WALNUTS = Within-Orbit Adaptive Leapfrog No-U-Turn Sampler

Nawaf Bou-Rabee (Rutgers & Flatiron)

joint work with Bob Carpenter (Flatiron), Tore Kleppe (Norway), & Sifan Liu (Flatiron).

arxiv:2506.18746 https://github.com/bob-carpenter/walnuts

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  - **Gradient-based:** also evaluate $\nabla \log \mu$ (e.g., MALA, HMC, NUTS).

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$$i \in \mathbb{Z} \quad \text{(integration time)}, \qquad h > 0 \quad \text{(step size)}, \qquad M \in \mathbb{R}^{d\times d} \quad \text{(mass matrix)}.$$

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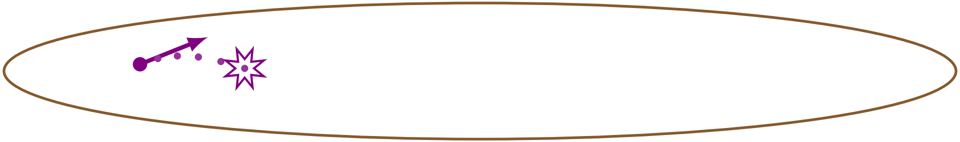
Why Integration Time Tuning is Tricky in HMC†



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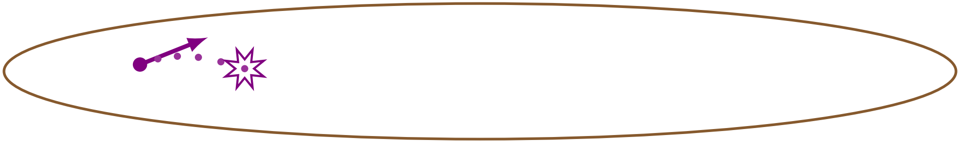

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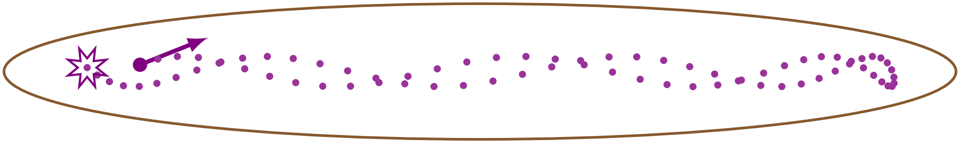

Too long: trajectory loops back, wasting computation

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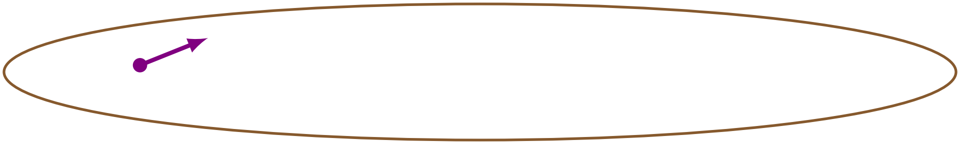

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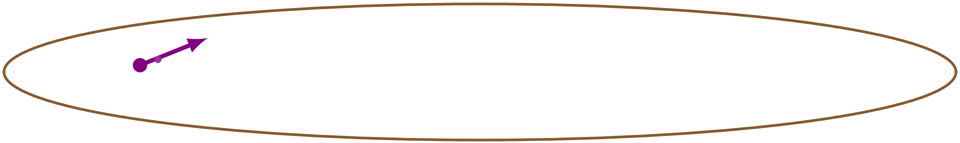

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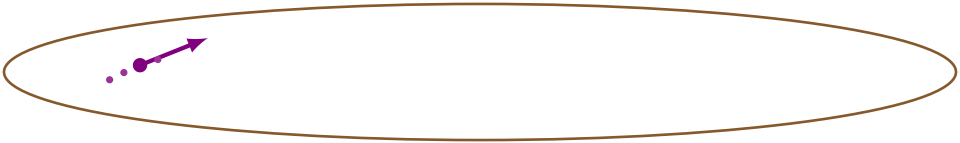

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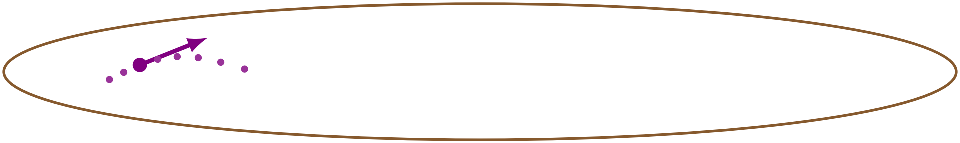

