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Paper summary

The Efficiency of Geometric Samplers for Exoplanet Transit Timing Variation Models

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March 6, 2019

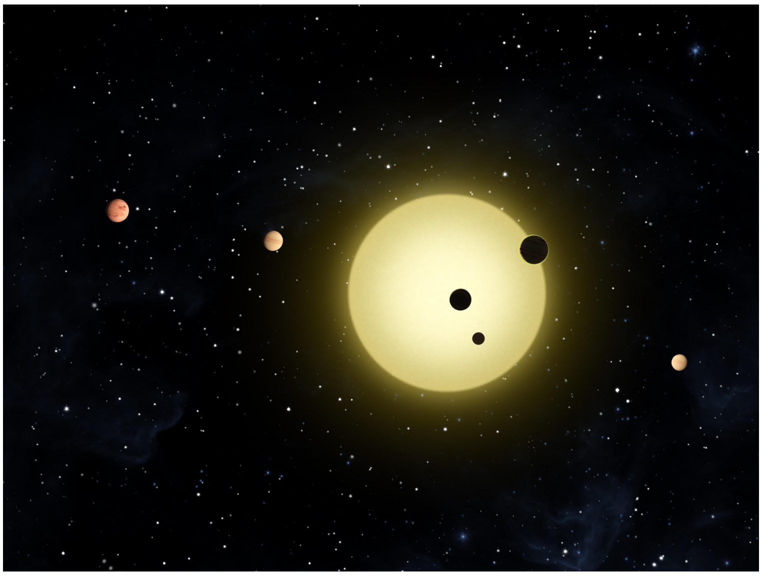

Figure 1: *Artist's impression of Kepler-11, which is a Sun-like star which has six planets in orbit. At times, multiple planets pass in front of the star at once. This image is based on observations by NASA's Kepler spacecraft on August 26, 2010. Credits: NASA/Tim Pyle.*

1. Introduction

The science of exoplanets investigates planets that are orbiting other stars than our own, and tries to describe their properties. In order to obtain the compositions of these planets, which can be inferred from their densities, a relationship between mass and radius is needed. There are two common methods to observe exoplanets; the first one is the radial velocity method, which measures small changes in velocity and position of the star that are caused by the gravitational influence of the orbiting planet. This method provides a measure of the planet mass. The second approach is measuring the star's decrease in brightness when a planet transits in front of it, thereby blocking some of its radiation. Figure 1 demonstrates this effect. Since the size of the planet determines the amount of starlight that is blocked from view, the transit method measures the planet's radius. Combining these two methods has proven to be difficult, because both are only suitable for planetary systems found in very specific, and often different, circumstances.

Fortunately, there is another approach that can be used to determine planet masses, for multiplanetary systems. The Transit Timing Variation (TTV) technique measures small deviations in transit times, which are caused by the planets' gravitational influence on each other. Astronomers have created dynamical models that can predict the transient times when planetary properties are known. However, inverting these models to obtain planetary properties from a measured TTV is not trivial. For a known TTV there exists degeneracy between the parameters of the model as well as multimodality in their posterior distributions. This is where Markov Chain Monte Carlo (MCMC) can step in to estimate the parameters that describe the planets.

2. Samplers

This paper investigates two different models to compute the TTVs from planetary properties, which will be discussed in the next section. Both of these models require 10+ parameters, therefore the task of running the MCMC is not an easy one, and it matters in which way the parameters are sampled from the distribution. One of the most basic forms of MCMC is the the Random Walk Metropolis-Hastings algorithm, which selects the next step randomly from a distribution centered around the current point. It could greatly improve the efficiency of the sampler if the next proposed step was chosen with some more knowledge of the target distribution, so this step would be more likely to be accepted. In the paper the authors investigate the efficiency of 6 different samplers that are applied to TTV data of exoplanets.

• **MALA** (Metropolis-adjusted Langevin algorithm). This sampler chooses a step based on the gradient of the posterior distribution, in order to reach the maximum faster.

