

Bayesian approach:

- Determine probability of RMSD value given a set of feature values
→ get also mean RMSD and uncertainty
- Estimate two contributions to probability and uncertainty:
 1. Physical variability (encoded in a model) – *cannot* be reduced with more samples
 2. Model uncertainty – can be reduced with more samples

Compare Bayesian results and machine-learning results in a couple of cases to validate the (faster) ML algorithm and estimate the uncertainty of its results

