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Probabilistic modeling of astrophysical time series: gravitational microlensing and occultation mapping of planets and moons

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Abstract

Scientific progress in modern astronomy research commonly relies on gathering large quantities of data using exceedingly precise instruments. The process which "generates" these data consists of the physical phenomenon of interest – for instance, an exoplanet blocking or twisting the light of a distant star, and the noise introduced by the measurement process and the presence of an atmosphere The task for an astronomer is to first construct a *model* which describes the entire process which generated the data and to then "fit" that model to data. All models only approximate reality and the researcher has to make a series of decisions during the model building process, everything from how to process the raw data to which results to put in the abstract of a paper. Advancements in computational statistics and machine learning in the past decade or so have made it possible to fit ever more complex models to data. These models are generally expressed in computer code which may contain complex numerical algorithms, such as iterative solvers and numerical integrals. In this thesis, I mostly focused on developing methods which enable *statistical inference* with these kinds of complex models in two particular domains within astronomy, gravitational microlensing and occultation mapping. The common theme between these two topics is that both deal with accurately measuring the brightness of distant stars as a function of time with the goal of inferring properties of exoplanets and stars. Broadly speaking, I believe the biggest contribution of this thesis is providing a new lens for looking at a particular set of old problems, a lens which incorporates recent advancements from statistics, machine learning and computer science. More specifically, I have developed a an open-source software package caustics[1] which enables fast and accurate computation of binary lens and triple lens microlensing light curves and simultaneously provides exact *gradients* of the code outputs with respect to all its inputs. This is significant because it for the first time enables the use of modern gradient based statistical inference algorithms such as Hamiltonian Monte Carlo with microlensing light curves. Microlensing is one of the major goals for the upcoming *NASA Roman* telescope and the existing modeling methods are completely inadequate for dealing with the scale of data which will come from *Roman*. I also propose a framework for dealing with issues which have plagued the field for decades – various pathologies in microlensing models and questions about the interpretation of statistical results. Besides microlensing, I have also delved into the field of occultation mapping of Solar System objects and exoplanets. Together with collaborators, I have developed a novel statistical method for reconstructing spatial maps of volcanic emission on Jupiter's moon Io using infra-red occultation light curves. I applied the same method to exoplanets to explore the exciting possibility of detecting weather changes on Hot Jupiters by reconstructing two dimensional maps of the emission surface from simulated *JWST* secondary eclipse light curves. I found that planetary scale changes in the emission pattern should be detectable with *JWST*.

[1] https://github.com/fbartolic/caustics

Chapter 1

Introduction

1.1 Context

The key idea of the scientific revolution in the 16th century was to carefully observe the world, build *models* which describe some aspect of the observed phenomenon, and finally and most importantly – test those models to see if they provide an accurate description of reality. Since the time of Galileo, this process gave rise to the modern world and revolutionised our understanding of the universe. Today we have amazingly accurate models of the universe. Einstein's theory of *General Relativity* which describes the universe at a large scale and the *Standard Model* which describes the universe at the atomic and subatomic scales, both of which were developed in the 20th century. In my opinion, the two most important questions for the physical sciences in the 21st century and beyond are the following:

- How do we combine the Standard Model and General Relativity to get a complete physical theory of the Universe?
- What is the origin and distribution of complex life in the Universe?

It used to be the case that conducting experiments with the potential to to change our understanding of fundamental physics was relatively straightforward and could be conducted by a single person or a small group of researchers. I have in mind, for instance, Kepler's observations of planetary orbits, Ernest Rutherford's experiments with atoms or Arthur Eddington's observations of the Solar eclipse with the goal of testing General Relativity. The data gathering process consisted of writing notes in a physical notebook and the analysis hardly required complex statistics. Today the situation is more complicated because much of the "low-hanging fruit" of scientific discovery (in the physical sciences) has been exhausted and the use of computers is absolutely central to the process. Progress today usually (but not always) requires coordination between many scientists, engineers and software engineers building highly complex experiments. Consider this list of some of the most notable scientific discoveries in the past few decades:

