Rediscovering Newton's gravity and Solar System properties using deep learning and inductive biases

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Introduction

We show how ML methods can exploit established scientific frameworks to discover accurate physical laws and unobserved properties, in an analogous fashion to how scientists develop theories consistent with observations. Our approach is based on the framework introduced by (Cranmer et al., 2019; Cranmer et al., 2020) which used a combination of graph networks (GN) (Battaglia et al. 2018) and symbolic regression. The key principle is that the "edge function'" within the GN has a correspondence to forces. By training a GN to simulate orbital dynamics from real data, we were able to extract the edge function and correctly infer the formula for Newtonian gravitation. We also structured the GN-based simulator to predict accelerations by multiplying the model output by a scalar variable fit during training (corresponding to *force = mass X acceleration*) and found the learned scalars were proportion to the orbital bodies' true masses.

Approach

Our two-step approach---training a GN-based simulator, then using symbolic regression to find analytical formulae for forces---is summarized in Fig. 1: The input is a GN with given distances as edges, and nodes with learnable scalar properties. The GN updates the edges of this graph to compute forces. We then sum over all forces acting on each body (assuming that $F_{i,j} = -F_{j,i}$) and divide by the nodes, to get accelerations. The loss function is obtained by comparing this predicted acceleration and the true acceleration. The function that the GN learned to update the edges is also used to recover an algebraic force using a symbolic regression algorithm.