• **HMC** (Hamiltonian Monte Carlo). The problem with using only the gradient of the distribution is that its direction will never be aligned with the desired trajectory around the maximum, but rather it will always point towards it. A nice physical analogy for this, one which is quite fitting to this paper, is a planet orbiting a star. The planet will also feel a gravitational gradient that is only directed towards the centre of its orbit, and is not aligned with its trajectory. A planet with zero velocity would therefore crash into its star. In the physical system this is prevented and a stable orbit is maintained because of exactly the right amount of *momentum*. HMC applies this idea to MCMC algorithms, by introducing an auxiliary variable called momentum to the system. Similarly to classical mechanics, the Hamiltonian of this system can be defined as the sum of potential and kinetic energy, and Hamilton's equations can be solved to propose a new position.

• **DEMCMC** (Differential Evolution MCMC) and **AIMCMC** (Affine-Invariant ensemble MCMC). Both of these sampling techniques employ multiple walkers that exchange information with each other, that determines the size and direction of the next step.

• **SMMALA** (Simplified Manifold Metropolis-adjusted Langevin algorithm). This method uses not only the gradient, and therefore the first derivatives, of the target distribution, but also their second derivatives in the form of the Hessian. A disadvantage of this method is that computing the Hessian can be quite time-consuming. This issue is resolved in the newly developed method by the authors of this paper, **GAMC** (Geometric adaptive Monte Carlo), which only uses the Hessian frequently in the beginning and gradually reduces its usage over time.

3. TTV models

Multiple models have been developed to model the TTV from planetary properties. In this paper, the two models that are used to investigate the efficiency of the samplers are the *Simple Sinusoidal model* and the *TTVFaster model*.

Simple Sinusoidal Model

This is one of the earlier, more basic methods to model exoplanet TTVs. It uses an analytical expression that combines sines and cosines to create a sinusoidal waveform:

$$\begin{aligned}\tau_m(N_m, p) =\ & t_{lin,m} + \\ & A_m \sin(f_{TTV} t_{lin,m}) + B_m \cos(f_{TTV} t_{lin,m}) + \\ & C_m \sin(2 f_{TTV} t_{lin,m}) + D_m \cos(2 f_{TTV} t_{lin,m}). \quad (1)\end{aligned}$$

As can be seen from the formula, there are six parameters for each planet. For a two planet system this results in 12 free variables. In the equation, $t_{lin,m}$ is the linear ephemerus for planet m, f_{TTV} is the frequency, equal to $f_{TTV} 2\pi/P_{TTV}$ (with P_{TTV} the superperiod of TTV signals).

Using this model, a synthetic data set was generated with true parameters that correspond to the well-known double planetary system Kepler-307, which can be seen in figure 2. To make the simulated data more realistic, 5 minutes of Gaussian white noise was added to each data point.

TTVFaster Model

TTVFaster is a semi-analytic model that approximates TTVs using a series expansion, which can be thought of as a sum of multiple sinusoids. The parameters this model uses are the planet-star mass ratio μ, orbital period P, initial transit time t_i and eccentricity vector components k and h, which describe how much the orbit deviates form a circle and what its inclination is. With the TTVFaster model, three synthetic data sets were generated. One of the same Kepler-307 planetary system, and two more challenging ones of the Kepler-49 and Kepler-57 systems. The second system is more complex because it has a total of 4 planets, so the orbits of the inner planets are also slightly perturbed by the outer planets. The last system was chosen because previous studies had found some bimodality in the posteriors for the eccentricity components h and k.

For both models, the ln-likelihood is of the form:

$$\ln\mathcal{L}_m = -\frac{1}{2} \sum_{i \in N_m} \left(\left(\frac{\tau_{m,i} - T_{m,i}}{\sigma_{m,i}} \right)^2 + \ln(2\pi\sigma_{m,i}) \right), \tag{2}$$

where $m = 1, 2$ denotes the inner and outer planets respectively, $\tau_{m,i}$ gives the transit time calculated from the TTV model and $T_{m,i}$ corresponds to the measured transit times, with $\sigma_{m,i}$ the measurement uncertainties. The total ln-likelihood is then obtained by summing $\ln \mathcal{L}_m$ for both planets.