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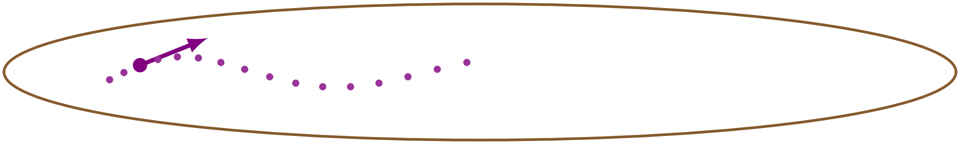

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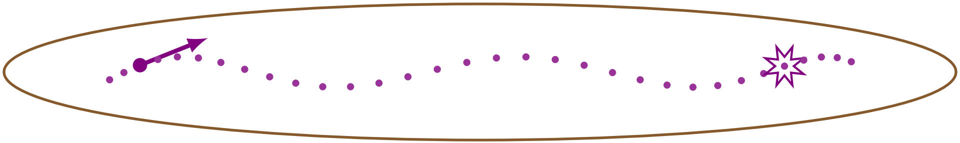

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- **However:** some important targets exhibit extreme variations in scale, e.g., Neal's funnel.†

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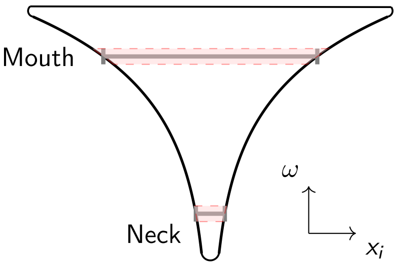

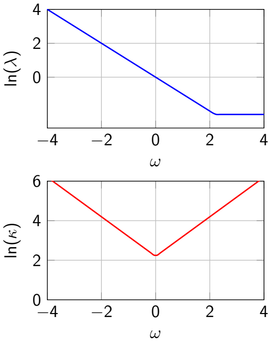

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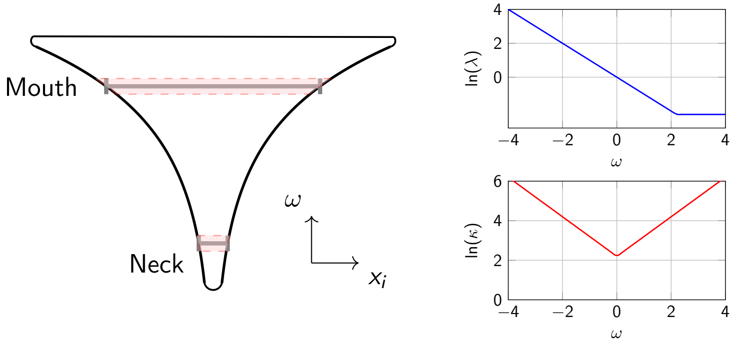

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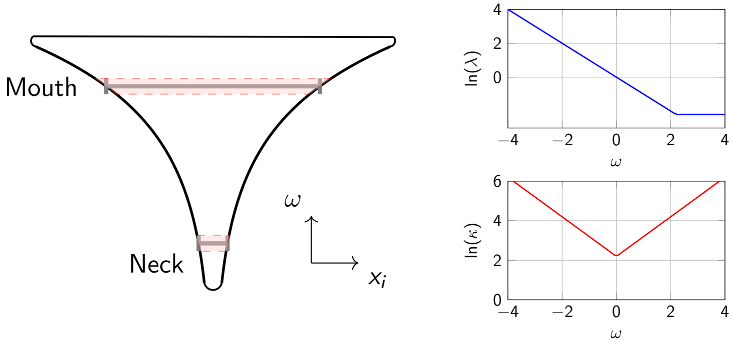

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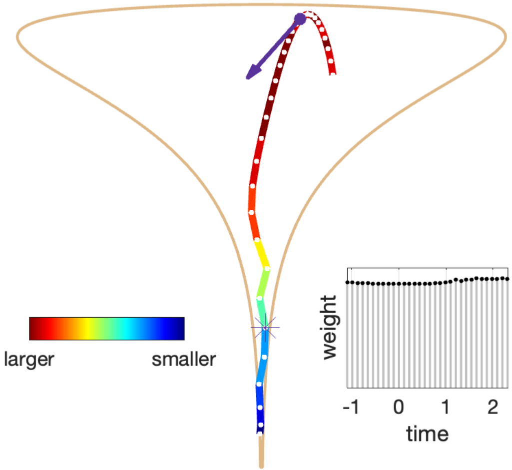
  - More forgiving with respect to tuning (e.g., macro step size).

