IACS Master of Data Science Thesis Proposal

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Title

Solving the Gravitational Equations of Motion with Neural Networks

Advisor

Pavlos Protopapas has agreed to act as my primary advisor.
Chris Rycroft has also kindly agreed to act as an informal ad-hoc advisor on specific questions as needed.

Abstract

The evolution of a gravitational system can be accurately simulated using classical numerical methods such as symplectic integrators. However, it is computationally expensive to simulate a large gravitational system to a high degree of precision. This thesis aims to determine whether a neural network can be trained to generate approximate solutions to small gravitational systems, i.e. two or three body problems. If good results are achieved on small systems, we might try to extend these results to larger systems. We may use our synthetic training set and software infrastructure to create an open competition on this problem along the lines of ImageNet in computer vision.

An interesting related problem is the identification of orbiting bodies by combining pairs of "tracelets" that have consistent orbital trajectories. Neural network techniques could prove to be more efficient at spotting patterns and identifying tracelets that are likely to belong to the same orbital body.

Motivation and Background

The equations of gravitational motion are a seminal achievement in physics and astronomy. They were the inspiration for the invention of differential calculus and have great practical importance even today in astronomy and applications related to space and satellites. They are a subject that has fascinated me since I was a child before I learned calculus.

Machine learning and neural networks have made great strides in recent years. A recent research focus has been using ML in science, and in particular in solving differential equations. This was a topic that featured prominently at the IACS ComputeFest this year. One principal motivation is to see what results can be obtained by applying ML to a well understood classical differential equation. The hope is that whether or not the results are intrinsically useful, they will be a stepping stone to learning about using ML techniques to solve differential equations in general.

There is more reason for optimism in the ability of ML to identify orbiting bodies based on photographs. This is currently a manually intensive process with a lot of human input and a large backlog of tracelets that have never been paired with other tracelets. This is qualitatively the kind of task at which neural networks have excelled. It is also tightly defined and of practical interest in the astronomical community.

Goals

My goals in this project are both scientific and personal. My primary goal is to gain experience doing meaningful scientific research. I am guardedly optimistic that a neural network could be trained to efficiently simulate both 2 body gravitational systems and "reduced" three body systems in which one body is significantly lighter than the other two. If we could do that I think the project would already be a moderate success. The full 3 body problem and the general n-body problem are much harder, and I don't think it's likely we will get a neural network to solve this in a useful way compared to classical numerical simulations. On the other hand, even if we can just get an approximation, it could provide useful insights into techniques for modeling differential equations with neural networks.

A related goal is to create the infrastructure to run a competition on solving the gravitational equations using neural networks. Competitions have been remarkably fruitful in driving progress in the field of machine learning. The success of the ImageNet competition in fostering advances in computer vision is perhaps the most prominent example. In addition to trying to solve this question myself, I have interest to share a training data set with the larger community in case others would like to try it. A considerable part of the work on this project may prove to be creating a large synthetic data set of many simulated gravitational trajectories. Another body of work will be to program a routine to automatically score a trained network. These two elements (a large data set and automated scoring program) could be the key resources enabling us to run a competition if we chose to move forward.

The problem of identifying orbital bodies from multiple tracelets perhaps offers better prospects to make an advance on the current state of the art in astronomy. On the other hand, it is narrower in its focus and less broadly applicable. I will need to see how things go and get input from my advisor to allocate time between these related questions. The primary goal if we pursue this avenue would be to take a real-world data set (e.g. images captured from optical telescopes from the Center for Astrophysics) and generate an output consisting of the orbital elements of likely bodies in the solar system. If we could create a code that made verifiable predictions about the orbits of heretofore unidentified bodies, I would be very pleased with that result.

Scientific Justification

I carefully considered whether to try to pick my own topic from first principles or to ask an advisor to suggest a topic that they are working on. I chose the latter course, because identifying promising research topics is difficult and I wanted to lean on the experience of an advisor. I also wanted the greater structure and support that comes from working on a research problem sponsored by a faculty member. Professor Protopapas has suggested these avenues of research, and I share his assessment that they are likely to lead to scientifically valuable results.

A number of important problems in computational science can be distilled down to numerically simulating analytically intractable differential equations. A prominent example is fluid dynamics. The classical numerical analysis community has made steady progress by improving algorithms and running on larger computing clusters, but we're starting to bump into limits of e.g. energy consumption for computations at the exascale. Machine learning and neural networks are a novel approach to these problems that is just starting to be tried. They have demonstrated enough success in other challenging problem domains that many researchers believe it is worth trying to use them for solving differential equations.

Literature Review

I will be completely honest here and acknowledge that I have not yet had the time to complete the necessary literature review. I discussed this topic with Professor Protopapas early in the semester. Since then, I have been struggling mightily to keep up with a full course load and my family commitments. I have made informal plans to begin work on this research topic with Professor Protopapas over the summer. As a result, I am confident that by the time the Fall 2019 semester begins I will either be in a strong position to write this thesis, or will be sufficiently chastened that I will have time to back out and complete a capstone project so I can graduate on time!