JUPE: JULIA™PACKAGE IMPLEMENTATION OF OPTIMIZATION ALGORITHM ANALYSIS USING LYAPUNOV FUNCTION

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ABSTRACT

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Gradient-based iterative algorithms are widely used method for solving optimization problems, with well-known applications including in the fields of machine learning and data science. Savings in computational capacity can be made if the best performing algorithm is chosen for the optimization problem being solved through algorithm analysis. JuPE, the main goal of this paper, is a Julia package that aims to provide a streamlined and simple way of performing analysis on gradient descent and two of its accelerated variants at solving a class of optimization problem using an approached based on Lyapunov functions.

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Dedication

I would like to dedicate this thesis to my family and close friends.

Acknowledgements

I would like to acknowledge...

Acronyms

FG Fast Gradient

1

Introduction to JuPE

Optimization problems can be in the broadest sense described as problems where an optimal solution is obtained using a limited amount of resources. Many problems that exist in the field of engineering and natural science can be categorized as optimization problems. For example, when mapping applications are used to navigate between two points, an algorithm tries to find the shortest path to a destination by choosing the direction of travel while under constraints such as traffic laws or avoiding road work. Gradient-based iterative algorithms are a prominant tool to solve large optimization problems. Their ability to efficiently optimize functions without requiring an explicit formula means they are extensively used in fields such as machine learning and data science. As the term encompasses many algorithms, each can solve any of the many types of optimization problems with varying levels of speed and accuracy, making it very useful the ability to compare algorithms on specified metrics and identifying the one best suited for a problem. But while these algorithms are widely used, their analysis have only been available to those with an in depth knowledge of the underlying math until recently [1]. The main work of this thesis presents a tool for analysis of gradient-based algorithms' performance characteristics accessible to non-experts.

JuPE (Julia Performance Estimation) is a computer program written in the Julia programming language that automatically and systemically finds the worst-case performance guarantee of an algorithm at solving a specified set of problem. After the program is given a class of functions, the algorithm to be analyzed and the performance metrics, it returns a guarantee speed at which the algorithm inputted can solve any function in the provided set.

1.1 Optimization problems and algorithms

In this paper, the optimization problem considered is in the form of finding the minimum point of a continuously differentiable function:

$$\text{minimize} \quad f(x) \tag{1.1a}$$

$$\text{subject to} \quad x \in X \tag{1.1b}$$

Where $f(x)$ is the optimization function and X is a constraint set. Here, x is the input and $f(x)$ is a measure of how close a solution is to being optimal. Well-known examples of this problem are large language models (LLMs) such as ChatGPT and machine learning models that enable self-driving features in automotives, amongst many others. These models are only possible due to the minimizing of loss functions, a fundamental part of their training where a function is used to quantify the dissimilarity between a model's output and the target values, and the model's parameters are modified iteratively in order to minimize the function and improve the model's performance.

While the minimum of any function can be found by traversing it, for large-scale and complex problems, it is more efficient to be optimize numerically using iterative gradient-based algorithms. These algorithms minimize a function by starting at an initial point and iteratively updating it using the gradient of the function at the last iteration until it reaches a local minimum. For example, the gradient descent (GD) algorithm updates x_k following this formula:

$$x_{k+1} = x_k - \alpha \nabla f(x_k) \tag{1.2}$$

Where x_0 is the initial point, k is the current iteration number, $\nabla\ f(x_k)$ is the gradient of f at the current point x_k, and α is the step size. Following this update formula, in each iteration, x moves toward the goal x_*

As an adjustable parameter of the algorithm, α can affect the speed at which the algorithm converges, or whether it converges at all: If α is too small, the algorithm will have to run many iteration before reaching the minimum, but if α is too big, overshooting can occur where the iterations oscillates on either sides of the minimum without converging. Accelerated algorithms exist that seek to solve the problem of overshooting, such as Polyak's Heavy Ball (HB) method which introduces a momentum that incorporates previous iterations of x:

$$x_{k+1} = x_k - \alpha \nabla f(x_k) + \beta(x_k - x_{k-1}) \tag{1.3}$$

Another algorithm that tries to solve GD's shortcomings is Nesterov's Fast Gradient (FG), which updates by evaluating the gradient at an interpolated point:

