Empirical Solution of the Brachistochrone Curve and Data Analysis of the Periodic Table

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1 Introduction

After spending some time working on my Final, I decided to focus on educational applications of python. I'm going back to teaching after this school year and I plan on implementing python in my high school courses because I wish that I was introduced to coding much earlier in my educational career. I decided to choose two topics out fundamental science education and build out some examples that I can use in my classroom and provide to others to use in theirs.

For the first portion, I will use "optimize" in order to test various solutions of the brachistochrone curve. Optimize is still difficult for me to use, so I had to rely on a tutorial to use it to correctly calculate a complete time integral of the various pathways tested. I will also admit that I was not able to fully achieve my desired goal for this section, as it was too lofty for my skill level, but I will discuss what I wanted to do and machine learning solutions I was able to find for the problem. I was able to read them over, but I wasn't able to get them to work in jupyter notebook.

For the second portion I use a combination of "pandas" and "seaborn" in order to analyze various trends of the periodic table. The periodic table properties of elements was the easiest to find yet robust data set that I could find. I put the data into an excel sheet and used the xlsl commands in order to read the periodic table data into python. I used various seaborn graphing options in order to visualize the various periodic trends. I teach chemistry next year and the graphs produced by seaborn are the best I've seen to represent classic periodic trends. Not only do I plan on using these graphs in my lectures next year, I also plan on making the use of this periodic table excel file in my chemistry class. Even chemists can benefit from a little python.

I'm not a python master, and I have to rely a lot on google and github but thanks so much for a great semester. I'm excited to develop the skills I've started in your class.

2 The Brachistochrone

The Brachistochrone is the solution to the deceptively simple question: what is the fastest pathway from a to b under some constant, downward acceleration? It is a combination of two greek words which literally translates to "shortest time". The problem was posed by Johann Bernoulli in June of 1696 as a challenge to the mathematical world of the time. Despite having retired from mathematics and science in order to be the Warden of the Royal Mint, Isaac Newton solved the problem and submitted his work anonymously to the Philosophical Transactions, a respected journal of the time.[Sanderson and Strogatz 2016] Newton determined that the fastest pathway for a particle under some gravity like acceleration is that of a cycloid, which is the path way traced by a point on the edge of a rolling circle. Newton submitted it anonymously but the solution was so good that Bernoulli said that he could "regonize the tiger by his claw".

$$C = \frac{sin(\theta)}{\sqrt{y}} \tag{1}$$

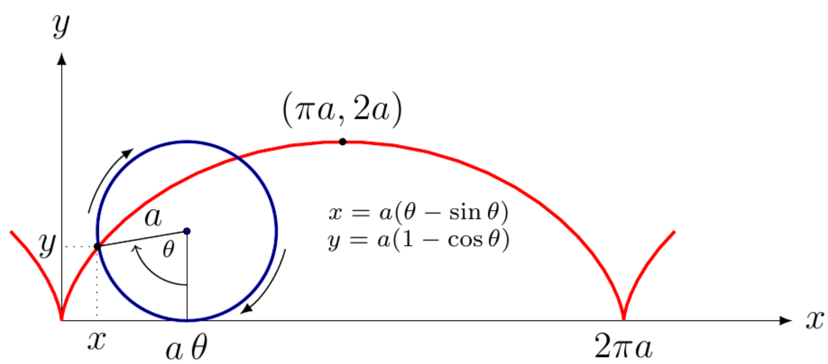

Figure 1: The red pathway is that of the brachistochrone curve. It is traced out by one point on the edge of a rolling circle. Traveling this curved pathway minimizes the time necessary for an object, accelerated by gravity only, to travel.

This solution is a classic problem given to upper division undergraduate students and starting out graduates in physics and engineering. It can be solved by several different models and approaches. It is most often solved as a differential equation problem, which is then time minimized. The resulting trigonometric functions produce a cycloid. However, other approaches exist which produce the same solution. In its original solution by Bernoulli, it was imagined as light traveling through glass of an ever increasing index of refraction as it travels downwards. The ever increasing index of refraction reflects the increasing velocity due to gravity. Bernoulli phrased it in this way because this is how the motion of light was phrased in the 1600's, as automatically traveling the pathway of minimum time. This approach using Snell's law also produces a brachistochrone curve!

Modern approaches (which I failed to implement) can use genetic algorithms in order to produce a brachistochrone curve. You start by giving the algorithm a goal of traveling from the origin to a designated location by random walk. Walks in the -y direction lead to the next step in the y direction becoming slightly larger in order to account for the acceleration due to gravity. Given an initial guess at a solution of a straight line from the origin to the designated location, over successive generations given the goal of minimizing time, this approach will also approach the brachistochrone curve. [Oller n.d.] In my opinion, this is the coolest solution but its important that all three approaches give the same answer.