Visualization of WALNUTS Transition Step



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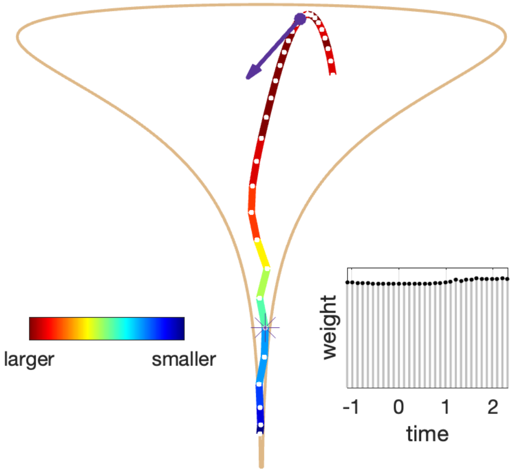

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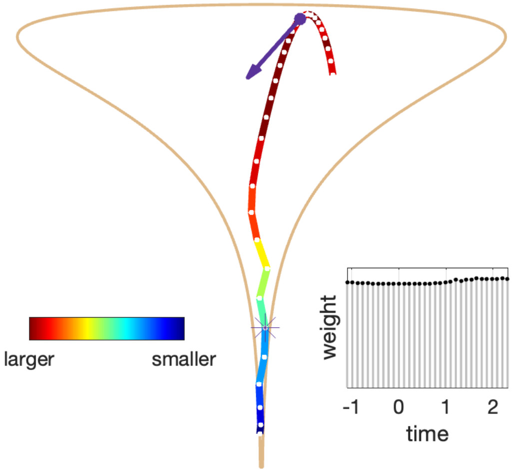

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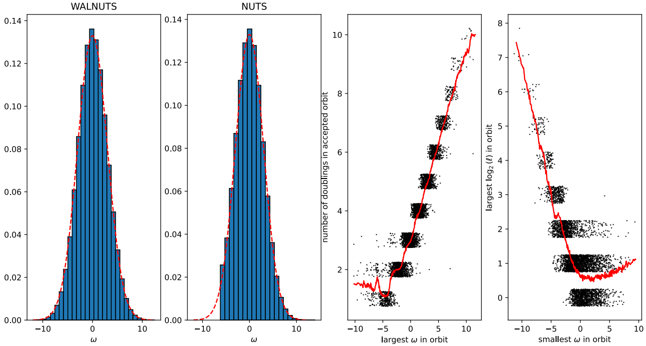

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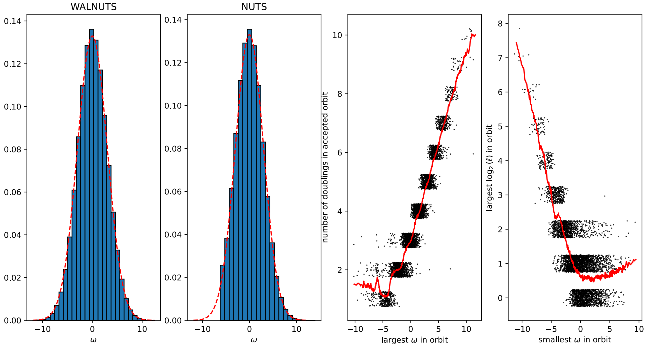

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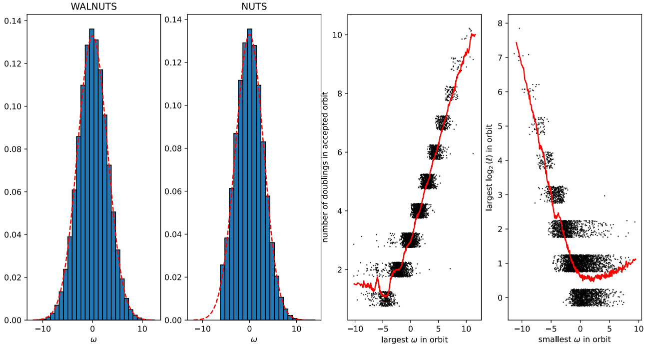

