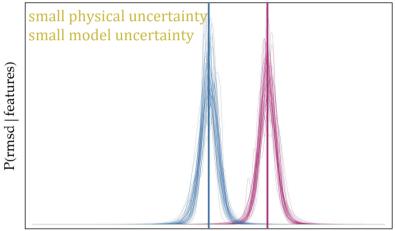
Bayesian approach:

Determine probability of RMSD value given a set of feature values
→ get also mean RMSD and uncertainty

P(rmsd | features)

- 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



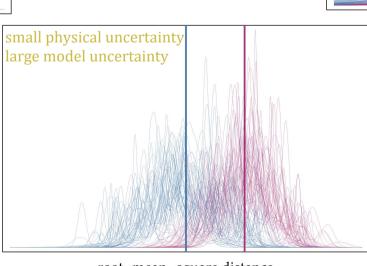
root-mean-square distance



root-mean-square distance

large physical uncertainty

small model uncertainty



root-mean-square distance