- Discovery of accelerated expansion of the Universe
- First sequencing of the human genome
- Detection of the Higgs Boson
- Paleogenomics studies of the origin of Homo Sapiens
- Detection of gravitational waves by LIGO

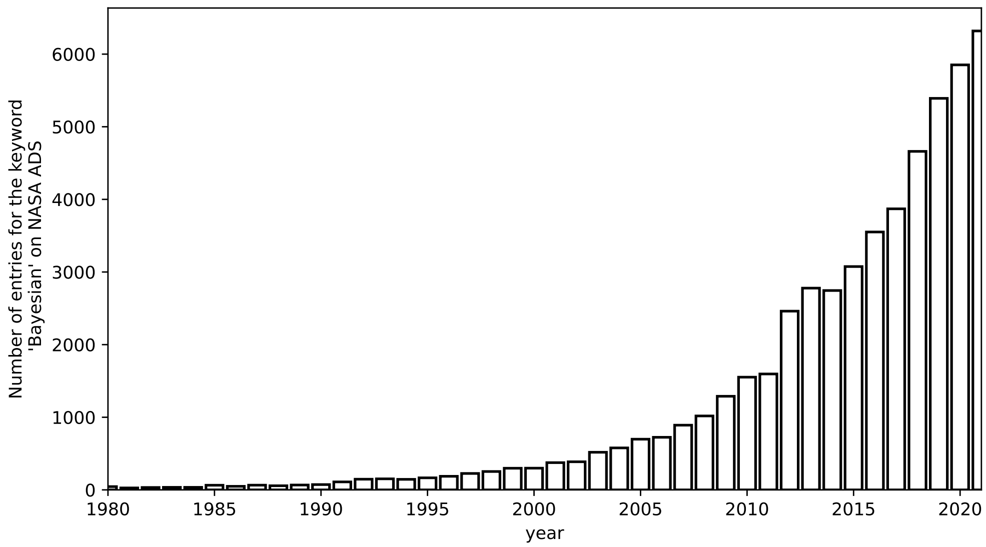

Figure 1.1: Number of NASA/ADS entries containing the keyword "Bayesian" per year.

- Reconstruction of the first image of a Black Hole

All of these discoveries required gathering substantial amounts of data and the use of relatively complex statistical analysis techniques. Computation and statistical analysis are now absolutely central the process of scientific discovery.

Simultaneously, in the past decade there's been a complete revolution in the field of machine learning/AI thanks to the advent of deep learning and neural networks. Besides the incredible progress on predicting patterns in language and vision, deep learning has also been used in science for things like solving the protein folding problem (Jumper et al., 2021) and in mathematics for the purpose of discovering novel conjectures and theorems Davies et al. (2021). Deep learning has been less useful in physics and astronomy so far but as I will argue in this thesis, some of the technologies which underlie deep learning such as automatic differentiation and GPU computing are going to be (if they aren't already) crucial for processing and understanding complex datasets in physics and astronomy.

There is another revolution worth mentioning. It is slightly less obvious than the one in machine learning but nevertheless significant. In the past two decades there has been a substantial increase in popularity of Bayesian statistics. Fig 1.1 shows that number of entries in the NASA/ADS database containing the keyword "Bayesian" each year is growing almost exponentially. One of the reasons that these methods are so popular now even though they have been invented many decades ago is that they used to be very computationally expensive and the algorithms necessary to do proper Bayesian analysis were somewhat underdeveloped. This has changed drastically in the past decade. I will discuss these methods in detail in § **??**. Much of this thesis is about applying Bayesian methods to problems in astronomy.

Having situated the work presented this thesis in the present moment and point out some scientific and technological changes that I think are relevant, I will now focus on astronomy in particular. The kinds of questions in astronomy that most excite me are those which lead us closer to answering one of those two fundamental questions I stated at the beginning of this chapter. The question about the origin of life in the universe in particular. Since the first discoveries of planets outside of our Solar System in the early 90s (Wolszczan and Frail, 1992; Mayor and Queloz, 1995) thousands more have been confirmed[1] using methods such as transits, radial velocity, microlensing and direct imaging. Thanks to gravitational microlensing we now know (Cassan et al., 2012) that there is an average one planet per star in the Milky Way. In addition to detecting the presence of the planets and inferring their properties such as mass, radius, and orbital period; it is now possible to measure the transmission and emission spectra of their atmospheres and even reconstruct crude maps of their surfaces[2] (Knutson et al., 2007; Majeau et al., 2012). With the James Webb Space Telescope, we might even be able to detect biosignatures in the atmospheres of Earth size planets.

