Robot Scientist for Droplet Friction Experiments

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For centuries, the (semi-)automation of science has been a dream for humankind, and recent advancements in artificial intelligence have brought us closer to achieving this goal. The goal of this work is to develop the first complete robot scientist in physics. For this, we bring together, up to now, disjoint research directions: (i) automation and autonomy in science and (ii) equation discovery. By integrating equation discovery, the results of the discovery process are understandable for human scientists. The proposed test system comes from the field of soft matter physics and involves studying the motion of droplets sliding down an inclined plane [1].

We envision a closed loop system which consists of 6 modules. The starting point is the **(1) fully automated droplet friction experiment**. The robot can freely choose between different liquids, surface materials, and tilt angles of the inclined plane. The sliding droplet is monitored with cameras, and its properties such as width w, mass m, length l, height h, viscosity η, contact angle θ, and speed v are measured. Additionally, the acceleration is calculated by using the time difference between the measurements. Using this acceleration, the friction force F_f is the difference between the gravitational force $F_G = mg\sin(\alpha)$ and the kinetic force $F_a = ma$. The calculated friction force is the target value in the next module **(2) equation discovery**. Here, the robot scientist seeks an equation that directly calculates the friction force based on the measured droplet characteristics. The most promising equations for different experimental setups are used to **(3) find a master equation**, which abstracts from the individual experiments and is a general equation that describes all experiments. The difference (residuals) between the general equation and the measured friction forces are modeled with a **(4) Gaussian process**. The Gaussian process estimates the error surface and its uncertainty for the entire feature space. Combining both makes it possible to trade off exploration vs. exploitation, find areas where all proposed equations have difficulties, or separate suggested equations. In the next step, the robot scientist **(5) decides which data point to measure next**. Finally, a **(6) prediction for this requested data point** is given either via a neural network that models the experiment or an experiment planner module, which designs an experiment to measure the real friction force.

Currently, two equations are given in the literature to calculate the friction force in a droplet $F_f = w\gamma k(cos\theta_r - cos\theta_a)$ or $F_f = F_0 + \beta w\eta v$, where k, F_0 and β are setup dependent constants. These equations have been developed by humans over years of scientific work. In a first step, we simulate the friction force experiment, but with the real data from the experiment and noise added. The robot scientist is already able to rediscover the first equation using modules 1 (simulated experiment), 2 (equation finding), and 4 (Gaussian process). As soon as the automation of the experiment is completed, we will investigate if the robot scientist confirms one of the two proposed equations, or even suggests a new equation.

References

[1] Xiaomei Li et al. “Kinetic drop friction”. en. In: *Nat Commun* 14.1 (July 2023). Number: 1 Publisher: Nature Publishing Group, p. 4571.

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