

MSM Agent MVP Report

Grade: WARN

Warnings

- ITS only weakly stable (rel_std_max=0.53)

Data summary

- trajectories: 28
- total_time_ns (approx): 14000.00
- dt_ns_effective: 0.5000

Key metrics

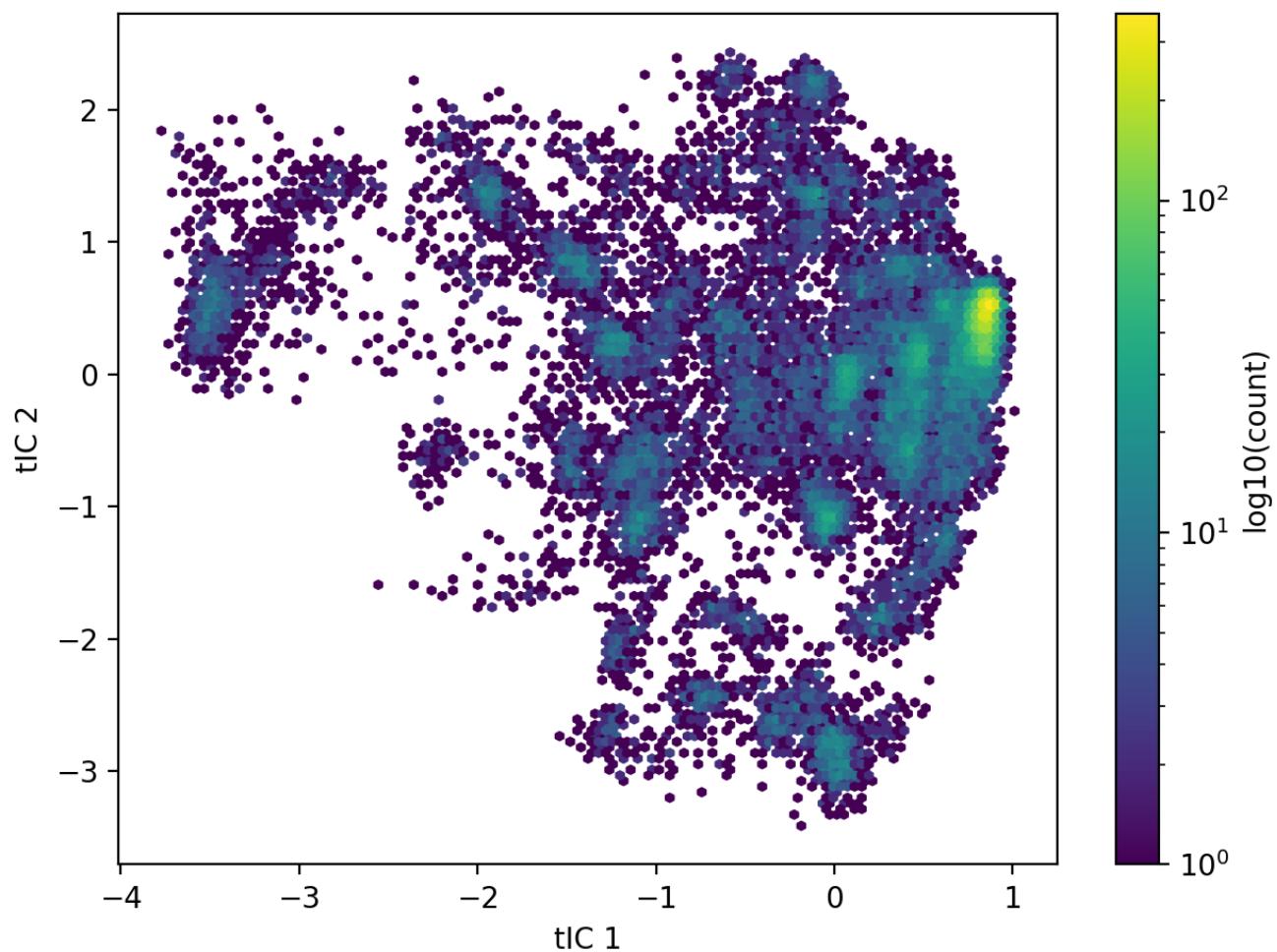
- tiny_frac: 0.000
- avg_out_degree: 7.63
- ITS rel_std_max(top-k): 0.534