Answering a grand question such as "are there biologically produced complex molecules in this exoplanet atmosphere" will not be easy even with cutting-edge instruments such as the James Webb Space Telescope. It will also almost certainly not be a clear yes or no kind of answer; rather, it will require a deep understanding (i.e. good *models*) of the physics of exoplanet atmospheres, stellar variability, the response of the instrument, sophisticated statistical analysis of the drawing on multiple independent pieces of evidence and clear definitions of what it means to have detected something. To build a good model for the thing we really care about requires understanding also the the things we may intrinsically care less about (instrumental systematics, details of stellar variability, variations in Earth's atmosphere etc.).

A large fraction of this thesis (with the exception of Chapter 5) is focused on building the necessary infrastructure (computation, statistics, interpretation) which should enable new discoveries in exoplanet (and planetary) science. Wherever possible I try to approach these problems from first principles thinking but with a heavily computational/statistical approach with a healthy dose of pragmatism. In the next two sections I will provide a brief introduction to specific areas I worked on and end the chapter with an outline of the following chapters.

1.2 Gravitational microlensing

"Do not bodies act upon light at a distance and by their action bend its rays, and is not this action strongest at the least distance?" asked Newton (1704). Much later in 1912, even before he published his theory of General Relativity, Einstein predicted the that a distant light source could be magnified by a foreground mass relative to an observer on Earth if the two objects were very precisely aligned (Renn et al., 1997). At the time Einstein concluded that this *gravitational lensing* effect was unobservable and did not even bother publishing the result until 24 years later a young amateur scientist R.W. Mandl convinced him to write a short paper on the subject (Einstein, 1936). In that paper he stated that *"Of course, there is no hope of observing this phenomenon directly. First, we shall scarcely ever approach closely enough to such a central line. Second, [the angles] will defy the resolving power of our instruments"*. Still, the consensus at the time was that this was unobservable.

The first definitive observation came in 1979 by Young et al. (1980) who observed a double image of the quasar Q0957+561 and concluded that the two images correspond to the same object whose light was distorted by a foreground gravitational lens in the form of a massive galaxy. That the same effect could be used to detect the presence of planets orbiting around their host stars was first theorized by Liebes (1964) who wrote that *"the primary effect of planetary deflectors bound to stars other than the Sun will be to slightly perturb the lens action of these stars"* although he was also sceptical about the possibility of detection, saying that *"associated pulses would be so weak and infrequent and of such fleeting duration – perhaps a few hours – as to defy detection"*. Gravitational lensing as a method for discovering exoplanets really took off with the work of Paczyński

[1] At the time of writing the NASA Exoplanet Archive contains more than 5000 exoplanets.

[2] The subject of Chapter 5.

Figure 1.2: Stellar field of a microlensing event GLE-2012-BLG-0406 (centered), imaged by one of Las Cumbres Observatory's 2m telescopes, showing the high density of stars typical in microlensing observations. Credit: Y. Tsapras. Taken from http://microlensing-source.org/pictures/.

(Paczynski, 1986b,a; Mao and Paczynski, 1991) who also coined the term *microlensing*, which refers to gravitational lensing in a regime where the images of the background object cannot be resolved but one can nevertheless measure its magnification as a function of time.

Microlensing as a method for detecting exoplanets has some unique aspects. First, it's a one-off event which happens on a timescale of a few minutes up to several months depending on the distances to the background star and the lensing star and the mass of the lens. In addition to the fact that there's only one chance to observe such an event for it to happen at all requires extremely precise alignment between the lens and the background star and the chance of observing a stellar microlensing event is about one-in-a-million (CITE) for a typical star within the Milky Way. To observe a planetary signal is about an order of magnitude less likely than that. Hence, obtaining a decent sample of planetary events requires continuous monitoring on the order of 10^8 stars at the time which way microlensing observations that to focus on the densest region of the Milky Way – the galactic bulge. Figure 1.2 a picture from of such a dense stellar field. Finally, in the vast majority of cases we do not detect any light from the lens itself, the collected photons are from a background star completely unrelated and distant from the lensing star. This is very different from other exoplanet discovery methods and it means that we only obtain dynamical properties of planets such their masses and periods.