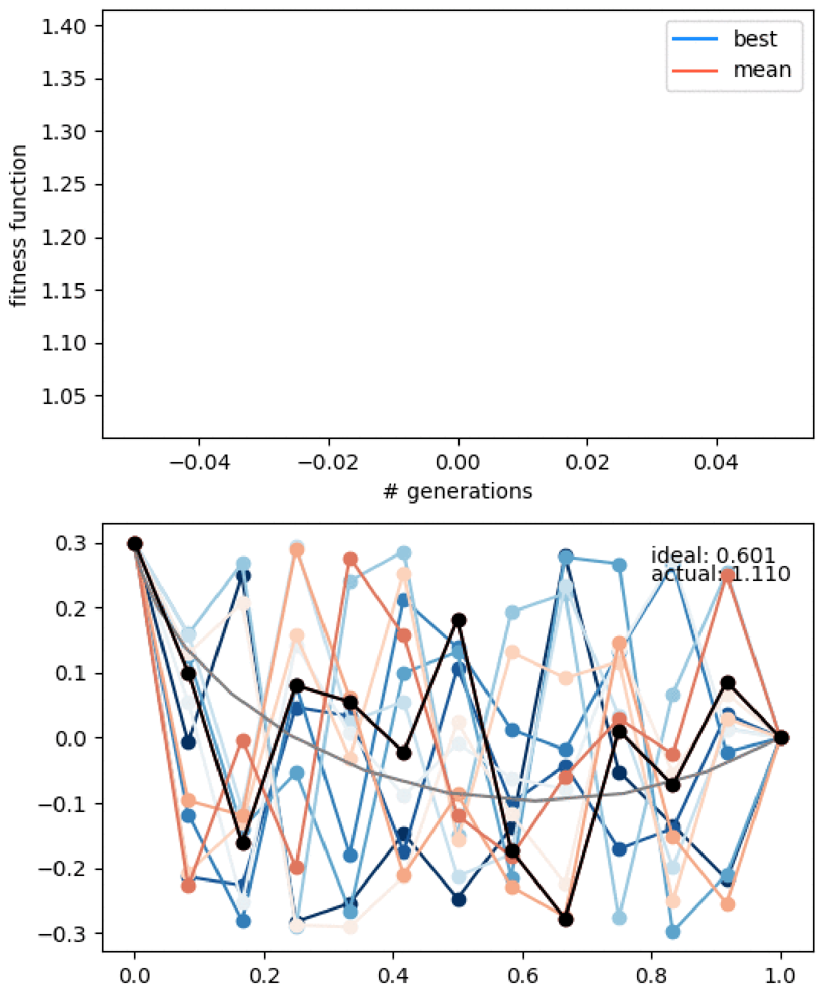

Figure 2: First generation of a genetic algorithm figuring out the brachistochrone, written by Oller. At this stage, the random walks are very random.