Suggestions

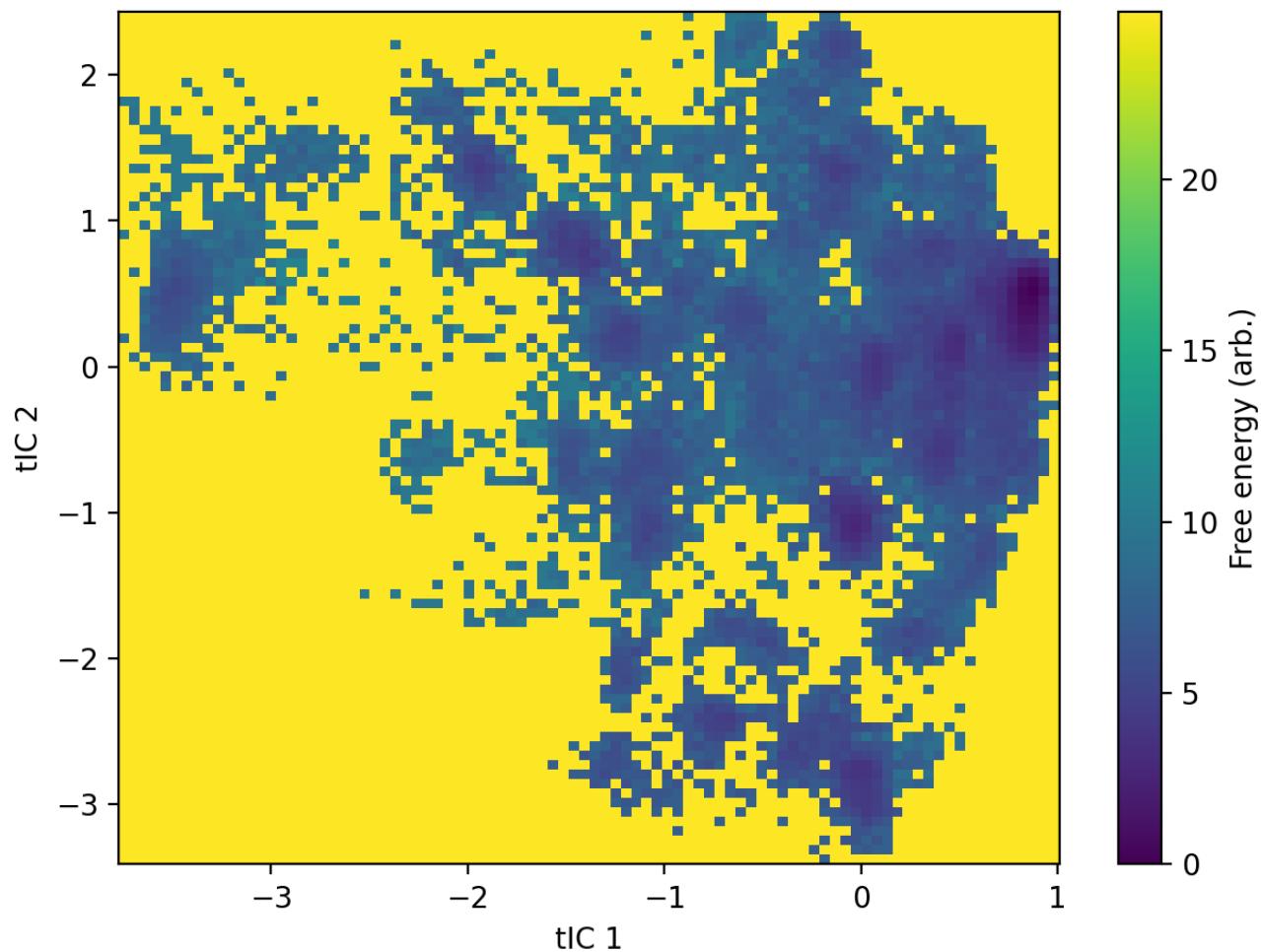
- Try increasing tICA components (4→6/8) and/or increasing MSM lag list to find plateau.
- If still unstable, consider adding contact features (dihedral-only may miss slow modes).