The aspects that make microlensing events that make them difficult to observe also mean that it provides a unique lens onto exoplanet systems. Relative to other methods such as transits and radial velocity, microlensing is sensitive to planets located at substantially greater distances, well outside of our Solar System neighborhood and even potentially to Milky Way's satellite galaxies such as the Magellanic Clouds and the nearby Andromeda galaxy (CITE). Microlensing is also sensitive to very to very small planets and planets which are further out from the star than those typically detected using transits and radial velocity. Microlensing surveys such as OGLE (Udalski et al., 1993) and MOA (Muraki et al., 1999) have been continuously monitoring crowded stellar fields in the Milky Way since the 90s[3] discovering thousands of stellar events and dozens of planetary events. In order to detect planetary deviations in the observed light curve it essential to have high cadence observations of the source star. The way surveys have traditionally worked is that once a particular star started to become magnified many additional small telescopes would start observing it to obtain denser coverage and sometimes space-based observatories get involved as well. The vast majority of microlensing events analyzed so far consist of observations from multiple observatories, each with its own unique aspects such as noise properties, cadence and photometric quality.

Future surveys such as the ground based Rubin Observatory (Ivezić et al., 2019) telescope and the space based Roman Telescope (Penny et al., 2019) and Euclid (Bachelet et al., 2022) will detect tens of thousands of events in total. Although most of past work in the field focused on characterizing individual events binary lens events, answering questions about *populations* with these new (but also existing) datasets requires scalable data analysis methods and algorithms and a clear set of guidelines on how to interpret the analysis products. This is a substantial challenge because microlensing events are notoriously difficult to model. Even though the datasets are relatively simple, consisting of multiple time series photometric light curves in different bands, the parameter space of even the simplest models is highly non-linear, correlated, relatively high dimensional and there are often near perfect degeneracies in the solutions.

The assumptions that existing methods for modeling microlensing events rely on are often opaque and unquestioned. Discussions on model "degeneracies" (Song et al., 2014; Hwang et al., 2019; Skowron et al., 2018; Dominik, 2009), correlated noise (Bachelet et al., 2015; Li et al., 2019) and model comparison (Hwang et al., 2018; Dominik et al., 2019) have been ongoing in the microlensing literature for decades without a clear solution and proper framing of the issue. In this thesis I will revisit these kinds of questions while taking into account many recent developments in the fields of computational statistics and machine learning. My main contributions are the following:

- I wrote an open-source Python package `caustics` which enables fast and accurate computation of binary and triple lens microlensing light curves using contour integration. The code runs on both CPU and GPU architectures, and crucially, for reasons that I will elaborate in subsequent chapters, it supports *automatic differentiation* of all outputs with respect to all input parameters which enables the use of statistical methods which are orders of magnitude more efficient than existing approaches. The code can easily be extended to support quadruple lensing and arbitrary intensity profiles for the source star.

- I have revisited the topic of degeneracies in the posterior probability distributions which appear in the context of microlensing and propose solutions to these problems.

- I have extended the complex polynomial root solver from Cameron and Graillat (2022) such that it can be executed on GPU architectures and that it supports automatic differentiation. This enables the evaluation of 1M lens equation solutions for point source binary and triple lenses in seconds using a CPU and miliseconds using a GPU.

- I propose an approach to statistical inference on a population of microlensing events which different from existing methods and has some advantages.

- I briefly discuss the issue of correlated noise in microlensing light curves and propose ways to account for it using Gaussian Processes.

[3] Initially the focus was on finding dark matter candidate particles – so called MACHOs (Massive Compact Halo Objects).