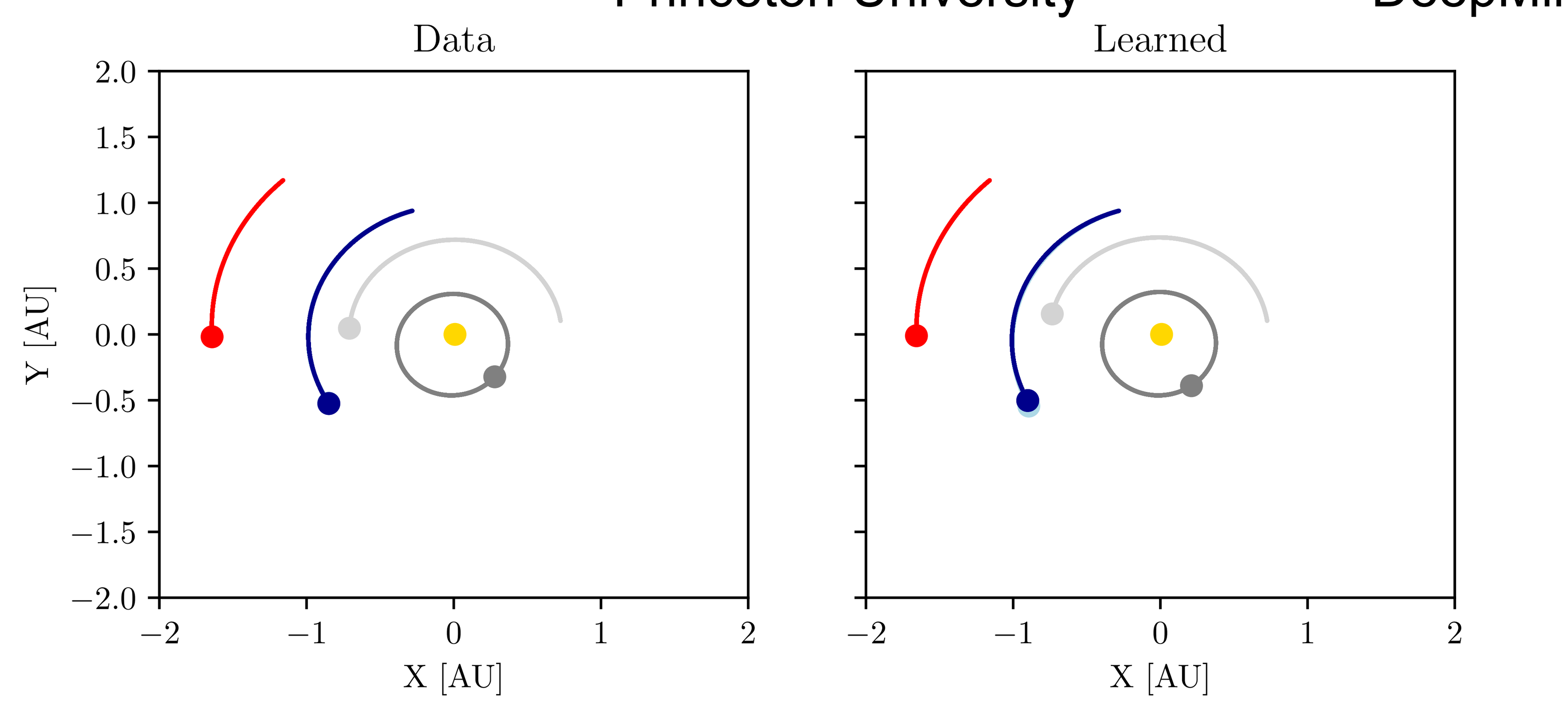

Fig. 2: *Left:* data from the bodies of the inner Solar System. *Right:* same bodies evolved from same initial conditions using the learned interaction.

Methods

- **Data:** We use Solar System data from NASA's HORIZONS On-Line Ephemerys System. We extract orbits for the Sun, all planets, and the moons that have a mass above $10^{18} M_{\odot}$. In total, our problem consists of 31 bodies, listed in Fig. 3.
- **Loss function:** Due to the varying orders of magnitude in our target data (accelerations), we weighted the loss function by the true accelerations.
- **Spherical coordinates & exponentials:** To deal with the large data ranges, we converted vectors to spherical coordinates, and took the logarithm of the magnitudes. We also exponentiate the learned scalars before converting forces to accelerations.
- **Data augmentation:** During training, we perform a random 3D rotation of the data at each step. This allows us to augment the data, and solves the issues of incomplete orbits in the data.
- **Different biases:** We attempted to repeat the process relaxing the *Force = mass X acceleration*, however in this case our algorithm learns an arbitrary function of the mass, which means the symbolic regression no longer works.

Results & Conclusions

Our MLP successfully finds an interaction between bodies that matches the observed acceleration. This shows that GNs can learn interactions not only from simulations, but also from real data (Fig. 2).

The scalar properties learned by our MLP, which are learned during training and multiplied by the forces to compute the accelerations, are shown in Fig. 3 along with the masses per body. When applying the symbolic regression we recover Newton's law of gravity.

Our results show that our two-step approach is a viable tool for discovering physical laws from real observations. Even though the law we discovered is already know, the purpose of this work is to confirm that known laws are *discoverable* with our method. This is a key step toward building more sophisticated tools for automating the process of scientific discovery, in particular data-driven theory formation and evaluation.