Figures

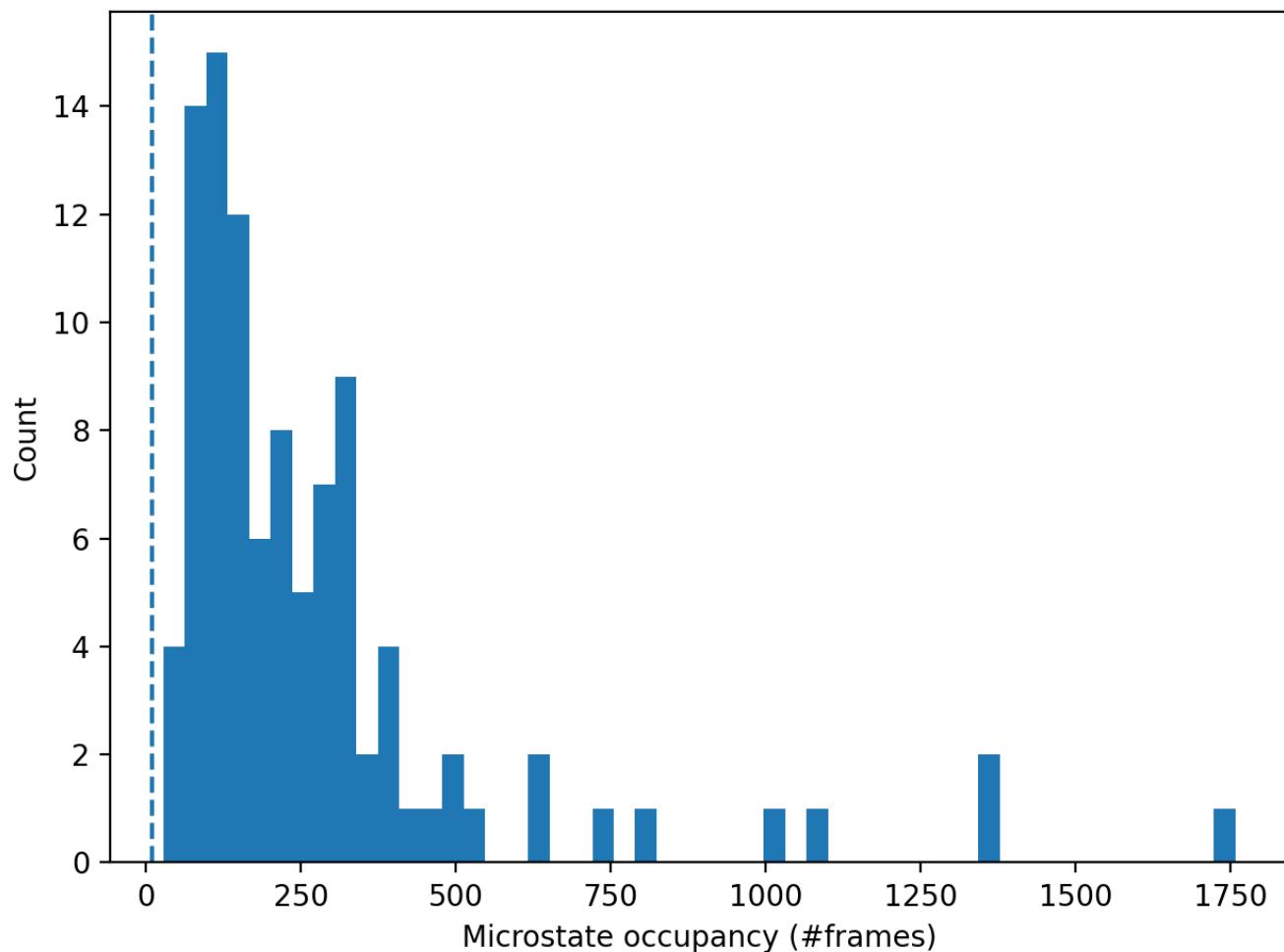
tica_density