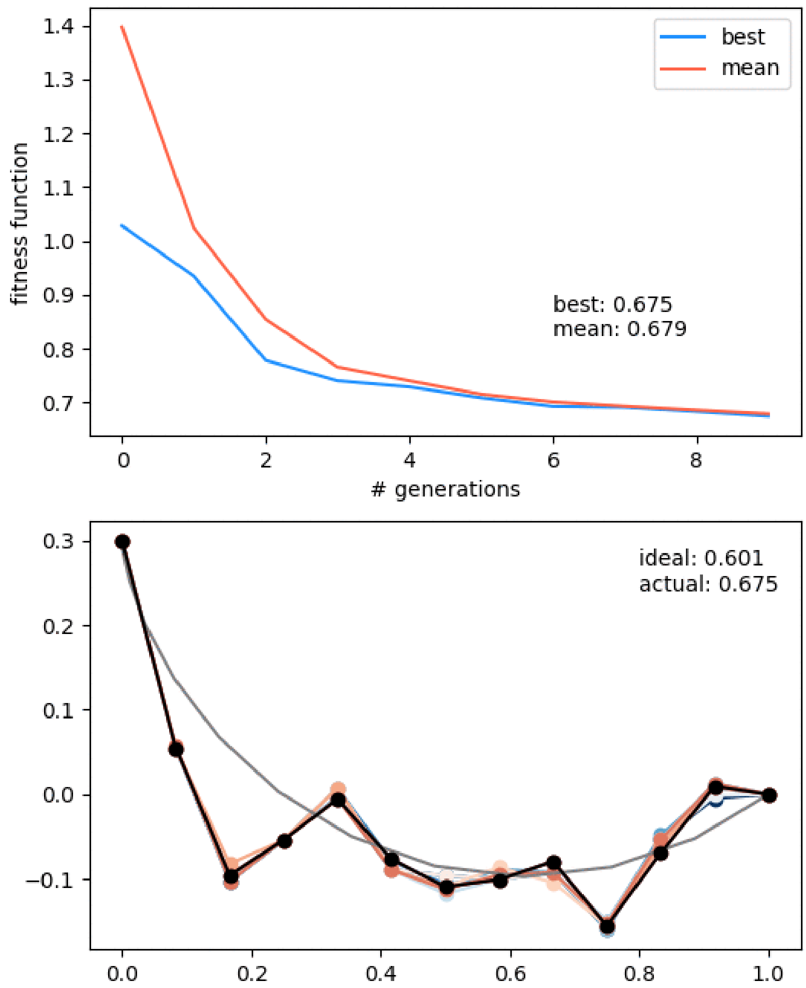

Figure 3: Eighth generation of a genetic algorithm figuring out the brachistochrone.

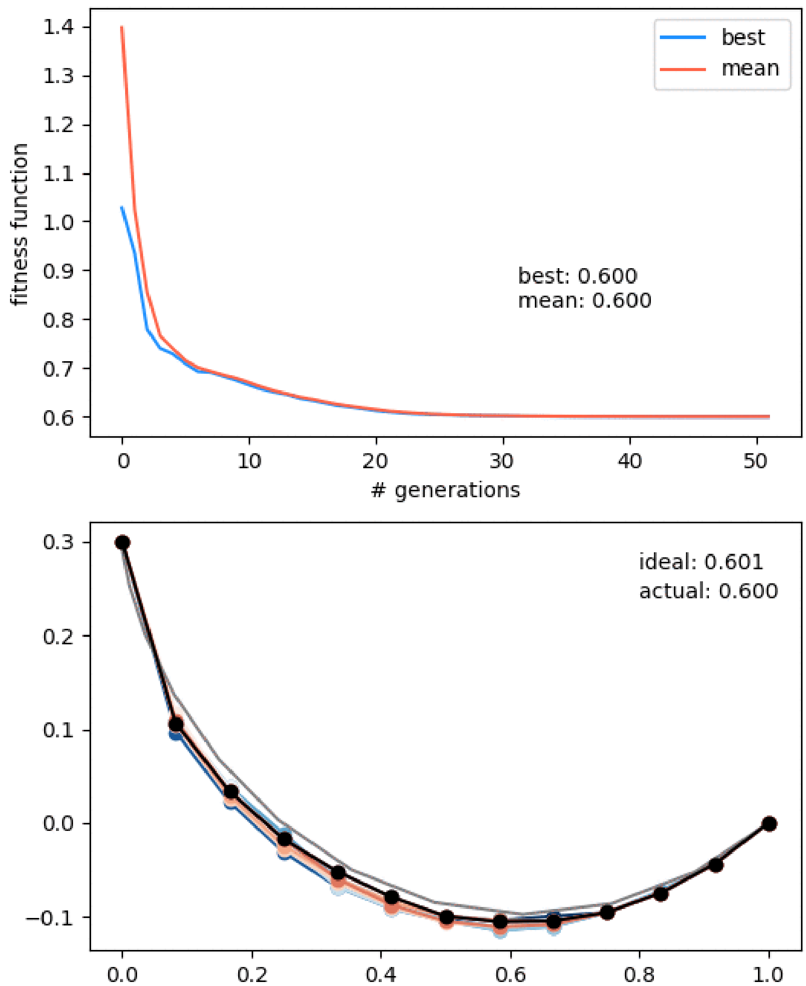

Figure 4: Fiftieth generation of a genetic algorithm figuring out the brachistochrone. At this point, all the versions of the random walk have converged to the analytic solution.

So, for my attempt at arriving at the same solution, I went with the classic differential solution and used optimize in order to determine the angle used to calculate the constant value for the cycloid solution. [Hill 2017] Along with the cycloid solution, a circular pathway, a parabolic pathway, and a linear pathway are also tested, then time integrated in order to find the total time of travel along the path. This approach is flawed because it only includes these four intuitive solutions to be tested, and we often see in physics that human intuition is not only imperfect, but often leads us astray. It leaves open the possibility that there may be some other, even faster pathway that we didn't think of. The existence of an analytic solution and the convergence of the genetic algorithm approach let us know that isn't true in this specific case, but in cases where an analytic solution doesn't exist make the genetic algorithm the most attractive approach.

