Exoplanet atmosphere evolution: emulation with random forests

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ABSTRACT
Atmospheric mass-loss is known to play a leading role in sculpting the demographics of small, close-in exoplanets. Understanding the impact of such mass-loss driven evolution requires modelling large populations of planets to compare with the observed exoplanet distributions. As the quality of planet observations increases, so should the accuracy of the models used to understand them. However, to date, only simple semi-analytic models have been used in such comparisons since modelling populations of planets with high accuracy demands a high computational cost. To address this, we turn to machine learning. We implement random forests trained on atmospheric evolution models, including XUV photoevaporation, to predict a given planet’s final radius and atmospheric mass. This evolution emulator is found to have an RMS fractional radius error of 1% from the original models and is ~ 400 times faster to evaluate. As a test case, we use the emulator to infer the initial properties of Kepler-36b and c, confirming that their architecture is consistent with atmospheric mass loss. Our new approach opens the door to highly sophisticated models of atmospheric evolution being used in demographic analysis, which will yield further insight into planet formation and evolution.

Key words: planets and satellites: atmospheres - planets and satellites: physical evolution - planet star interactions

1 INTRODUCTION

The observed exoplanet population is dominated by planets with ages of 1-10 Gyr (e.g. McDonald et al. 2019; Berger et al. 2020). Thus, it is distinctly separated in time from the formation process that happened early, in many cases within the first ~10 Myr of the planet’s life. In order to connect observed exoplanets to their origins we rely on the computation of evolutionary models to describe their possible histories.

This issue is perhaps most pertinent for the small (1-4) R½, close-in exoplanets (periods ≤ 100 d) that are now thought to represent one of the dominant exoplanet populations (e.g. Howard et al. 2012; Fressin et al. 2013; Silburt et al. 2015; Mulders et al. 2018; Zink et al. 2019). In many cases these planets are known to host H/He dominated atmospheres (e.g. Weiss & Marcy 2014; Jontof-Hutter et al. 2016; Benneke et al. 2019). Therefore, their proximity to the host star means they’re vulnerable to atmospheric mass-loss, wherein the extreme irradiation drives powerful hydrodynamic outflows that cause the planet’s atmosphere to lose mass (e.g. Baraffe et al. 2005; Owen & Jackson 2012; Erkaev et al. 2016; Owen & Alvarez 2016; Kubyshkina et al. 2018). It is now well established that this atmospheric loss sculpts the close-in exoplanet population and is thought to play a dominant role in creating both the exoplanet desert and radius gap (e.g. Owen & Wu 2013, 2017; Ginzburg et al. 2018; Owen & Lai 2018; Gupta & Schlichting 2019; Wu 2019; Owen 2019; Gupta & Schlichting 2020). However, the formation scenario for this planetary population is uncertain, and strongly debated (Bean et al. 2021). These planet’s bulk properties (mass and radius) vary significantly over their lifetimes due to a combination of cooling and mass-loss (e.g. Lopez et al. 2012; Owen & Wu 2013). Thus, computation of their evolution is critical to unravelling their formation, since one can statistically constrain a planet’s formation properties by determining which initial conditions can evolve into the planet we observe today (Rogers & Owen 2021).

However, atmospheric-loss driven evolution is convergent: there are many initial planetary conditions that can evolve into an exoplanet with observationally indistinguishable bulk properties. This convergent evolution arises from both cooling and mass-loss. An initially hotter, higher entropy planet cools faster, meaning it reaches the same thermodynamic state as a planet that started cooler, with a lower entropy. Similarly, planets with a more massive initial atmosphere are larger, and as such can drive more powerful outflows, meaning it reaches the same atmospheric mass as a planet that started with a less massive atmosphere.