$$x_{k+1} = x_k - \alpha \nabla f(y_k), \tag{1.4a}$$

$$y_{k+1} = x_{k+1} + \beta(x_{k+1} - x_k) \tag{1.4b}$$

1.2 Algorithm analysis

Let us consider the problem of minimizing a simple quadratic function:

$$f(x) = x^2/2 - 3 * x + 4 \tag{1.5}$$

Using (GD) and equation 1.2, substituting step size α with values 0.2, 0.5, and 2, and picking a starting point of x_0. By solving the problem with each variant of the algorithm and counting the number of iterations each runs for before reaching within 0.001 of the true minimum, we can measure the iteration complexity:

It can be seen how different tunings on the same algorithm can achieve drastically different speed and accuracy optimizing a function, or whether it can solve for the minimum at all. Considering there exist many other first order methods in addition to the three in 1.1, each infinitely adjustable by changing the step size or by changing the number of past iterations used, being able to predict how an algorithm will perform before solving an optimization problem can mean a more accurate solution can be found and in fewer iterations. And while the example is of a simple function where overshoot can easily be identified and the number of iteration needed to find the minimum is small, the benefit of using an optimal algorithm only increases as the problem gets bigger and more complex. Looking again at the example of training large language and self-driving models, as more training data is available, the training process which has been going on for years will need to continue for many more, all of which consumes vast amounts of computational power. As a result, even a small improvement in the performance of the algorithm used can lead to large savings in time and energy.

Considering the quadratic function example, while it yielded an analysis of the algorithms' performance, it required solving the optimization problem. Not only would this be computationally costly for any problem large enough to warrant being optimized numerically in the first place, any benefit finding an algorithm better at solving that problem is negated as the problem has already been solved. Additionally, any analysis result is applicable only

to one function and cannot be reliably used to derive a first-order method's performance on any other problem.

Due to these limitations, it is more efficient to analyze algorithms' performance at solving a broader set of problem. As a result of their widespread application, popular iterative gradient-based algorithms have been extensively analyzed. For example, [2] presents the Adam algorithm and compared its performance to that of its peers by conducting experiments and drawing conclusions based on emperical evidence. While this approach can provide useful insights into how an algorithm performs, there exists other approaches toward analyzing algorithms such as [3], [4], and [5] that aim to find a mathematically provable performance guarantee of an algorithm over a class of functions. This worst-case guarantee is how JuPE perform analysis and will be refered to in this paper as algorithm analysis: Given that a characteristic that a set of functions might share (such as being convex or quadratic), algorithm analysis would return the worst-case performance measure that guarantee the algorithm analyzed would perform as good or better solving every function within said set.

1.3 Julia programming language

JuPE is written in the Julia programming language, a high-level programming language designed specifically for high-performance numerical computing. Julia's compiler performance has been benchmarked to be faster than many other languages used for numerical computing while rivalling C, a language often used for its high efficiency [6]. Julia accomplishes this while being a high-level language with simple syntax rules that resembles existing popular languages, making it easy to code with and to understand.

Julia was also chosen as it is designed for numerical computing, supporting matrices as well as UTF-8 encoding, making it possible to use scientific notation: variables and functions as they exist in the code and as the user inputs them into the program can use math symbols or Greek letters. This makes Julia excel at communicating mathematical concepts, which simplifies both the process of coding the program and understanding its mathematical underpinnings.

Julia was also chosen as it is open-source and available for free. As JuPE is a package designed for expert and novice users alike to install and use, it made sense to choose Julia as it available on many of the popular platforms such as macOS, Windows, and Linux.

1.4 Overview

JuPE performs worst-case algorithm analysis when three main inputs are provided: The class of functions in question, the algorithm being analyzed, and a performance measure. The package then performs the algorithm analysis and returns the fastest guaranteed convergence rate.

Users can pick from one of the algorithms provided in the package or create their own iterative first-order algorithm by specifying how it is updated. The class of functions can be provided by detailing the characteristic of the set, such as 1 strong 10 smooth convex function. Users can specify a performance measure, which can be how far the iterate x_k is from the goal x_* or any quadratic combinations of the iterates. Throughout the process, the user never has to change the code of the package or understand how JuPE works, making it an easy to use black box tool.

