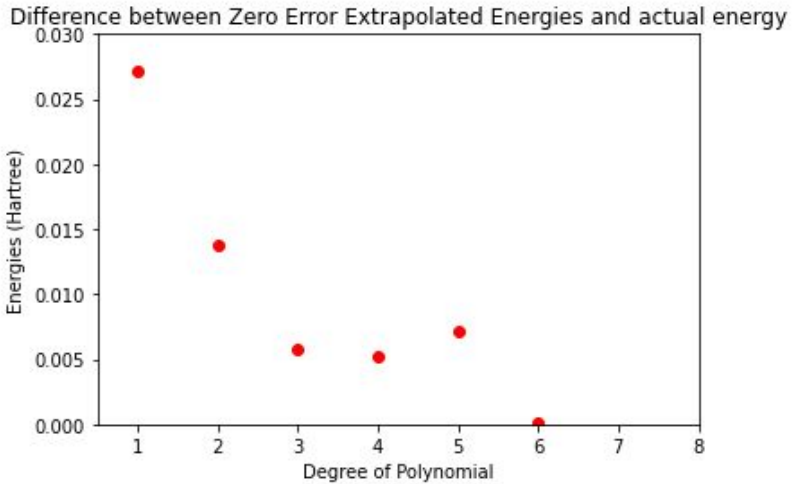
Statistical Analysis of VQE Extrapolation

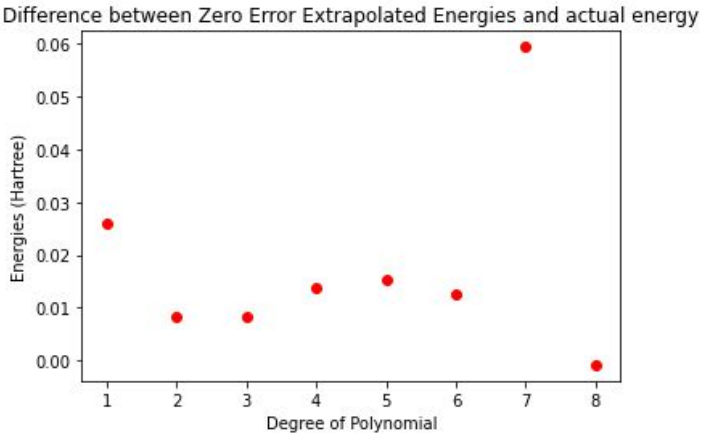
Meeting With Prof. Schnetzer and Rikab
June 29, 2020

Whether the statistical analysis being done is reasonable?

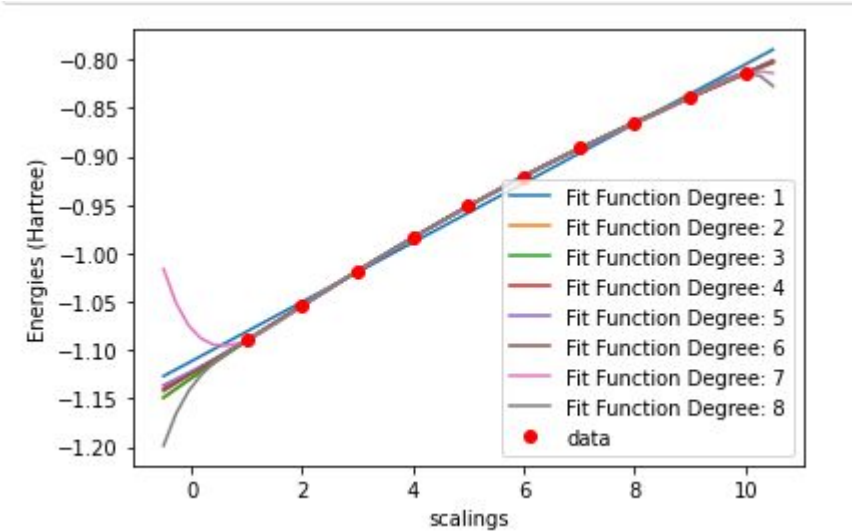
Most Important Thing

How to measure errors on zero noise energy?