1.3 Occultation and phase curve mapping

Interestingly, the second topic I will cover in this thesis has a history not unlike that of microlensing. It was proposed in the early 20th century and it was only much later that technology caught up with the idea. Back in 1906, Russell (1906) pointed out that certain features in light curves of Solar System satellites may be attributed to inhomogeneities of their surfaces. The key idea is that although at any given time we only observe the total light from an unresolved satellite or planet, different portions of the surface are visible at different times so we may expect that some of the information about the surface intensity (be it emission from heat or reflected Sunlight) gets imprinted onto the light curve. Russell (1906) also considered the inverse problem – can we learn something about the surface of these objects starting from a light curve? The method he proposed is now known as *phase curve mapping* and it was first attempted by Lacis and Fix (1972) who analyzed photometric light curves of Pluto in reflected light attempting to constrain variations in the *albedo* of the surface with inconclusive results.

Later works such as Buie et al. (1992); Young and Binzel (1993); Young et al. (1999) went a step further by using not only phase curves but also light curves of mutual *occultations* of Pluto by its moon Charon to reconstruct albedo maps with greater success. The major advantage of occultations relative to just phase curves is that more information about the surface is encoded into the light curve because of the sharp limb of the occultor sweeping over the disc of an occulted body and blocking the reflected light. More importantly for this thesis, Spencer et al. (1994) was the first to observe the occultations of Jupiter's moon Io by another of Jupiter's moons – Europa, and also occultations of Io by Jupiter itself. These observations were conducted using near-infrared telescopes such as NASA's Infrared Telescope Facility (IRTF) to observe emitted light from Io's surface which is covered with many time-varying and bright volcanic features. The observing campaign of Io has yielded insights into the the nature of its volcanic activity and it continues to this day. I will return to the subject of Io in great detail in Chapter 4.

A natural question arises, can we do this with objects outside of the Solar System? The answer is yes. Knutson et al. (2007), Majeau et al. (2012), and de Wit et al. (2012) used Spitzer mid-infrared observations of secondary eclipses of the Hot Jupiter HD189733b and found that surface emission is best described by the presence of a large hot spot on the dayside of the planet which is longitudinally offset from the substellar point. Similarly, Stevenson et al. (2014), produced temperature maps of the Hot Jupiter WASP-43b, Demory et al. (2013) mapped the Hot Jupiter Kepler-7b in reflected light and Demory et al. (2016) mapped the thermal emission from the Super Earth 55 Cancri e. These studies were only able to capture longitudinal variations in intensity. Real exoplanet atmospheres of are certain to have three-dimensional spatial inhomogeneities in emission more complex than a single hot spot due to the presence of clouds, zonal jets, storms, waves etc. (Showman et al., 2020).

In recent years there have been significant advances in statistical modeling of phase curves and eclipse light curves. Most notably, Luger et al. (2019) introduced the `starry` code which enables analytic computation of phase curves and occultation light curves for bodies with arbitrary emission maps expressed in a spherical harmonic basis (an idea dating back to Russell (1906)) and Luger et al. (2021) expanded the algorithm for the (considerably more complicated) case of reflected light. In this thesis, I will present the work I've done in collaboration with other researchers from the planetary science and exoplanet communities on using `starry` to map the surface of Io and investigate the prospects for detecting fine spatial structure in the atmospheres of Hot Jupiters using JWST phase curves and eclipse light curves. My contributions to this area are the following:

- I have developed a novel model for inferring emission maps of Io from occultation light curves.

First part of this project is published in Bartolić et al. (2022) though I haven't managed to complete the second part.

- I have investigated the problem of eclipse mapping of exoplanets using the starry framework, focusing in particular on the possibility of detecting planetary scale storms on Hot Jupiters using JWST. I found that it extremely difficult to infer maps of higher resolution than a dipole order but that should still be sufficient for detecting large scale weather and climate change in the atmospheres of these planets.

The application of the occultation/eclipse mapping method to Io can be seen as the best case scenario for the application of the same method to exoplanets. I will show that even in the case of observing a bright object right in our neighborhood, this is by no means and easy task. Our ability to reconstruct the surface features of Io sets a sort of upper limit on what is possible with exoplanets.

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