MCMC exercise

Calculation errors

- Statistical error: $Staterr = \left\langle \left| \langle f \rangle_{sampled} - \langle f \rangle_{true} \right| \right\rangle_{runs}$
- Standard error: $Stderr = \frac{\sigma}{\sqrt{N}} < Staterr$

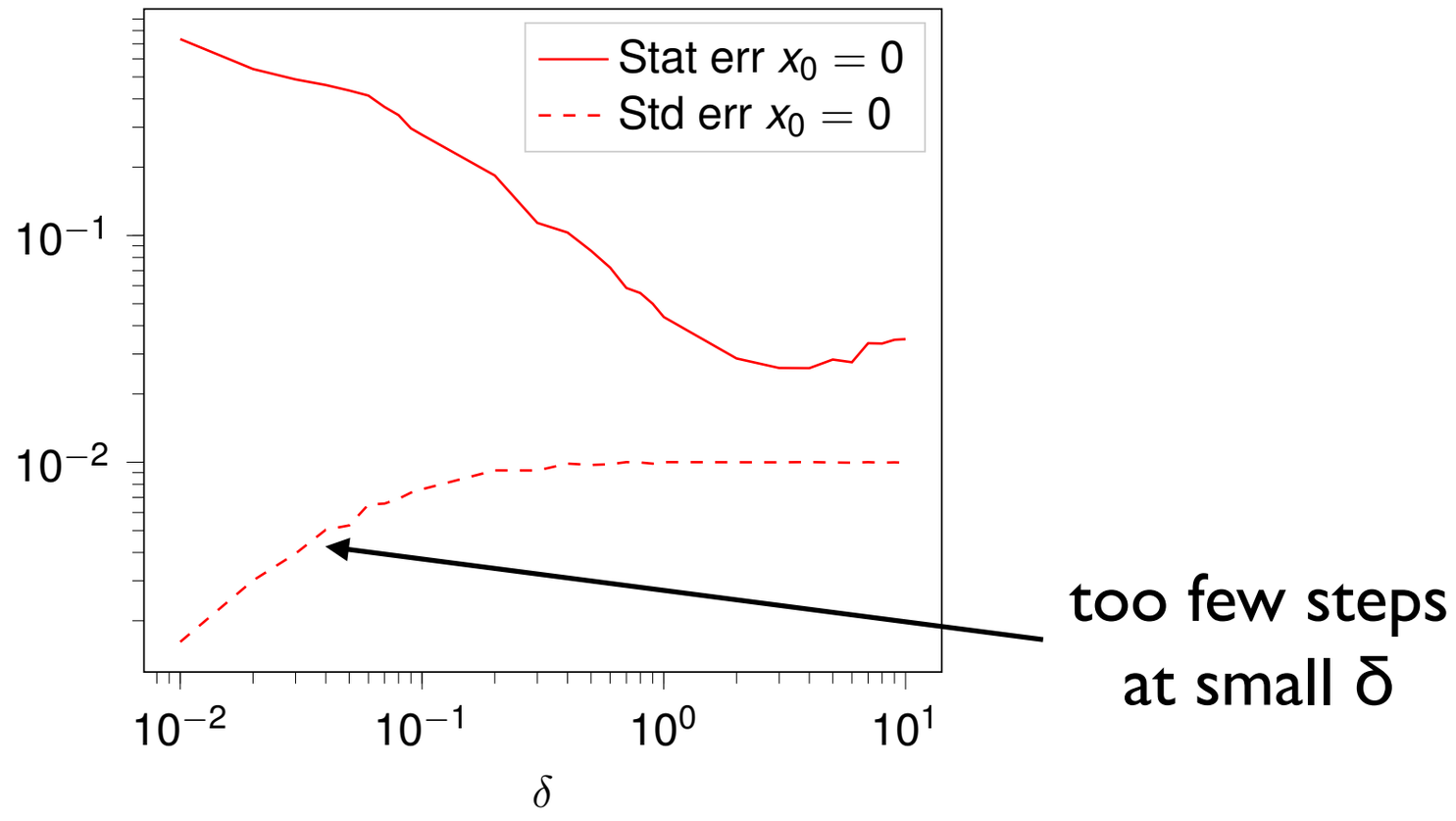
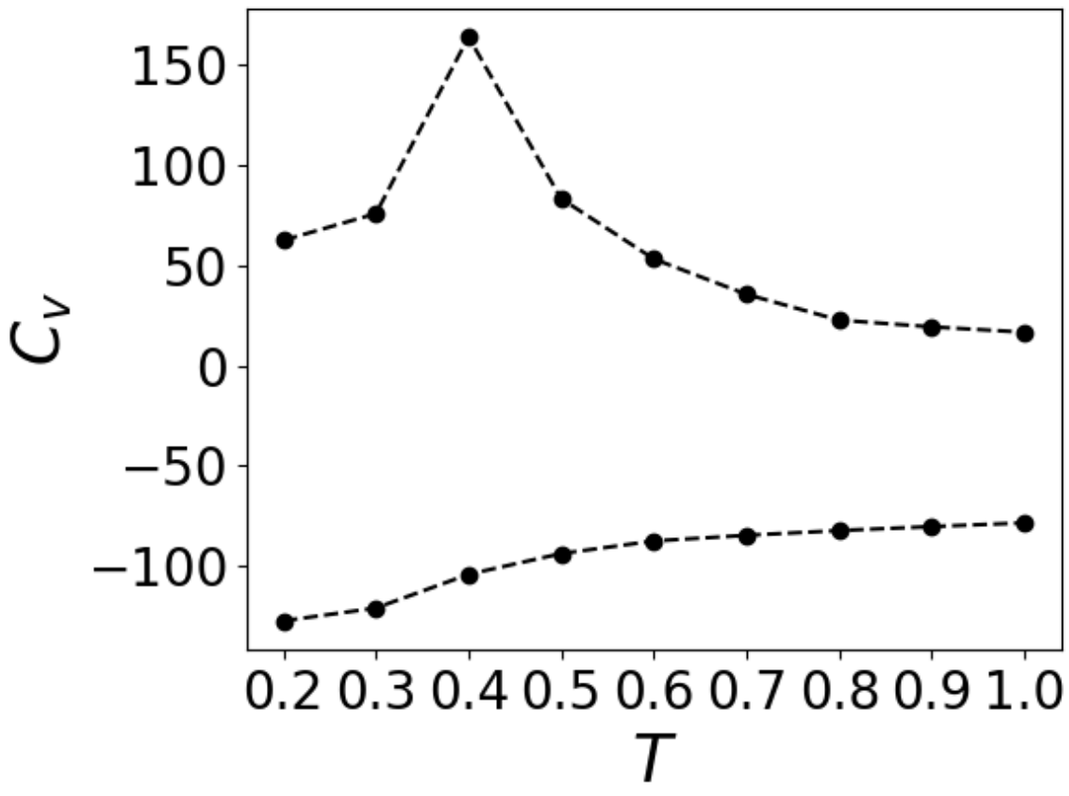