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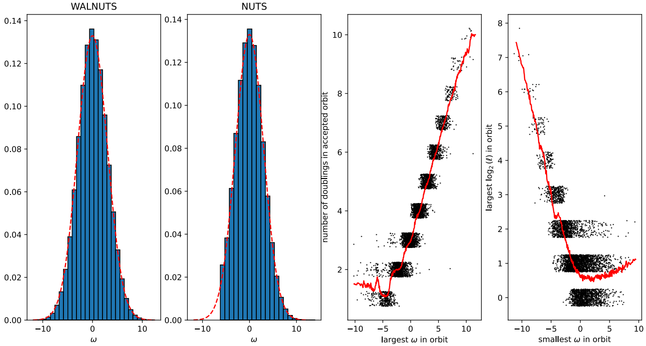

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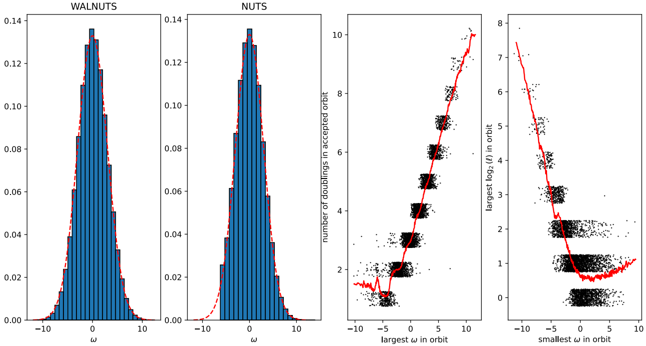

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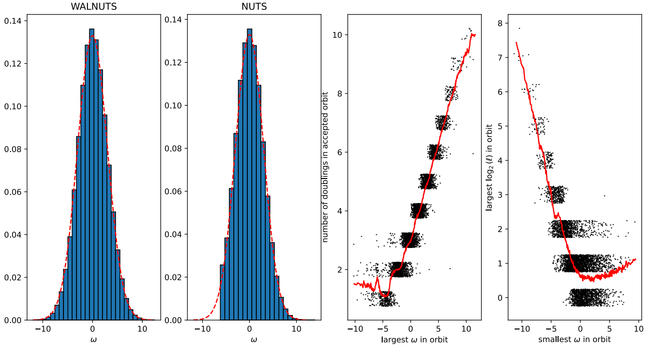

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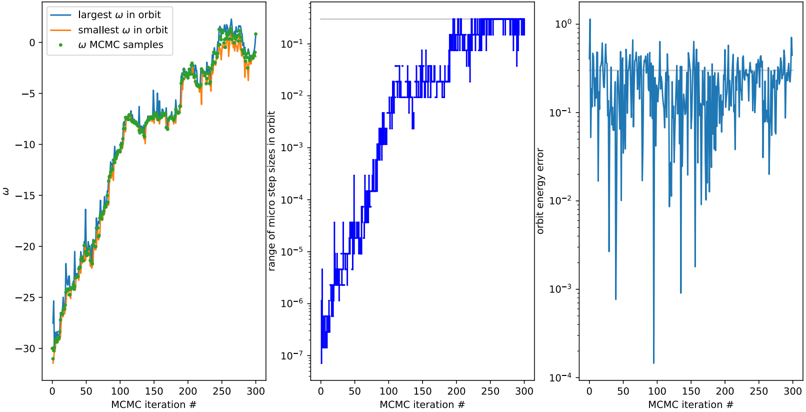

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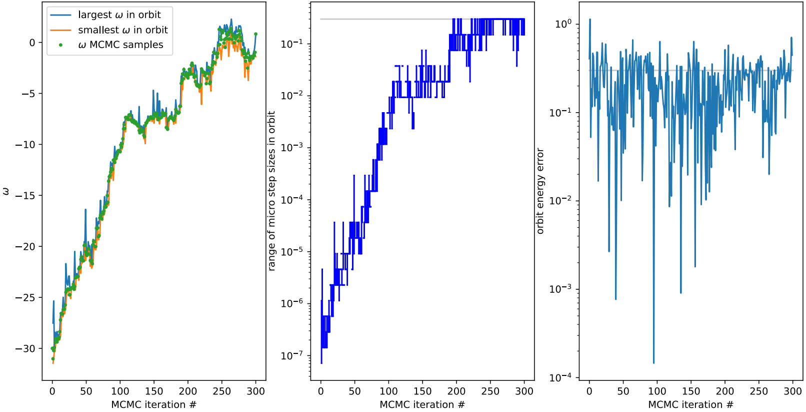