Nevertheless, this convergent evolution does not mean a planet’s initial conditions are completely lost. In fact evolutionary modelling can provide important constraints that are inaccessible using only measurements of mass and radius for an evolved planet. Specifically, evolutionary modelling in both the photoevaporation and core-powered mass-loss scenario has indicated the core-composition of sub-Neptunes is an “Earth-like” iron-rock mixture (e.g. Owen & Wu 2017; Wu 2019; Gupta & Schlichting 2019; Rogers & Owen 2021). Furthermore, the link between planet radius, entropy and mass-loss mean a planet’s initial thermodynamic state is not completely lost. Specifically, a lower bound on a planet’s initial cooling time (the Kelvin-Helmholtz timescale) can be determined because a planet with an even shorter cooling time would be larger and would have lost too much mass (e.g. Owen 2020).
However, to fully and statically characterise these plausible initial planetary conditions requires the computation of a large number of evolutionary models, and to do this at a population level is extremely computationally challenging. For example, to extract population level constraints on the exoplanet population at formation Rogers & Owen (2021) evaluated $\sim 10^{10}$ planetary evolution models. To make this computationally feasible, a simplified, semi-analytic evolutionary model was used. However, even in this work, it could only be applied over a narrow range of stellar mass and expected correlations (for example between core-mass and initial atmospheric mass) were not taken into account.

Thus, if we desire to be able to use evolutionary models for population level statistical inference we must consider a new, more computationally efficient approach. This is all the more pertinent if we want to use accurate evolution models that include, for example a real equation of state, radiative transfer with atmosphere models and self-gravity. Fortunately, machine-learning provides an answer. Instead of solving the planetary structure and evolution equations for each planetary model one wishes to evolve, we can use a machine-learning model to emulate the planet’s evolution. In this letter, we construct an exoplanet evolution emulator which is trained on models of XUV photoevaporation, testing it on the mass-loss benchmark system Kepler-36.

2 EVOLUTION EMULATOR

As a demonstration, we choose to train the evolution emulator with the semi-analytic model of the evolution of an exoplanet’s H/He atmosphere from Owen & Wu (2017). This model calculates the evolution of a planet’s photospheric radius and atmospheric mass-fraction as its primordial H/He atmosphere cools and experiences mass-loss due to XUV driven photoevaporation. We refer the reader to Owen & Wu (2017); Rogers & Owen (2021) and references therein for the technical details of this model.

To emulate the atmospheric evolution we turn to supervised machine learning. The goal is to predict the photospheric radius and atmospheric mass-fraction as its primordial H/He atmosphere cools and experiences mass-loss due to XUV driven photoevaporation. We refer the reader to Owen & Wu (2017); Rogers & Owen (2021) and references therein for the technical details of this model.

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![Flowchart to demonstrate the atmospheric evolution emulator.](image)

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2.1 Emulator design

The design of our emulator, as shown schematically in Figure 1, is a two step-approach with all adopted algorithms taken from scikit-learn (Pedregosa et al. 2011). In the photoevaporation model, the transition from a sub-Neptune (i.e. cores with extended H/He atmospheres) to a super-Earth (i.e. stripped cores) is quick since the mass-loss timescale drops rapidly for atmospheric mass fractions $\lesssim 1\%$, resulting in a runaway process (Owen & Wu 2013; Lopez & Fortney 2013; Owen & Wu 2017; Mordasini 2020). Thus, the outcome of exoplanetary evolution is essentially bimodal. This bimodality motivates our two-step approach: we begin by implementing a random forest classifier to determine whether a given planet will evolve to become a super-Earth or a sub-Neptune. Since the planets that become super-Earths have a negligible atmospheric mass fraction, the final radius for these is simply given by the mass-radius relation of the stripped cores. For the sub-Neptunes we employ a second machine learning algorithm, in this case a random forest regressor, to predict the final radius and atmospheric mass fraction of a the sub-Neptune. We note that random forests were chosen over other machine learning algorithms such as support-vector machines and gradient-boosted linear regression. These alternative algorithms yielded inferior performance or required more training to achieve the same accuracy as our random forest approach.

To train the machine learning models, $10^6$ planets were simulated to 5 Gyrs with the semi-analytic photoevaporation model of Owen & Wu (2017), with the input parameters $\{P, M, M_\text{core}, \rho, X_\text{init}\}$ uniformly drawn such as to sample parameter space evenly. In this case, the bounds were as follows: $P \in [1, 100]$ days, $M_\star \in [0.5, 1.5] M_\odot$, $M_\text{core} \in [0.6, 20.0] M_\oplus$, $\rho \in [-1.0, 1.0]$ and $\log X_\text{init} \in [-4.0]$. Random cross-validation was used to optimise the performance of the random forest classifier and regressor, which yielded highest accuracy when both contained 19 decision trees.