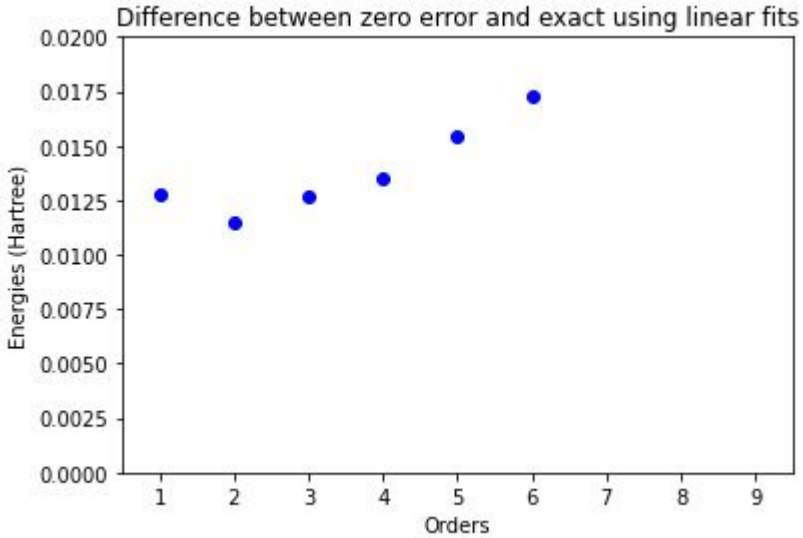


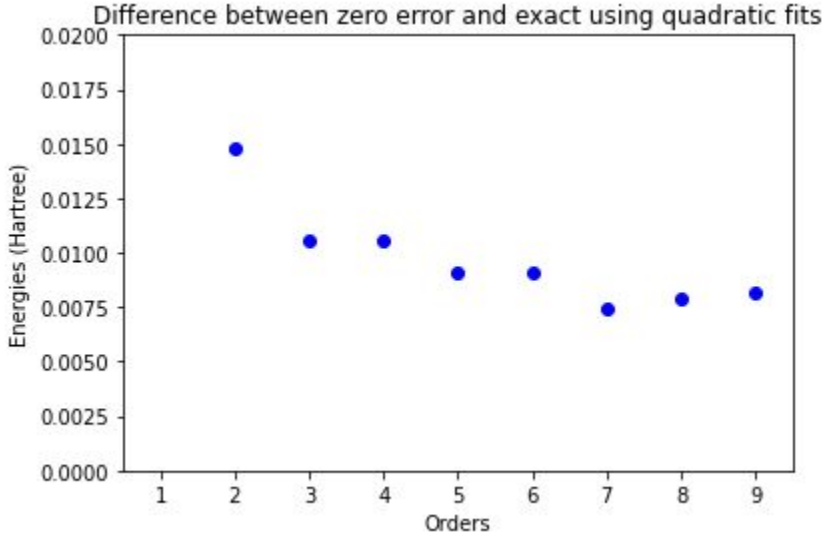


Is it worth using polynomial fitting? Or should we just rely on Richardson Extrapolation which is just linear fitting?



Does it seem reasonable to pursue how a particular polynomial performs (in approximating zero noise energy) with different orders?