In the next chapters, we will 1) discuss the mathematical approach that JuPE utilize, 2) break down the code structure of the program and how it functions, and 3) show some of the analysis that the package has done.

2

Literature Review

Substantial literature has been published that aim to evaluate and compare the performance of algorithms using emperical evidiencce. In [2], a frequently cited paper, the author designed and conducted experiments where metrics such as cost per iteration of commonly used algorithms are recorded. The result gives a general idea of different algorithms' characteristic solving different problems.

There exist in the literature many approaches to deriving a performance bound of first-order optimization algorithms. In 2014, Drori and Teboulle first introduced the method of representing a class of function with constraints, reformulating the problem of analyzing an optimization method into a semidefinite program (SDP) whose size is proportionate with the number of iterations the algorithm is run. [3]. The paper coined the term Performance Estimation Problem (PEP) and showed that by solving convex semidefinite problem, a worst-case numerical bound on an algorithm's performance solving that class of function can be derived. Taylor, Hendrickx and Glineur built upon this work by introducing the ideas of creating a finite representation for a class of smooth strongly convex functions using closed-form necessary and sufficient conditions. While the above mentioned two approaches give the performance bound in the form of a guarantee how close x_k is to the goal x_* after a fixed number of iterates, the method used in this package proves that the performance measure inputted by the users decreases at a guaranteed rate throught out the optimizing process.

IQCs here

Of the methodologies above, PEP has been implemented into a computer program in PESTO, a MATLAB toolbox and PEPit, a Python package. The program when given a first-order method, a class of function, a performance measure, and an initial condition, will find the worst-case performance automatically. PESTO and PEPit follows the PEP methodology and presented an easy way to analyze gradient-based algorithms.

The main contribution of this thesis paper is to create an alternative computer program similar PESTO and PEPit that aims to provide an accessible and fast way to analyze the performance of first-order methods for a guaranteed convergence rate, leveraging the approach presented in [7], in the Julia programming language.

3

Lyapunov-based approach

JuPE performs algorithm analysis by using the technique layed out by Van Scoy and Lessard in [7]. While JuPE is a blackbox tool, understanding the mathematical approach on which it is based is prequisite to understanding the package's code and functionalities.

The steps of this technique, which will be discussed in detail over the sections of this chapter, consists of 1) viewing the algorithm as a Lur'e problem, 2) Replacing the nonlinear gradient with interpolation conditions that represent the class of smooth strongly convex functions, 3) Use lifting matrices to tighten to the interpolation condition representations, and 4) Prove whether a convergence rate is guaranteed by solving a convex semidefinte program.

3.1 Iterative algorithms as Lur'e problems

The first step in the technique is to view optimization algorithms from a control theory perspective: As iterative gradient-based algorithms uses the gradient of the function to update x, they can be reformulated into a linear time-invariant (LTI) system (how the algorithm update) in feedback with a static nonlinearity (the gradient of f) at point x. Using a block diagram, the algorithm can be seen as:

Here, G represents the LTI system, while y and u are input and output of the gradient nonlinearity. For example, (FG) equation 1.4 can be rewritten to match this view as:

$$x_{k+1} = x_k - \alpha u_k, \tag{3.1a}$$

$$y_{k+1} = x_{k+1} + \beta(x_{k+1} - x_k), , \tag{3.1b}$$

$$u_k = \nabla f(y_k) \tag{3.1c}$$

The algorithm can then be put into state-space representation as:

$$\xi_{k+1} = \begin{bmatrix} (1+\beta) & -\beta \\ 1 & 0 \end{bmatrix} \xi_k + \begin{bmatrix} -\alpha \\ 0 \end{bmatrix} u_k, \tag{3.2a}$$

$$y_k = \begin{bmatrix} 1+\beta & \beta \end{bmatrix} \xi_k, , \tag{3.2b}$$

$$u_k = \nabla f(y_k) \tag{3.2c}$$

The LTI system G can be expressed with four matrices that change in value depending on the algorithm and size depending on the number of past states used to update x. For (GD), (FG), and (HB) as they are described in 1.1, these matrices are:

Beyond the three listed examples, this step can be applied to any other first order methods. Deriving an LTI system represented by matrices out of an algorithm not only creates a representation easy to understand and operate on, but also in next sections enable the representation of the past states of an algorithm and the forming of a Lyapunov function that will guarantee a convergence rate.