Swapping a physical model for a machine learning emulator will dramatically decrease the computational expense of calculations. In our case, it was found that for an equivalent set of planets, the emulator has a computational speedup factor of $\sim 400$. This speed-up is all the more impressive as our standard evolutionary model was heav-
ily optimised, whereas no such optimisation was undertaken on the evaluation of the emulator. This indicates that speedups of $\gtrsim 1000$ are potentially achievable.

However, the trade-off for an improved speed is the introduction of output error. Overall, the accuracy of the classifier was found to be 99.98%, with very occasional planets being misclassified as a sub-Neptunes when they should be super-Earths. This latter point highlights a drawback of the semi-analytic model in which planets with low atmospheric mass fraction are inaccurately modelled, which we discuss in Section 4. The RMS fractional error for the sub-Neptune regressor was 1%. This value is significantly smaller than typical radii measurement uncertainties of $\sim 5\%$ (Fulton & Petigura 2018), implying that it is suitable for use in comparing large number of evolutionary models to the observed properties of bulk exoplanets. The RMS fractional error in final atmospheric mass fraction was found to be 0.5% and since the mass of a planet is dominated by the core, this introduces a negligible error in final mass. In Figure 2, we show planets in the radius-period plane evolved using the semi-analytic photoevaporation model in orange and evolution emulator in blue. One can see that the occurrence is near-indistinguishable. We also show the errors of the emulator in Figure 2, which are largest for larger planets with higher initial atmospheric mass-fraction. Despite constructing a training sample with uniformly drawn parameters, this does not evenly sample $R_1^g$ or $X_1^g$-space. Since the majority of planets evolve to smaller radii, this area of parameter space is more sparsely populated in the training data and hence accuracy is lower here.

### 3 INFERRING PLANETARY INITIAL CONDITIONS

The primary goal for developing an evolution emulator is its use in demographic analysis. This task is left for future work in which the emulator would be trained on more accurate models of atmospheric evolution, as discussed in Section 4. However, we test the emulator here by implementing it to infer the initial conditions of Kepler-36b and c (Carter et al. 2012; Vissapragada et al. 2020). This archetypal system consists of an inner super-Earth (Kepler-36b) with orbital period of 13.9 days, with observed mass and radius of $3.83 \pm 0.11 M_\oplus$ and $1.50 \pm 0.06 R_\oplus$ and an outer sub-Neptune (Kepler-36c) at 16.2 days with mass and radius of $7.13 \pm 0.18 M_\oplus$ and $3.68 \pm 0.06 R_\oplus$. This architecture is highly indicative of mass-loss, and is well explained by previous photoevaporation modelling (e.g. Lopez & Fortney 2013; Owen & Morton 2016; Bodenheimer et al. 2018). Due to its presence near resonance (Carter et al. 2012), allowing detection of large amplitude TTVs, it is one of the only systems in which both mass and radius are well constrained for a system with a super-Earth and sub-Neptune at present. In a similar manner to Owen & Morton (2016), we set up a Bayesian model in which we aim to place constraints on the core composition $\bar{\rho}$, core masses $M_{core}$ and initial atmospheric mass fractions $X_{init}$ required to evolve into the two planets that we observe today. Thus for our model parameters $\theta = (\bar{\rho}, M_{core,b}, M_{core,c}, X_{init,b}, X_{init,c})$ and observed mass and radius data $D = \{R_{obs,b}, R_{obs,c}, M_{obs,b}, M_{obs,c}\}$, we may write from Bayes’ law:

$$P(\theta|D) \propto P(D|\theta) P(\theta),$$

where $P(\theta|D)$ is the target posterior, $P(D)$ is the prior and assumed to be flat for core masses and core compositions and log-flat for initial atmospheric mass-fractions. Since both planets were formed in the same environment, we follow Owen & Morton (2016) and assume the core composition is the same for both planets. The likelihood function $P(D|\theta)$ is modelled as a Gaussian:

$$P(D|\theta) \propto \prod_i \exp\left(-\frac{(R_{\theta,i} - R_{\text{obs},i})^2}{2\sigma_{R_i}^2} - \frac{(M_{\theta,i} - M_{\text{obs},i})^2}{2\sigma_{M_i}^2}\right),$$

where $i = \{b, c\}$ and $\sigma_{R_i}$ and $\sigma_{M_i}$ are the measurement uncertainties in radius and mass from transit and TTV observations for each planet. We evaluate the posterior by calculating the radius and mass of Kepler 36b and c for a given set of parameters $\theta$ using the evolution emulator. In addition, we also take the observed orbital periods and stellar mass from the planetary system which is used as model

![Figure 2. Left: The radius gap computed with the semi-analytic model of XUV photoevaporation (orange) and with the evolution emulator (blue). Contours represent relative occurrence and individual planets are plotted in black. Right: A population of planets are shown with their periods and final radii according to the semi-analytic model, with arrows pointing to this position as predicted with evolution emulator. They hence represent the error between physical model and emulator for each planet. Note that the majority of planets do not have arrows since the error is negligible. Colours represent the initial atmospheric mass fraction. Whilst the average RMS error for the emulator is 1% (as most planets have radii of either 1.3 or 2.5 $R_\oplus$), the right-hand histogram shows this error as a function of radius. A typical radius measurement uncertainty is shown in black, taken from the value in the CKS catalogue (Fulton & Petigura 2018).]
input. To account for the measurement uncertainty in these quantities, we randomly redraw them from their associated errors every time the likelihood function is evaluated. To sample the posterior we use the affine-invariant Monte Carlo Markov Chain (MCMC) package (Foreman-Mackey et al. 2014). We run the chain with 100 walkers until convergence is confirmed with a chain of 50 auto correlation times.

In Figure 3, we show marginalised posteriors for the core composition, core masses and initial atmospheric mass fractions for the Kepler-36 system, as calculated by the evolution emulator. We also show posteriors which have been calculated with the semi-analytic model, which yield very similar results. As found in Owen & Morton (2016), both planets are inferred to have a core composition consistent with that of Earth ($\rho_\text{c} \approx 3.3$), with Kepler-36b being a stripped core with an upper limit on its initial atmospheric mass fraction of $\sim 1\%$. Kepler-36c, however, is inferred to have a core mass of $6.5 \pm 0.2M_\oplus$ which originally hosted a H/He atmospheric fraction of $\sim 20\%$. This was then partially photoevaporated, producing a sub-Neptune with a substantial remaining H/He atmosphere.

4 DISCUSSION

The results shown in Figures 2 and 3 clearly show that the evolution emulator is capable of reproducing the demographics and constraints provided by the semi-analytic model, whilst crucially being dramatically quicker to compute. We note that the work of Owen & Morton (2016), which also placed constraints on the initial conditions of Kepler-36b and c, implemented evolutionary models of photoevaporation using the stellar and planetary evolution code MESA (Paxton et al. 2011, 2013). Whilst being more accurate than the semi-analytic model adopted for training in this work, the computational expense was far greater since a grid of simulations were produced and interpolated in the MCMC sampling. The number of simulations required to train the two-step emulator is less than required to perform interpolation since information on the entire parameter space is used to inform the final output, making the process more efficient. Furthermore, it is important to emphasise the issue of over-fitting is not of concern in this machine learning application, since the models do not introduce noise that the emulator may be unintentionally trained on. This is because a single set of planetary and stellar conditions always produces the same planetary evolution track.

The adopted semi-analytic model of planetary structure is known to perform poorly when the atmospheric mass fraction falls to small values, such that the radiative zone of the atmosphere starts to dominate both the radius and envelope mass. Since the evolution emulator can be trained on more complex simulations that do not suffer from such issues, one could construct and train the emulator on a suite of planetary evolution simulations that incorporate appropriate radiative transfer, equations of state and self-gravity (e.g., those determined by MESA Owen & Wu 2013; Chen & Rogers 2016; Kubyshkina et al. 2020). One could also incorporate additional physics from alternative mass-loss models such as core-powered mass-loss (e.g. Ginzburg et al. 2018; Gupta & Schlichting 2019; Rogers et al. 2021) to investigate how the two mechanisms compete.