In order to arrive at the cycloid solution for the time optimized pathway, the following differential equations must be solved:

The total time of travel, which is our objective function to minimize is,

$$t = \int_{P_1}^{P_2} \frac{ds}{v} \tag{2}$$

Where ds is an arc length element, v is velocity and it's integrated from one position to the other. In this equation velocity can be found by using conservation of gravitational potential energy:

$$v = \sqrt{2gy} \tag{3}$$

If we use the origin as a starting point, then ds can be represented by,

$$ds = \sqrt{dx^2 + dy^2} = \sqrt{1 + y^2} dx \tag{4}$$

So our time function is given by

$$t = \int_{P_1}^{P_2} \sqrt{\frac{1 + y^2}{2gy}} dx \tag{5}$$

Equations of this form can be solved by the Beltrami identity [Weisstein n.d.]

$$f - y\frac{df}{dy} = C \tag{6}$$

$$C = \frac{1}{\sqrt{2gy}\sqrt{1 + y^2}} \tag{7}$$

Substituting C and squaring both sides leads to the following differential equation

$$[1 + \frac{dy}{dx}^2]y = \frac{1}{2gC^2} \tag{8}$$

This differential is solved either by using Euler's equation or a proper ansatz, but the following equations are solutions to the differential:

$$x = \frac{1}{2}[(\frac{1}{2gC^2})^2(\theta - sin(\theta))] \tag{9}$$

$$y = \frac{1}{2}[(\frac{1}{2gC^2})^2(1 - cos(\theta))] \tag{10}$$

And these parametric differential equations are the parametric equations of a cycloid. The optimize function was used in order to calculate the constant angle and constant value C based on the desired final position so that the cycloid passes through the desired final position.

For the other pathways used in the comparison the following pathways were used for the slower curves. A circular pathway which intersects both the origin and the desired final position:

$$r = \sqrt{x^2 + y^2} \tag{11}$$

A linear pathway whose slope causes it to pass through the desired final position. There's no intercept because it passes through the origin.

$$y = mx \tag{12}$$

A parabolic pathway which passes through the desired final position. It contains the parameter c which was minimized to give the shortest length pathway from the origin.

$$y = \sqrt{cx} \tag{13}$$

Given a final position of (-1, 0.5) I was able to calculate the time it would take to travel each pathway from the origin.

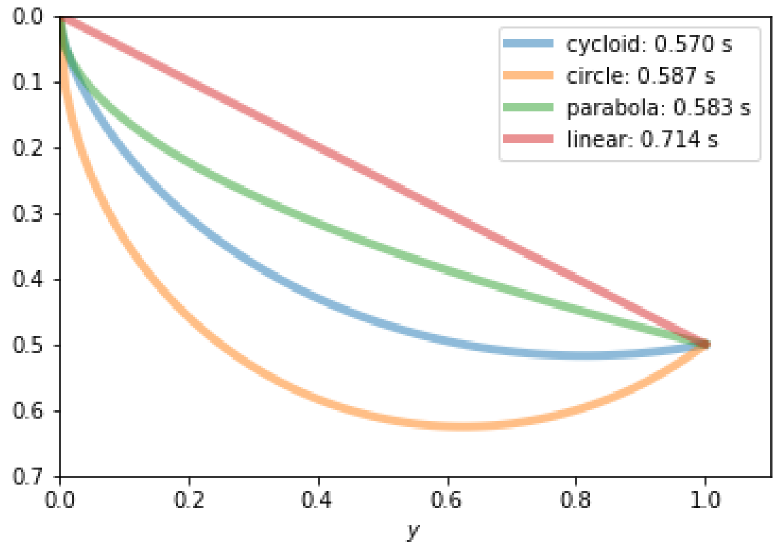

Figure 5: The results of the brachistochrone race. According to this simulation, the cycloid is the fastest pathway and the linear pathway is the slowest. This agrees with all other versions of the solution.

Despite not being able to make something that arrives at this solution by using a genetic algorithm, I'm happy with the final result. This is a good fundamental exercise in python and in using both optimize and integrate functions. I plan on using this python exercise for my AP Physics 1 course, in conjunction with a demonstration I have that shows the same principle with wooden curves and marbles. We run the demonstration and take videos, then perform video analysis on the demonstration in order to get a very good calculation of the time interval. The solver could be given the exact same parameters as the dimensions of the demonstration to have the solver serve as the hypothesis for the experiment while the video analysis produces data for analysis.

I believe that I can use python to step up my lesson design game, especially in the development of laboratory activities like this one.

I also like this example and activity as a learning experience because it's one of those lessons that easy to remember by coupling it with an interesting historical anecdote about why the problem was posed and how it was originally solved. The anecdote behind this one is as high quality as the story about how Gauss was whipped by his teacher for cooking up the arithmetic series formula in a single class period. Not every student will remember the series formula but if they remember the anecdote, they'll know what to google in case it ever comes up.

This example also has built into it physical fundamentals and lessons about misleading intuition that are widely applicable to mechanics problem solving in general. Even if a class is below the mathematical level of the example, the discussion is still worth having as part of any mechanics course and having the hypothetical calculation pre-made as software quickly overcomes the gap in mathematics that students may have with the solution, allowing you discuss the concepts and principles behind it.