3.2 Interpolation condition

For the remainder of this paper, we will focus on the only class of function currently supported by JuPE, m strong L smooth convex function $f \in F_{m,L}$.

In the field of robust control theory utilized by this Lyapunov-based approach, while an LTI system is relatively simple, the nonlinearity representing the gradient of the function cannot be efficiently solved. As a result, our approach replaces the nonlinearity with a set of conditions on its input and output, which provides necessary and sufficient conditions under which there exists a function $f \in F_{m,L}$ that interpolates a given finite set of argument-function value-gradient triplets. These interpolation conditions depends on the characteristics of the function class and was first formulated in [4] and reformatted in [7]:
Theorem 1 ([4], Thm. 4; [7], Thm. 3)**.** Given index set I, a set of triplets $(y_k, u_k, f_k)_{k\in I}$ is $F_{m,L} - interpolable$, meaning there exists a function $f \in F_{m,L}$ satisfying $f(y_k) = f_k$ and $\nabla f(y_k) = u_k$ if and only if:

$$2(L-m)(f_i - f_j) - mL||y_i - y_j||^2 + 2(y_i - y_j)^T(mu_i - Lu_j) - ||u_i - u_j||^2 > 0 \text{ for } i, j \in I$$

Where the Euclidean-norm of a vector x is denoted as $||x||$. Basing on this theorem, [[7], Cor 4] presented a non-negative linear combination of inequalities to create a tight representation of the class of function, which can be rewritten in a way easier to implement into code as:

Corollary 2 ([7], Cor. 4)**.** Given a function $f \in F_{m,L}$ and let $y_k, ..., y_{k-l}$ be a sequence of iterates; $u_{k-i} = \nabla f(y_{k-i})$ and $f_{k-i} = f(y_{k-i})$ for $i \in 0, ...l$. Then the inequality:

holds for all $\Lambda \in \mathbb{R}^{(l+2)*(l+2)}$ and $\Lambda >= 0$, and $\Pi(\Lambda)$ and $\pi(\Lambda)$ are defined as:

This step in the methodology is similar to that in [1]. By using interpolation conditions, the gradient of smooth strongly convex class of function inputted is represented by non-negative inequalities. This combined with the use of Lyapunov-functions to prove convergence rate which will be presented in 3.4 allows analysis to be done be solving a convex program

3.3 Lifting algorithm

3.4 Lyapunov function certification

$$V(x) =< P, X[x; u] >=< X^T P, [x; u] > \tag{3.3}$$

4

Code Components

To in order to perform algorithm analysis with JuPE, the user need to follow the folliowing 3 steps:

1. Choose from a supported list the class of function to be optimized.
2. Define an algorithm to be analyzed .
3. Specify a performance measure.

Figure 4.1: Analysis Example

```
m,L = 1,10
α = 2/(L+m)
@algorithm begin

        f = DifferentiableFunctional{Rⁿ}()
        xs = first_order_stationary_point(f)
        f' ∈ SectorBounded(m, L, xs, f'(xs))

        x0 = Rⁿ()
        x1 = x0 - α*f'(x0)

        x0 => x1

        performance = (x1-xs)^2
end

@show rate(performance)
```

In the example code, the user while using JuPE's provided macro to simplify the input process:

- Defined the class of function f and its gradient f' by calling one of the provided functions, in this case 1 smooth 10 strong convex functions.
- Set the global minimum goal as a stationary point x_s
- Defined an initial state x_0 and specified the algorithm with which the state is updated using algebra - gradient descent with a step size 2/11 in this example.
- Set the performance measure as the norm distance between the updated point and the goal $(x_1 - x_s)^2$.