In this work, the emulator was trained with input parameters of orbital period, stellar mass, core mass, core density and initial atmospheric mass fraction. As a further improvement, one could include additional parameters such as the cooling timescale of the planet, efficiency of photoevaporation and the final age of the system. We note that the likelihood function is evaluated. To sample the posterior we use the affine-invariant Monte Carlo Markov Chain (MCMC) emulator (dashed), yielding very similar results.

Figure 3. Marginalised posteriors are shown for the composition, core masses and initial atmospheric mass fractions of Kepler-36b (top row) and Kepler-36c (bottom row). These are calculated with the semi-analytic model of XUV photoevaporation from Owen & Wu (2017) (solid) and the machine learnt evolution emulator (dashed), yielding very similar results.

Kepler-36b, $P_b = 13.9$ days, $R_b = 1.50 \pm 0.06 R_\oplus$, $M_b = 3.83 \pm 0.11 M_\oplus$

Kepler-36c, $P_c = 16.2$ days, $R_c = 3.68 \pm 0.06 R_\oplus$, $M_c = 7.13 \pm 0.18 M_\oplus$
that this latter variable has little effect on the final radius of a planet under the photoevaporation model since the majority of mass-loss occurs during the first ~ 100Myrs. Since the majority of observed exoplanets, including Kepler 36b and c orbit main-sequence stars, it implies that age is not a dominant parameter. However, the small fraction of planets that the emulator misclassifies are those that are being stripped on Gyr timescales. Therefore, adding age as a parameter is likely to reduce this error since the emulator will learn this trend. Furthermore, if additional physics is included such as core-powered mass-loss which operates at much longer timescales, one would also require system age as an input.

5 CONCLUSIONS

We have shown that an emulator, trained on a model of the evolution of an exoplanet’s H/He atmosphere, is capable of accurately predicting the final properties of an exoplanet at a fraction of the computational expense of standard evolutionary models. Given the exoplanet evolution results in a bimodal population of super-Earths and sub-Neptunes, we implement an emulator that consists of a random forest classifier which separates planets which are either stripped, or maintain their primordial H/He atmosphere. Whilst an additional random forest regressor is used to predict the radius and atmospheric mass fraction of the planets which host atmospheres. We find that the fractional RMS error introduced in final radius is ~ 1%, when compared to the original model, significantly smaller than even the best measurements of an exoplanet’s radius (for example using asteroseismology, e.g. Van Eylen et al. 2018). The computational speed up factor is ~ 400 even without any optimisation.

As a test-case, we use the evolution emulator to infer the initial conditions of Kepler 36b and c (Carter et al. 2012; Vissapragada et al. 2020). We find results that are consistent with that of Owen & Morton (2016), in which the inner planet is stripped, whilst the outer planet has maintained a H/He atmosphere which was originally ~ 20% before photoevaporation took place.

Although the emulator is clearly accurate and fast, there are many aspects in which it may be improved. Instead of simple evolutionary models, sophisticated numerical simulations with higher accuracy should be used for training. Furthermore, other parameters such as system age and initial cooling timescale may be used as inputs. Finally additional physics may be included in the training data, such as core-powered mass-loss (Ginzburg et al. 2018; Gupta & Schlichting 2019).

Overall, this work has demonstrated that this tool is well-suited for demographic inference analyses such as that of Rogers & Owen (2021), in which the photoevaporation model was used to infer the core mass, core composition and initial atmospheric mass fraction distributions of the entire California Kepler Survey (Fulton et al. 2017). This analysis required the modelling of 10^{10} planets and was hence extremely computational expensive, despite only using the simple exoplanet evolution model of Owen & Wu (2017); Owen & Campos Estrada (2020). Implementing an evolution emulator will remedy this issue and thus allow investigation into potential correlations between distributions and the imprint of competing mass-loss mechanisms on the demographics of exoplanets.

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DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding author.

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