4. Methods

The samplers were evaluated on their sampling performance near the posterior maxima, so a burn-in period was ran first to put the starting points close to their optimal values. One of the problems with sampling from the posteriors of these models is that there are orders of magnitude differences between the values of the parameters. This makes it very difficult to choose a proper step size for the samplers. Also, there is quite a high correlation between some of the parameters, which leads to a slow sampling of the full parameter space. These issues were solved by applying a linear coordinate transformation, in order to rotate and scale the parameter space.

The efficiency of the six different samplers was compared by running 10,000 iterations on the four generated data sets, after burn-in. Two factors were taken into account when determining the efficiency: how well the posterior distribution was sampled from, and how long it took the samplers to complete the 10,000 iterations. The first point was investigated by looking at the Effective Sample Size (ESS) of the MCMC chains, which gives the number of effectively independent draws from the posterior distribution. A high ESS means that the chain has mixed well and therefore has a good estimate of the posterior distribution. For each sampler, two measures were computed: the mean ESS over the total elapsed time, and the minimum ESS over this time. For a high efficiency, these measures should give a high outcome. The sampler that was found to perform best was also used in a longer run to compute the posterior distributions of the parameters, so they could be compared to the true values of the models.

5. Conclusions

For the first data set, which was generated using the Simple Sinusoidal model, the **HMC** sampler is a clear winner, generating by far the highest ESS/time values. This sampler works really well if the posterior distributions are Gaussian. For the first data set made with the TVVFaster model (the Kepler-307 one), both the **HMC** and the **MALA** samplers score high. Figure 3 shows a corner plot of the posterior distributions of all the parameters. It can be seen that most of the parameters are uncorrelated, except for the eccentricity components h and k, and more weakly the planet mass ratios. The Kepler-49 system required a smaller stepsize and this led to another winner: the **GAMC** sampler performed the best for this data set. Finally, for the Kepler-57 system both **GAMC** and **DEMCMC** had the best efficiency. Altogether, this research shows that different samplers are suited for different scenarios. Choosing the right sampler can make a significant difference in computing time: the best performing samplers only took hours to converge, as opposed to weeks for the worst performing ones. Some samplers, such as GAMC and DEMCMC performed consistently alright for all the data sets, so these would be a safe choice. In future studies, the authors would like to investigate the effects of the sampler choice on the burn-in period and on more complex N-body TTV models.

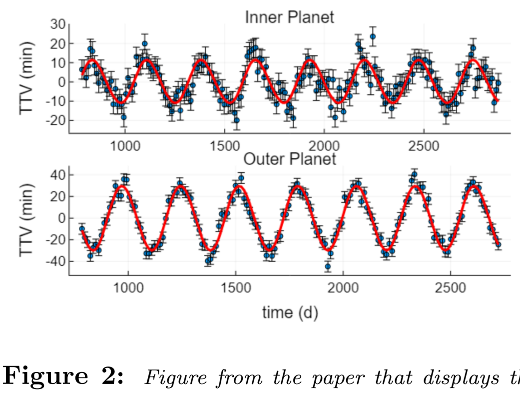

Figure 2: *Figure from the paper that displays the simulated data set from the simple sinusoidal model, with 5 min of Gaussian white noise. The red line shows the model's true parameters.*

