Statistical Analysis of VQE Extrapolation

Meeting with Professor Schnetzer and Rikab
July 1, 2020

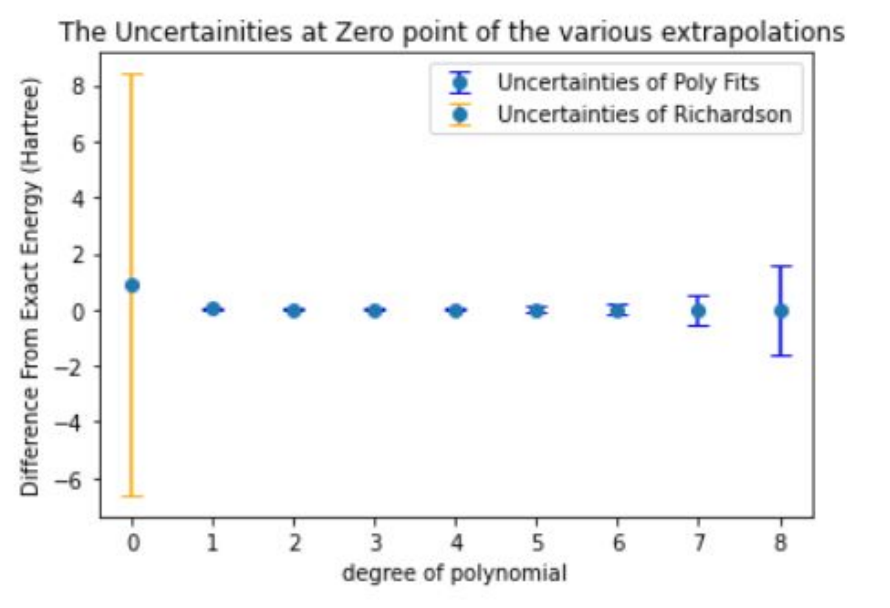
Methods: Monte Carlo *Uncertainty* Calculation

1. Obtain 100 samples of energies for a certain distance computed at each of the 10 noise scalings (1, …, 10)
2. For each of the 10 plots, calculate the mean and standard deviation of each and then construct a gaussian using that data.
3. From the resulting 10 gaussians, sample a point from each and extrapolate the zero noise energy either using richardson or some polynomial function.
4. Repeat Step #3 999 more times
5. The standard deviation of the 1000 zero noise energies is your uncertainty.

Key #1

The **greater** the **degree** of the polynomial, the **greater** the **uncertainty** of its zero noise approximation.

(Using Monte Carlo Method)



This is the opposite of what is suggested by computing zero noise uncertainties using ‘*covariance*’ method

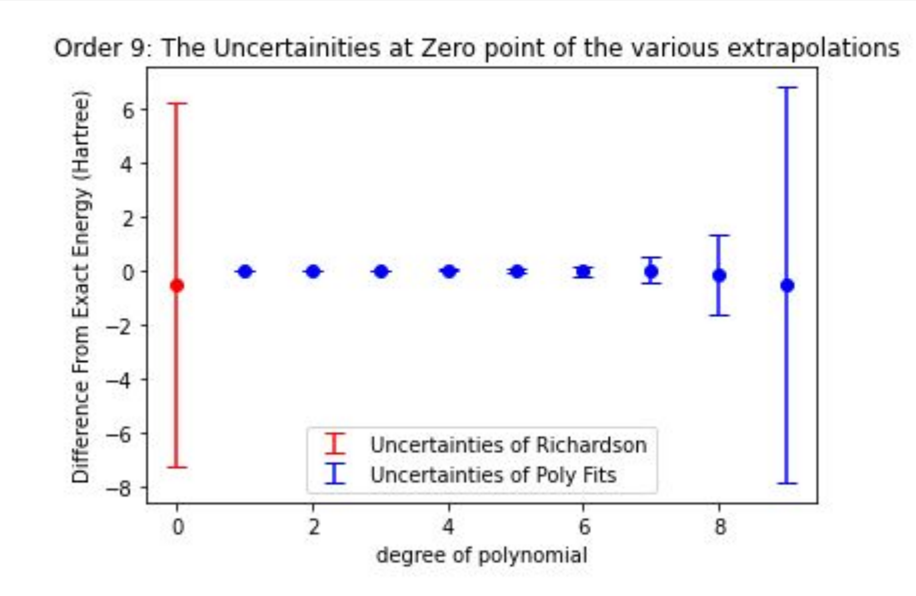
But if you use the ‘covariance’ method to calculate errors of fit at other points, the resulting error values can get really really big!

```
[0.0008505385155836958,
 4.742493961093152,
 213.6611033447164 8,
 2743.518106038691,
 18867.049301120802,
 88989.13130397731,
 325877.3827140574,
 994960.1224638921,
 2648800.617468519,
 6336152.560869853]]
```

Uncertainties of Degree 8 polynomial at the 10 noise scalings (1...10) using ‘covariance’ method.

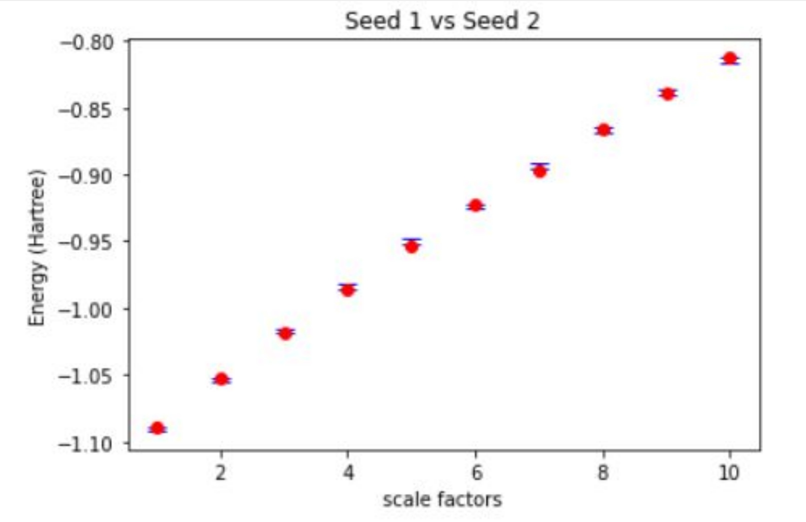
Key #2

Uncertainty of zero noise approximation by the **Richardson** Technique is similar to that by the **polynomial** with **no degrees of freedom**.



Key #3

Energies at 0.74 ang as a function of noise scaling factors do form a *roughly* linear pattern



- Seed 1: 100 samples each; Blue Error Bars
- Seed 2: 100 samples each ; Red Points