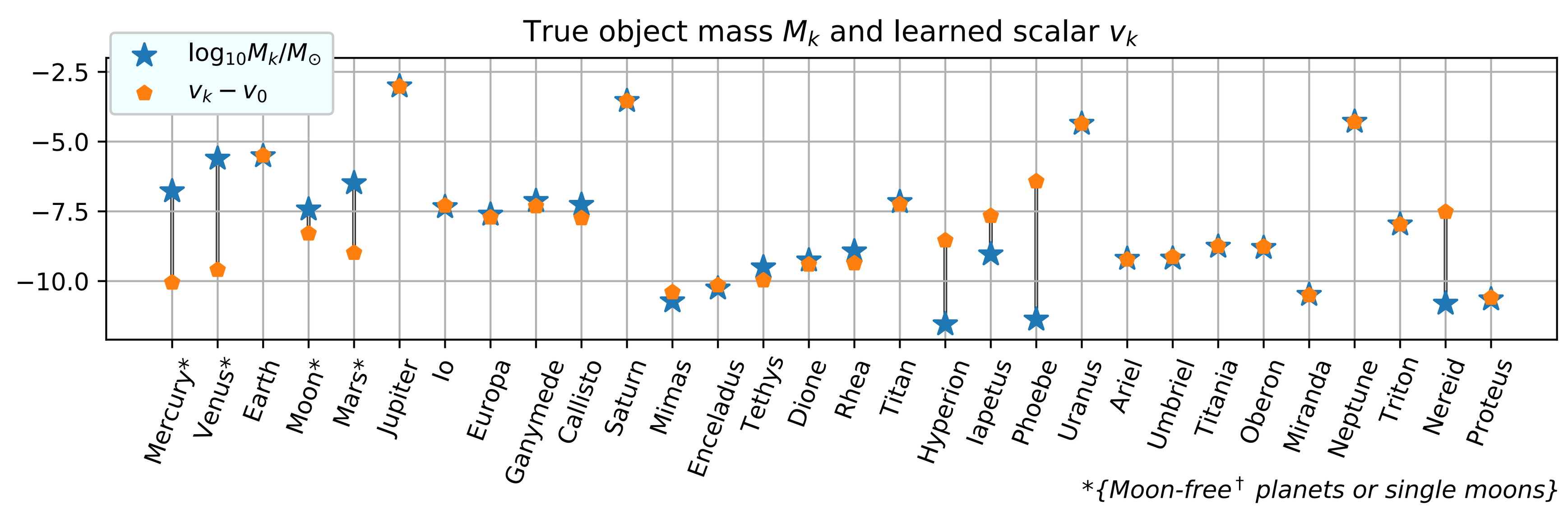

Fig. 3: Comparison of the learned scalars v_k relative to the Sun and the known logarithmic masses.

Main References

M. Schmidt and H. Lipson (2013). "Distilling free-form natural laws from experimental data." In: Science, 324(5923):81-85, 2009.

M. Cranmer et al. (2019). "Learning Symbolic Physics with Graph Networks.". In: arXiv e-prints, arXiv:1909.05862.

M. Cranmer et al. (2020). "Discovering Symbolic Models from Deep Learning with Inductive Biases.". In: arXiv e-prints, arXiv:2006.11287.

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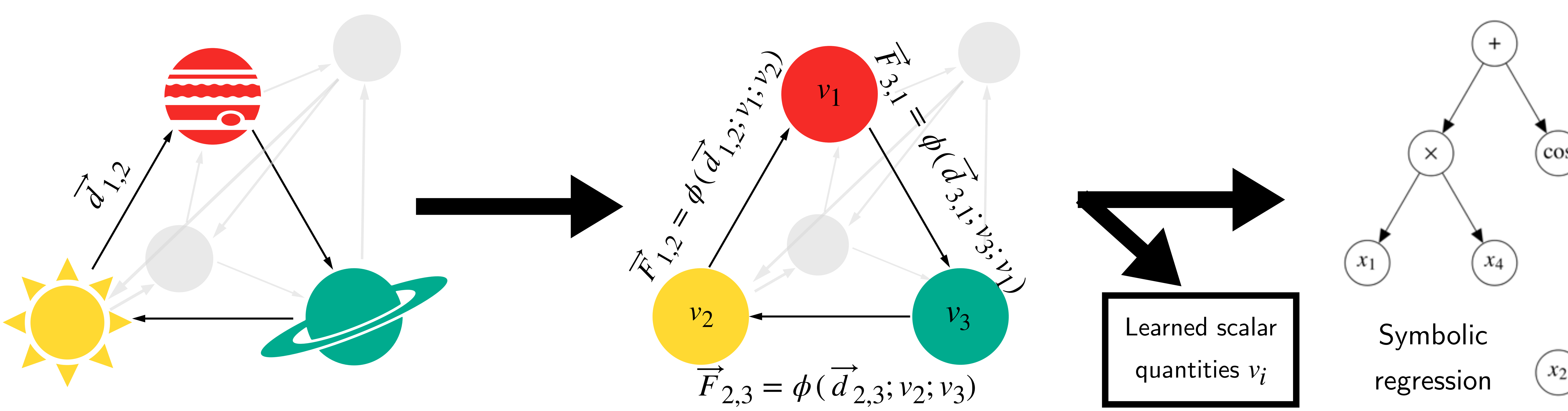
More references can be found in the paper.