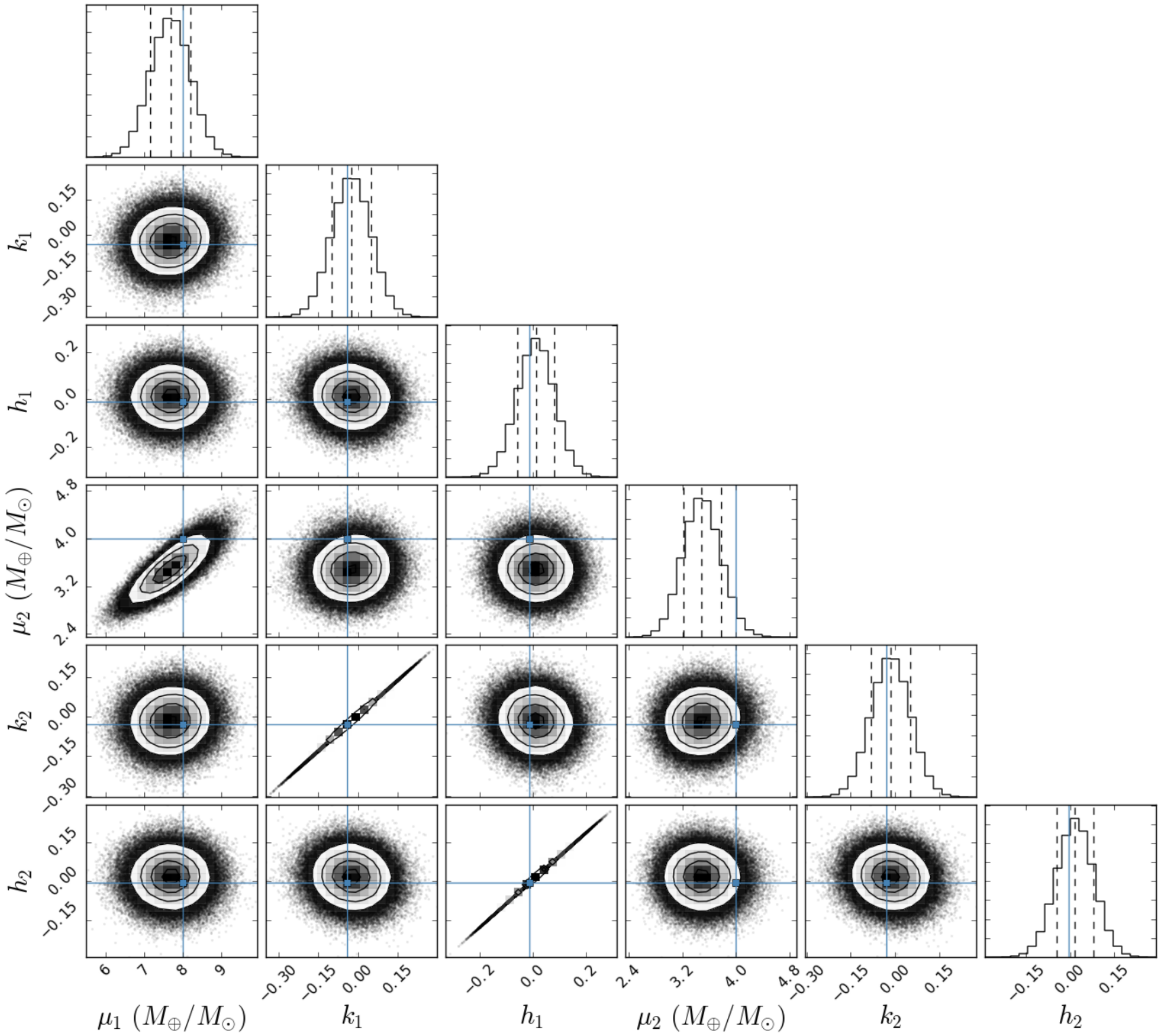

Figure 3: *Corner plot from the paper of the posterior distribution of the parameters from the TTVFaster model of the Kepler-307 planetary system. The HMC sampler was ran for 2 million iterations with a 500,000 burn-in period. The blue squares correspond to the true values of the parameters.*

References

- *The Efficiency of Geometric Samplers for Exoplanet Transit Timing Variation Models*, 2019, by Noah W. Tuchow, Eric B. Ford, Theodore Papamarkou and Alexey Lindo.
- *A Conceptual Introduction to Hamiltonian Monte Carlo*, 2018, by Michael Betancourt.
- *Markov Chain Monte Carlo Methods for Bayesian Data Analysis in Astronomy (Annual Review of Astronomy and Astrophysics)*, 2017, by Sanjib Sharma.