3 Data Analysis of Periodic Trends

For this second portion of the project I was going to analyze proton therapy experiment data using the tools that we've developed since the midterm. For the midterm I typed out by hand the data that I found from a paper on proton therapy so that I could use pandas to dissect it. I wanted to obtain a large data set so that I could perform a more robust data analysis and graphing exercise with seaborn in order to visualize trends. In attempting to find large CSV files or data frames with regards to proton therapy and the outcomes of the treatment, I found it basically impossible to find usable data. This is most likely due to the fact that medical trial information is closely controlled for the sake of patients rights, unlikely astronomical data which can be downloaded freely like we did a few weeks ago for laboratory activities. If I had more foresight, I'm sure I could have gotten properly censored data by emailing researchers directly but time is of the essence.

I decided to change it up and pull a large excel sheet of periodic table properties: the same data that is used for filling out element articles on wikipedia. The motivation was the fact that I'm teaching chemistry next year as part of my course load and periodic trends are an important component of any high school chemistry course. I wanted to try new ways of visualizing the various periodic trends. They're important for making predictions about reactivity, but without a motivation for the trends we're just asking students to memorize vocabulary. What better motivation is there than actual scientific data?

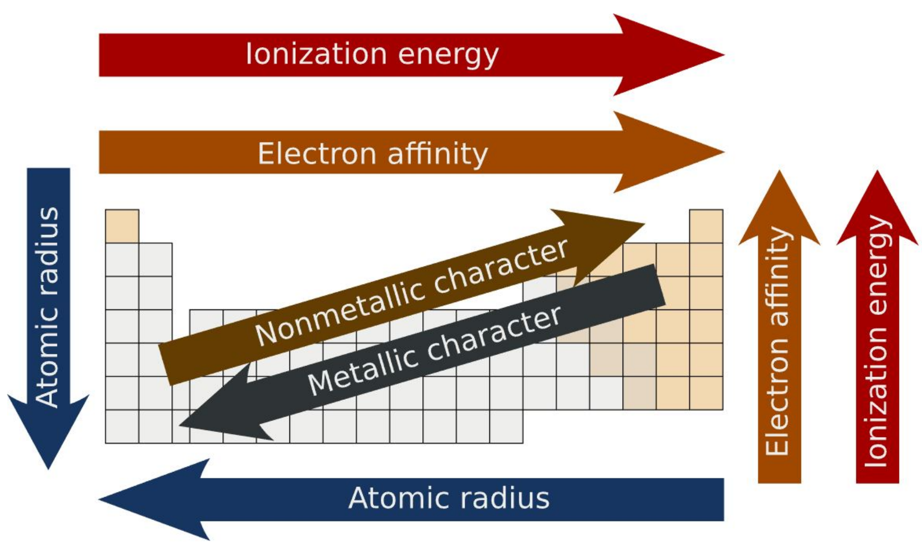

Figure 6: The classic periodic trends from the periodic table that allow students to predict reactivity and reaction types.

Moreover, the plots that seaborn makes are gorgeous. I've been fiddling with it since we were introduced to it in class a few weeks ago. I was able to read the excel sheet into python using pandas and separated the various properties of the elements into numpy arrays so that I could exercise the graphing utilities of seaborn and I was not disappointed. Below are some of these visualizations and explanations of each. These are only about half of the visualizations I made as some are just noise, with no underlying concept to explain them.

