymbol{\theta}^*$ as a starting parameter for the policy.



(a) ρ_{10}. Maximum residual ratio: 0.99922.



(b) ρ_{100}. Note the divergence in black, for low values of b.

Figure 6.5: Evolution of the residual ratio ρ_{10} and ρ_{100}, with the learned policy, depending on the problem parameters n and b.

Chapter 7

Summary and Discussion

In this thesis, we started with the idea of using numerical differential equations solver as an iterative solver for a linear system. More specifically, we turned our attention to a specific RK method, which has two parameters to chose from, which we called the solver parameters. We also chose a specific type of linear equation which arises from the discretization of the steady state, one dimensional convection-diffusion equation. This linear equation depends on two parameters, which we called the problem parameters. The goal was then to see if we could optimize for the solver parameters, as a function of the problem parameters, to maximize the convergence rate of the method. To do that, we used reinforcement learning. In particular, we applied the classical REINFORCE algorithm to our problem. Using the implementation in this thesis, we observed that the implemented solution works, with limited results. In particular, if we use the parameter that we learn, it is possible for the solver to diverge for some problem parameters. There are some avenues to improve these results, in particular:

- On the technical front, the implemented algorithm is very elementary, and suffers from the issue of high sample variance, being a Monte Carlo method. This issue can be addressed by more better algorithms.
- The policy used was a linear function of the problem parameters. We may want to explore if choosing a policy taking into account interactions between the problem parameters, or applying some transforms to them before fitting a linear policy. It is also possible to fit a neural network to the policy.
- Possible incremental improvements can also be made. This involves for example experimenting with the reward function design, or setting a decaying learning rate to improve convergence of the RL algorithm.

At last, we need not restrict ourselves to just one type of solver. We could potentially train an intelligent agent to chose which numerical solver to use, depending on the problem.

There is on the other hand one glaring issue with the way that reinforcement learning was applied to this problem. A core philosophy of reinforcement learning is that the states, actions and rewards are all interdependent. This interdependence was absent in this thesis, with the state transition being random, no matter the action taken. While it was possible to adapt this philosophy as presented in this thesis, this somewhat hampers the utility of using reinforcement learning over other methods. In particular, one may wonder if the implementation presented here is essentially "gradient descent, with extra steps".

It is therefore preferable to change how the problem is approached. One approach could be train an agent to dynamically change the solver parameters over successive iterations for some specific set of parameters. In that case, the agent would need information about the evolution of the residual, which complicates the modeling problem. Another approach would be to make use of meta learning [25], where instead of directly finding the optimal solver parameters, we learn how to find them efficiently.

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