Figure: Average statistical error on 200 runs compared with average standard error as a function of δ with 10000 samples, a warming time of 100 steps and $x_0 = 0$

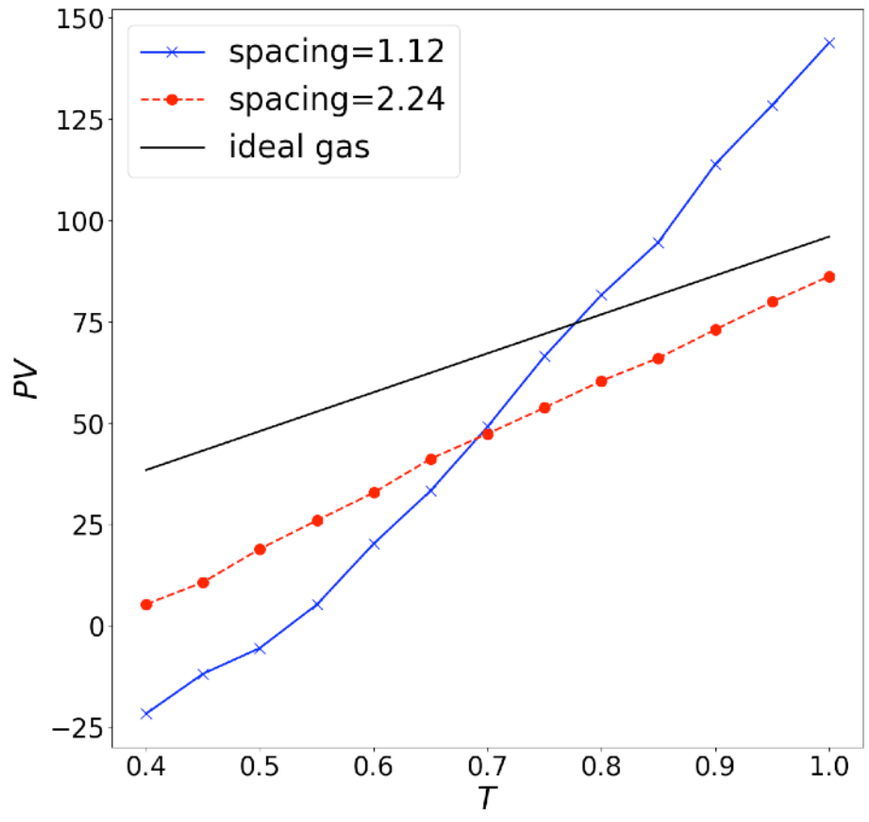
MD exercise

- Conclusions:
  - A very narrow range of time steps with visible energy drift before things explode
  - In the microcanonical ensemble to total energy (E_{pot}+E_{kin}) sets the accessible energy
    - The results depend very much on the initial E_{pot} , so on the initial coordinates
  - Sampled confirmations, heat capacity and pressure point to a phase transition

MD observables



Bug in pressure code: E_{kin} missing, corrected PV result:



Low T: attraction dominates: P negative, $P < P_{ideal}$
High T: E_{kin} dominates: P positive,
repulsion/exclude volume makes $P > P_{ideal}$