With the calling of the "rate" function, JuPE derives every necessary input from the performance measure and performs analysis automatically to return a rate of 0.6687164306640625, which can be seen in Figure 4.2. This means for the provided algorithm and every function in the class, the convergence rate of the performance measure is guaranteed to match or exceed the result worst-case guarantee rate.

Figure 4.2: Analysis result

```
rate(performance) = 0.6687164306640625
```

JuPE performs algorithm analysis by following the set of instructions presented in section 3 to create and solve an optimization problem and derive a performance certification. Implementing a mathematical procedure as code presents a list of challenges which includes being able to understand and differentiate between variables, represent concepts such as gradients or states, or formulating and solving a convex optimization problem, while keeping the users' interaction with the program simple. This chapter goes into the code that constitutes JuPE and enables these functionalities.

4.1 Expressions

Expressions are data structures acting as the smallest building block upon which every other concepts are built. An expression data structure contains the following fields:

Label When an expression is defined, the variable name used is stored in the expression as a string

Value Stores the value or decomposition of an expression.

Constraints When a constraint is applied to an expression, such as an expression being positive or negative semidefinite, the constraint is stored in the 'constraints' field.

Oracles When an expression is defined by sampling one or multiple oracles, the oracles used are stored in the expression data structure

Next When a state is defined as the 'next' state of another state, it is stored in the original state under the 'next' field.

Value and Decomposition

Each expression contains in its 'value' field either a scalar value, a vector value, or a decomposition dictionary. Depending on the content of the 'value' field, expressions can be categorized as:

Variable expressions an expression defined to be in a field. Its value is empty and its decomposition is itself.

Figure 4.3: Example of a variable expression

```
x0 = Rⁿ()
@show(x0)
x0 = Variable{Rⁿ}

Vector in Rⁿ
        Label: Variable{Rⁿ}
        Oracles: LinearFunctional{Rⁿ}
        Associations: Dual => LinearFunctional{Rⁿ}
```

Decomposition expressions formed by performing algebra on other expressions. Its value is a decompostion data structures containing how many of each variable expressions forms the decomposition expression.

Figure 4.4: Example of a decomposition expression

```
decomposition_exp = (x0-xs)²
@show decomposition_exp
decomposition_exp = -<x0,xs> + |x0|² - <xs,x0> + |xs|²

Scalar in R
        Decomposition: -<x0,xs> + |x0|² - <xs,x0> + |xs|²
```

In the

Fields

In example 4.3, expression 'x0' is defined to be in field R^n, a field pre-defined in JuPE which encompasses n-dimensional.

Algebra

Expressions in JuPE belong in an inner product space, which is a set of elements that can be vectors or numbers. Inner product spaces allow a list of operations, all of which are supported by JuPE, including:

Addition or subtraction between expressions Vectors and numbers can be added together in an inner product space. In an addition operation, if both expressions of the operation posess a 'value', they are added to create the value of a new resulting expression. Otherwise, the result is a new expression is created whose decomposition is the merging of the expressions being combined's decompositions.

Multiplication or division between an expression and a scalar This operation scales the value or decomposition of an expression by the scalar value.

Figure 4.5: Example of addition, subtraction and scalar operation

```
@algorithm begin
        x0 = R^n()
        y0 = R^n()
        a = x0-2*y0
        b = a+2*x0
end
@show(a)
a = a

Vector in R^n
        Label: a
        Decomposition: -2 y0 + x0
        Associations: Dual => a*
@show(b)
b = b

Vector in R^n
        Label: b
        Decomposition: -2 y0 + 3 x0
        Associations: Dual => b*
```

Inner product operation between two vectors In an inner product space, the inner product of two vectors result in a scalar.

Squared norm An expression of the normed vector vpace type can be squared to produce a an inner product space expression.