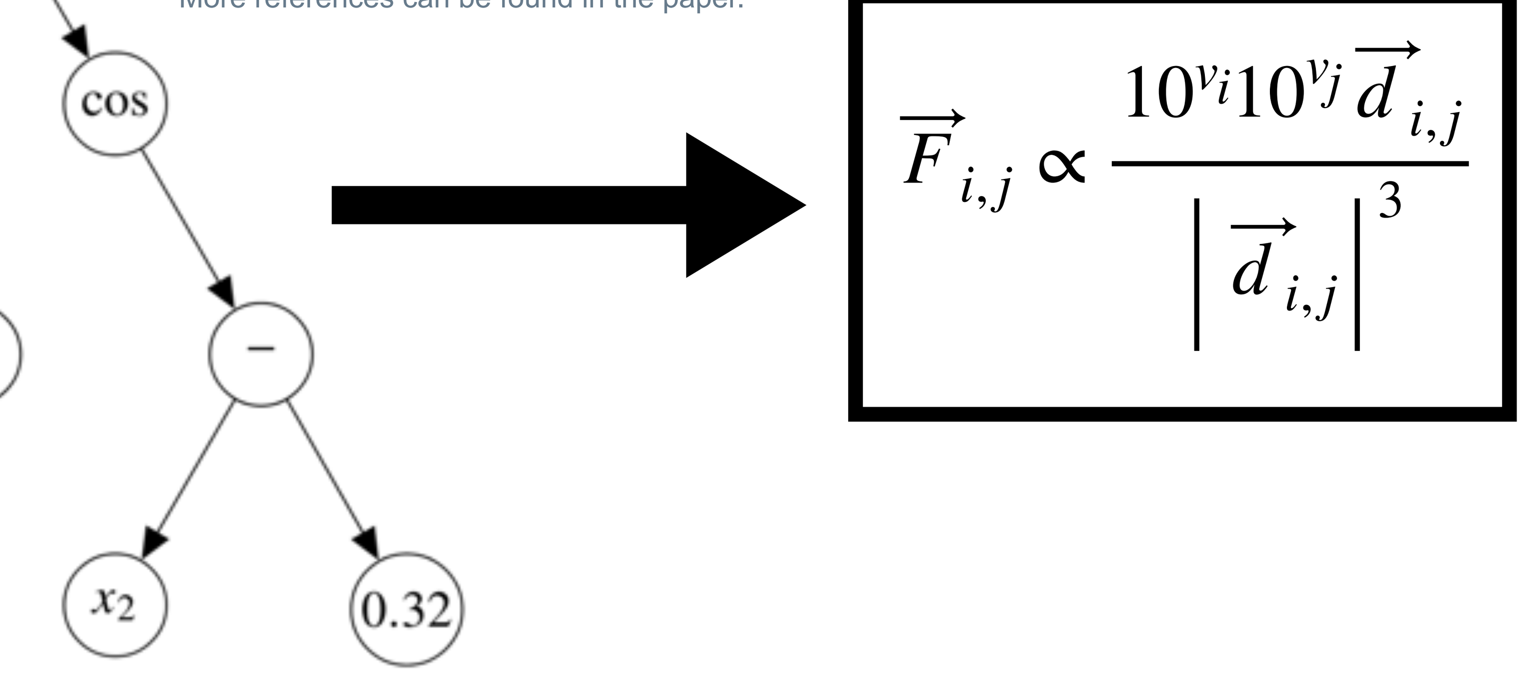


Fig. 1: Summary of our two-steps approach.