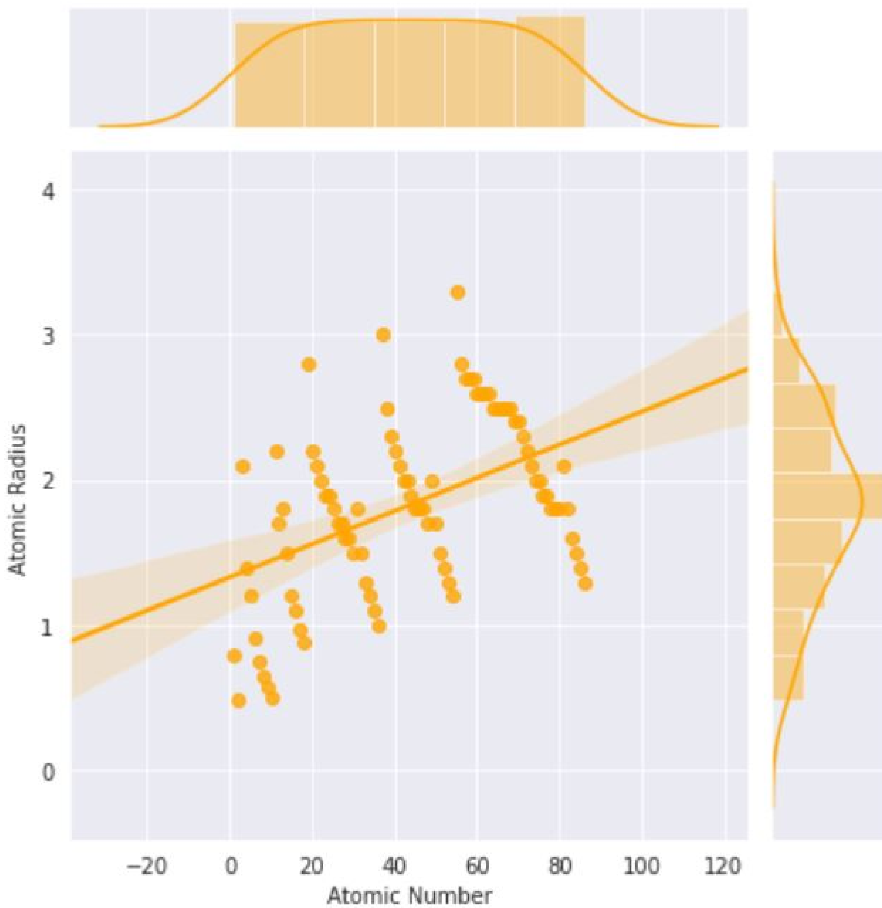

Figure 7: The classic trend of atomic number versus atomic radius. Generally the radius increases with atomic number but there is a large periodic fluctuation within the trend. These bands are the groups of the periodic table where the noble gas of the row has the smallest radius, increasing until the halogen of the row.

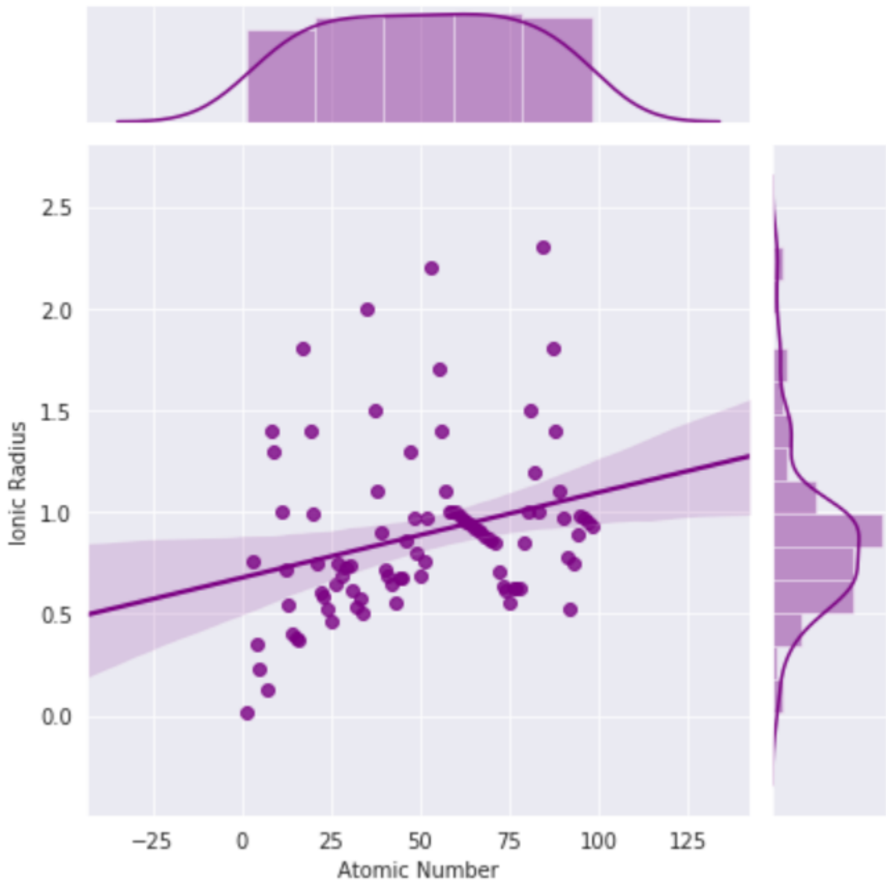

Figure 8: The trend of atomic number versus ionic radius. Generally, the ionic radius increases at the size of the nucleus increases as indicated by the linear trend however this is a large periodic fluctuation within this trend. That periodic fluctuation is due to the effect of shielding as electron orbitals complete. Each minimum is associated with a Noble gas and the largest radius is element 87 Francium, which matches the classic trend.