Figure 4.6: Example of an inner product between two vectors and norm of vector

```
@algorithm begin
        inner = x0'*y0
        norm = x0^2
end
@show(inner)
inner = <y0,x0>

Scalar in R
        Label: <y0,x0>
        Oracles: x0*
@show(norm)
norm = |x0|^2
Scalar in R
        Label: |x0|^2
        Oracles: x0*
```

4.2 Oracles

As JuPE perform analysis over sets of functions using only constraints on the $\nabla(f)$ block of, the block can be treated as a blackbox. In JuPE, these blackboxes are represented by oracles, data strucutres containing the relation and constraint information between expressions. Each oracle represent a class of function and can only exist if there exist interpolation conditions for said class. Oracles can be sampled at an expression to return another expression, establishing the relation information between the two expressions. As an oracle is sampled, JuPE uses the set of interpolation conditions to create every constraints on the two expressions. In 4.1, by calling the SectorBounded function, an oracle containing the interpolation conditions for 1 strong 10 smooth convex functions is created and labeled f', and the oracle is sampled at points xs and x0 by defining f'(xs) and f'(x0) inside the labeling macro.

Inner product oracle

Different from other algebraic operations supported by JuPE, the inner product is derived by creating an oracle of one vector and sampling it at the other vector of an operation, returning a new variable expression. As both the transpose of a vector, which is used to calculate the inner product, and the gradient of a function uses the notation " ' ", oracles are used to assist in the formation of inner product expressions. In this case, the oracle is not based on any class of function and therefore attribute no constraint to the vector being sampled.

4.3 States

JuPE represents the states of an algorithm using expressions. As the user inputs the algorithm being analyzed, an initial state is created and an updated state is defined as some algebraic combination of the initial state and the gradient. The relationship between a state and its next state can be defined using the "=>" operation inside the labeling macro, as can be seen in 4.1, and the next state is stored in the "next" field of a state expression.

4.4 Label

JuPE uses macro to keep the process of providing inputs to the program simple. As some of the programming rules of programming might be difficult to navigate for users who might not be used to programming, in order to make the process of using JuPE as accessible as possible, JuPE's macro:

Describe When an expression is referenced, JuPE will describe the expression and any relevant field without the user having to access it.

Define During the inputing process, users can define a new expression or oracle with only one line specifying its trait, instead of the usual steps of declaring a new object and filling in its fields that typically exist in programming. The macro will calls the necessary functions to create the object, assign every relevant field as well as updating every object associated with the one being created.

4.5 Constraints

As part of the analysis process, JuPE uses the interpolation conditions of the class of function inputted by the user to create constraints similar to section 3.2. To support constraints, JuPE uses data structures that include the expression constrained and one of the supported sets of values defined by the constraints.

When an oracle is sampled, a set of constraints on the expression being sampled and the result of the sample - the input and output of the black box - is created, and constraints are added as the oracle is sampled at more than one expression. For each constraint, the constraint is added to each variable expressions associated with it. The figure below shows the constraints created by the oracle in 4.1:

Figure 4.7: Example of oracle created constraint

```
vars, cons, orcs = variables_constraints_oracles(performance)
cons
        Set of constraints with 3 elements:
                0 <= 1.1 <∇f(x0),x0> + 2.0 <xs,x0> - 2.0 |x0|² + 1.1 <x0,
                0 <= R[|x0|² <xs,x0>; <x0,xs> |xs|²]
                0 <= R[|x0|² <∇f(x0),x0> <xs,x0>; <x0,∇f(x0)> |∇f(x0)|² <
```

In addition to being created by sampling oracles, constraints can also be defined by users. When analyzing any algorithm, constraints can be added to the initial condition of the algorithm. Any constraints added by the user is included in the formation of the optimization problem used to derive the performance bound.

Figure 4.8: Example of user added constraint

```
@algorithm begin
        (x0-xs)^2 <= 1
end
```

4.6 Performance measure

Part of JuPE's required inputs is the performance measure, the convergence rate of which JuPE finds the worst-case guarantee through algorithm analysis. In 4.1, the performance measure is set as $(x_0 - x_s)^2$, which is the norm or distance between the initial point and the

goal, which means the convergence rate guarantee returned is that of the distance between the point updated using gradient descent after each iteration x_k and the goal x_s.

4.7 JuMP

4.8 Lyapunov function formulation

5

Analysis Process and Result

After running JuPE to perform algorithm analysis on three algorithms (GD), (HB), and (FG) on classes of m strong L smooth convex function where the condition number L/m are chosen between 1 and 10, we get

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