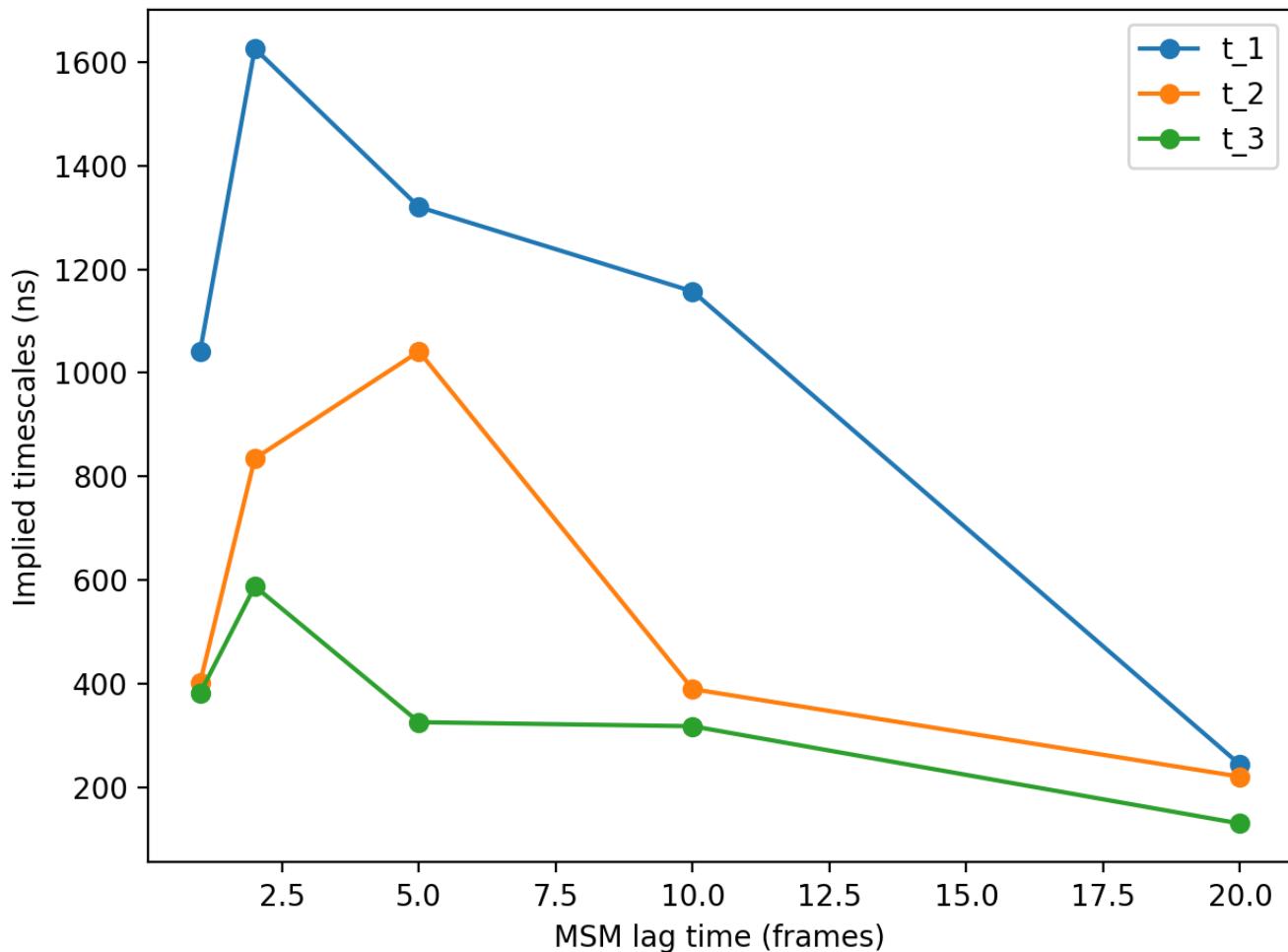
free_energy



occupancy



its



macro