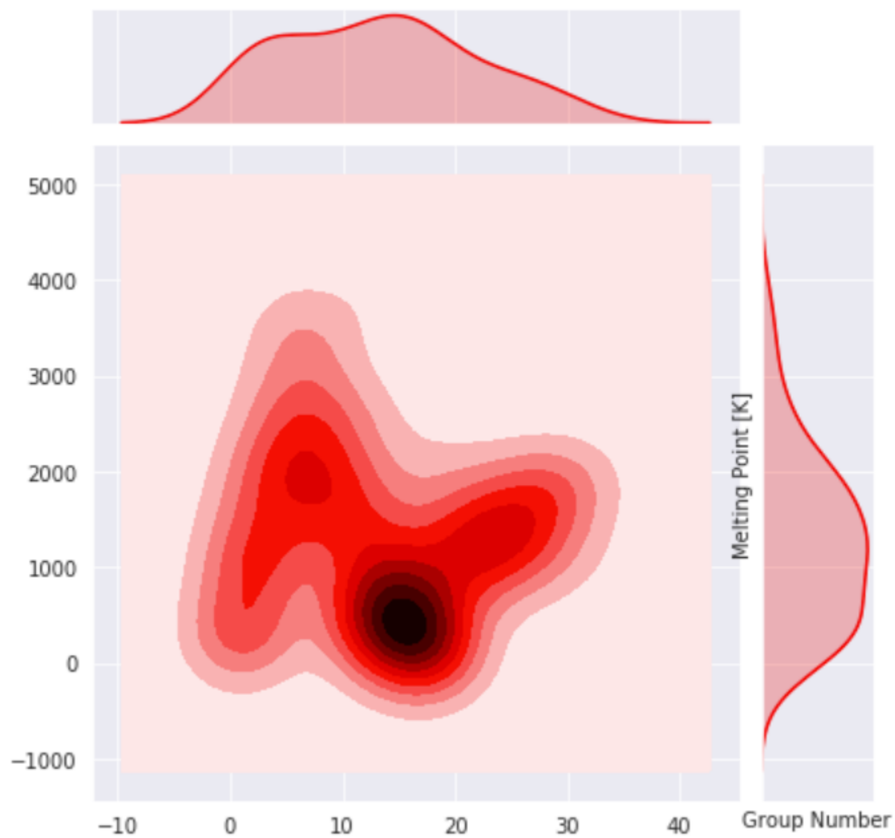

Figure 9: The trend of melting point versus atomic weight shows that in the melting point of the noble gasses at group 18 have by far the lowest melting points (which is why they're almost always gases). It's a good way to talk about the effect of them having complete electron orbitals, leading to non-interaction, leading to weak intermolecular forces, leading to low melting and boiling points. This graph also shows that in the middle of the table (the transition metals) have a particularly high melting point.

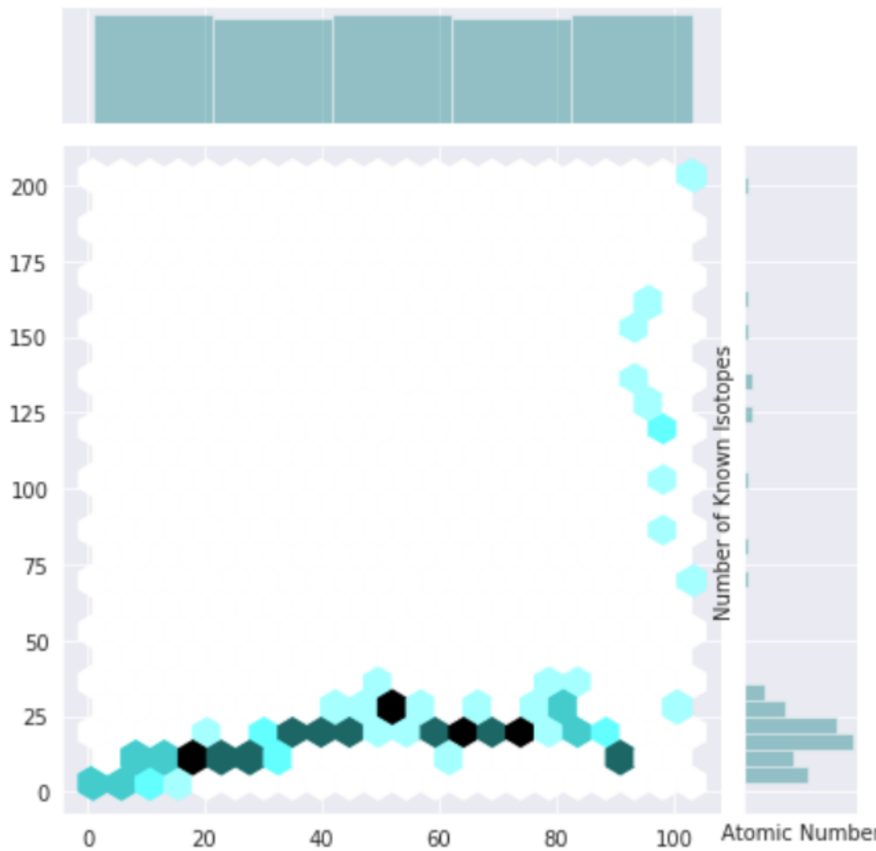

Figure 10: The trend of atomic number versus isotope count shows that the number of possible isotopes for any given element increases as the atomic number increases and blows up when you get the radioactive elements in the lanthanide and actinide series. It also the darkness used to represent clusters of higher than normal isotope count right around potassium, lead, and tungsten which tend to be the lighter radioactive nuclei discussed at the high school level.

