Root mean square analysis

$$\text{RMSD}(v, w) = \sqrt{\frac{1}{n}\sum_{i=1}^{n} ||\, v_i - w_i \,||^2}$$

- Root mean square deviation (RMSD)
  - describes the difference between two structures
  - usually based on a subset of atoms
  - *i* is an index over atoms
- Root mean square fluctuation (RMSF)
  - describes the fluctuations of a specific atom, e.g. alpha carbon, over the course of a simulation
  - usually described per residue, identifying relatively flexible regions of a protein
  - *i* is an index over configurations
- Both require structural alignment

- See RMS.ipynb, which shows different types of RMS analysis for a simulation of ubiquitin.

References

- Chodera, J. D. A Simple Method for Automated Equilibration Detection in Molecular Simulations. Journal of Chemical Theory and Computation 2016, 12 (4), 1799–1805. https://doi.org/10.1021/acs.jctc.5b00784.