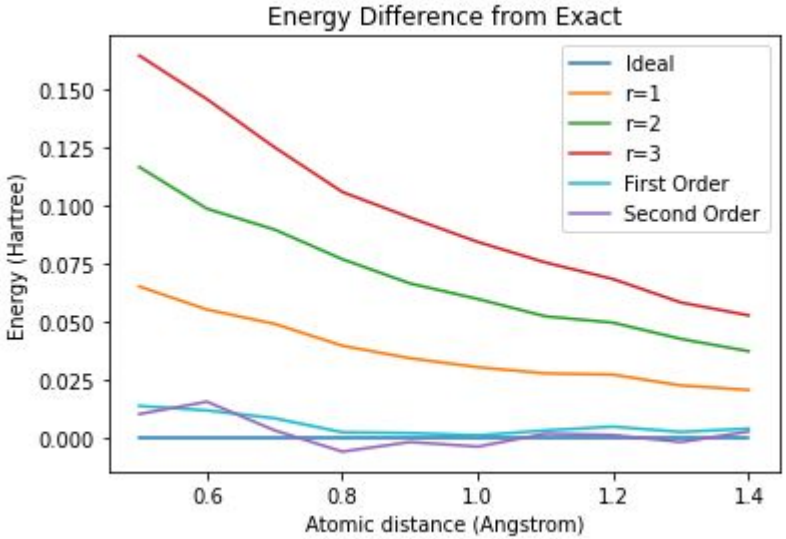


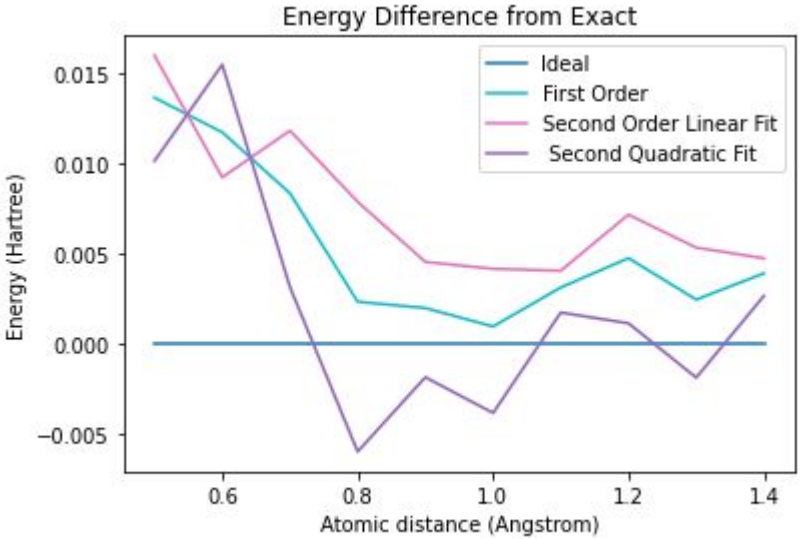
Does F test give us more information about comparison between 2 models than the chi square goodness of fit test?

```
Chi Square Statistics for polynomial fit of degree 1:
18.026923902704052
Chi Square Statistics for polynomial fit of degree 2:
0.5203167938954442
Chi Square Statistics for polynomial fit of degree 3:
0.6016254055250366
Chi Square Statistics for polynomial fit of degree 4:
0.4177978715186657
Chi Square Statistics for polynomial fit of degree 5:
0.50635288892659
Chi Square Statistics for polynomial fit of degree 6:
0.6774125527663473
Chi Square Statistics for polynomial fit of degree 7:
0.5658580768674772
Chi Square Statistics for polynomial fit of degree 8:
1.0475905198032063
```

```
F stat for degree 1 vs 2:
270.16843452608595
More param is good!
F stat for degree 2 vs 3:
0.05396235567804251
More param is good!
F stat for degree 3 vs 4:
3.6399493133582186
More param is good!
F stat for degree 4 vs 5:
0.12556026296551012
More param is bad!
F stat for degree 5 vs 6:
-0.010076728818806788
More param is good!
F stat for degree 6 vs 7:
1.5914264395575415
More param is bad!
F stat for degree 7 vs 8:
0.08030392824436064
More param is bad!
```

Why should second order do worse than first order?





- 50 Samples on H_2 molecule

Suggestions

- Error on constant term
- Monte Carlo on Richardson Extrap
- Diff way to calculate f test using fit error
- Chi sq with cdf instead of pdf
- Error vs uncertainty
- More points ---fit is better in terms of uncertainty on param but not necessarily the zero noise energy
- Review Sci Py docs on curve fitting with errors.