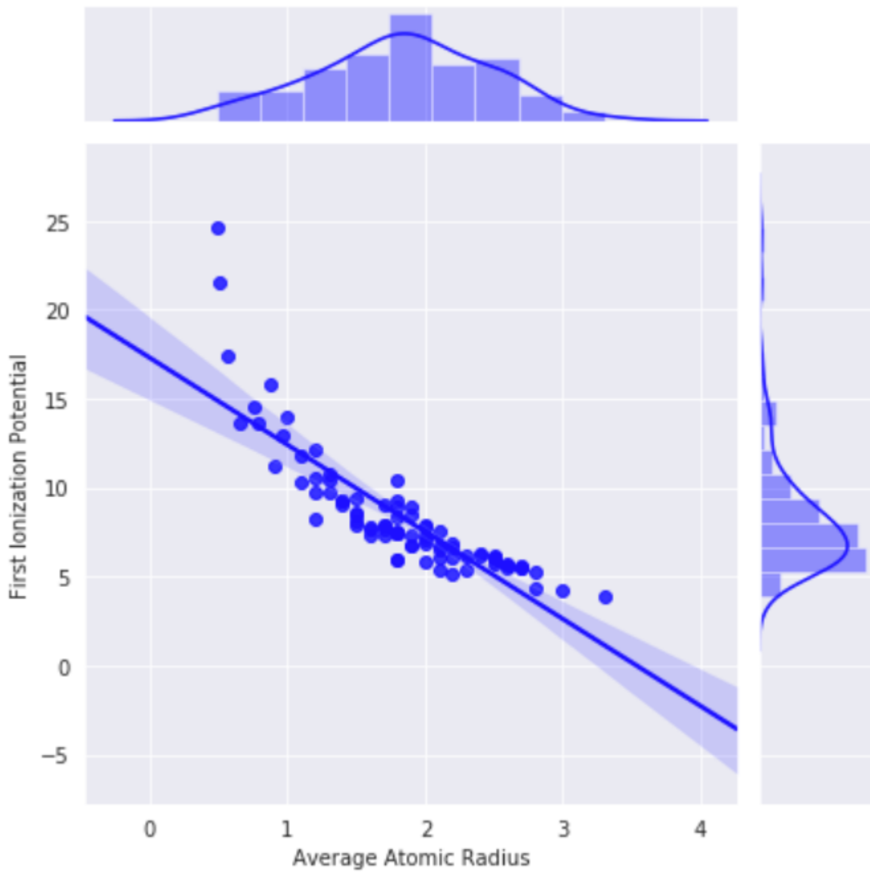

Figure 11: I saved the best for last. The trend of average atomic radius versus first ionization potential is very straightforward and aesthetic when visualized. This trend shows that the smallest atoms are harder to ionize while larger atoms are easier to ionize. This is due to the simple fact that the closer the negatively charged electron is to the positively charged nucleus, the more energy it requires to pull it away. The trend is fairly linear in the middle region but non-linear for very small and very large atoms. This is a good way to talk about how difficult it is to ionize helium since it has the double whammy of being both a noble gas with complete electron orbitals and being the tiniest noble gas.

It was a fun exercise rebuilding the known periodic trends using seaborn graphing utilities. It has a very attractive set of options for graphical representation of data, which is a big part of the battle when it comes to education. When used in conjunction with pandas, it's a very convenient way to visualize data from easily edited excel files. It's important for students to see real scientific data earlier in their education as most of the graphics they're shown are perfect algebraic functions with no deviation whatsoever. They should learn early that real science is messy.

When I get back to teaching next year not only do I want to use LaTeX in order to write my assignments now that I know how useful it can be, but I also want to prepare a majority of the graphics used in my coursework and material in python using seaborn and sympy now that I know that its possible. It's eye opening to see how textbook quality graphics are generated and how straight forward it really is.

Moreover, being able to quickly visualize data is a good way to take a first pass at detecting trends. If I ended up doing nuclear research or teaching a nuclear physics course, this would likely be a good way to show off the data made available from the National Nuclear Data Center made available by Brookhaven National Laboratory. They have reams of data available for almost every known isotope, which is effectively a periodic table worth of data for each and every element. These techniques could be used to quickly visualize the valley of beta stability, or the other established nuclear data trends.

References

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