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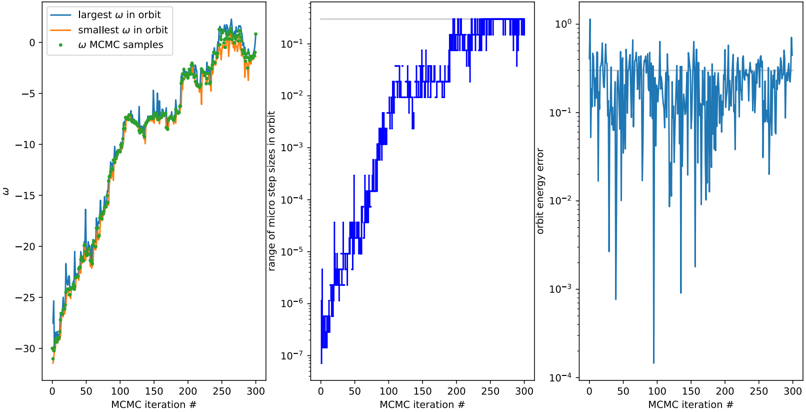
Cold-Start Diagnostics: WALNUTS in Neal's Funnel

- **Setup:** Initialized deep in the neck: $\omega = -30$, $x_i = 0$ for $i = 1, \ldots, 10$.



- **Left:** WALNUTS samples of ω (green) with orbit spans (lines).
- **Center:** Adaptive micro step sizes $h\ell^{-1}$ per orbit; gray line shows macro step size $h = 0.3$.
- **Right:** Energy error remains tightly controlled per orbit; dashed line shows $\delta = 0.3$.

WALNUTS: Transition Step

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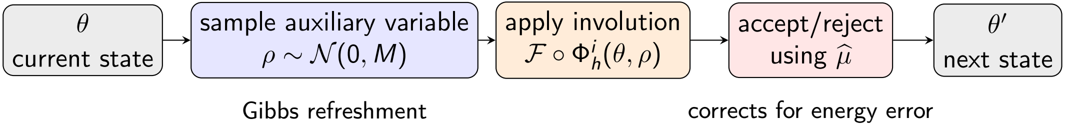
Contrast with HMC



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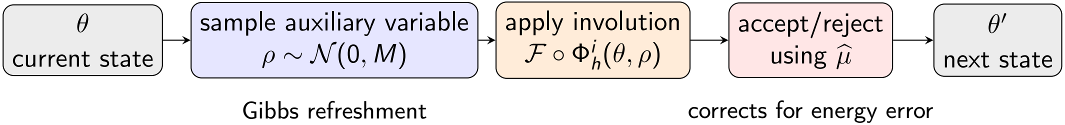
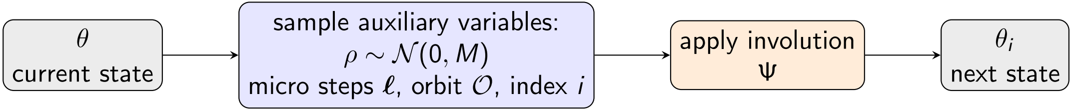
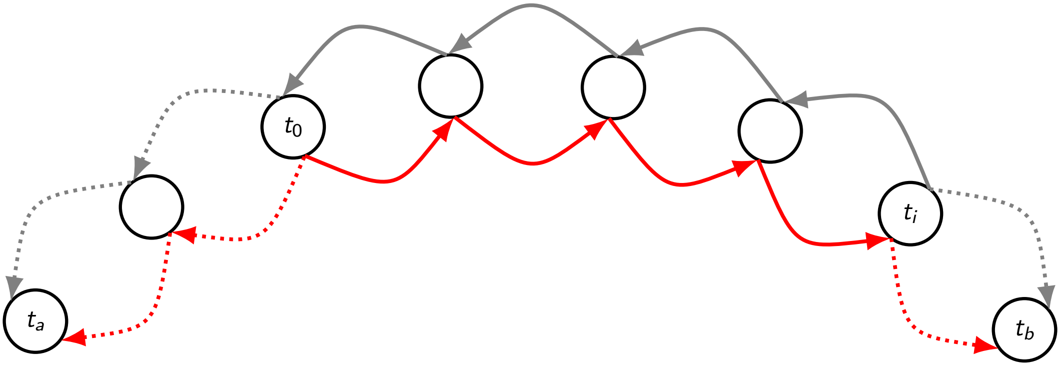




no Metropolis correction is needed since Ψ preserves the joint density

WALNUTS: Orbit Construction



Red: forward orbit from (θ_0, ρ_0).

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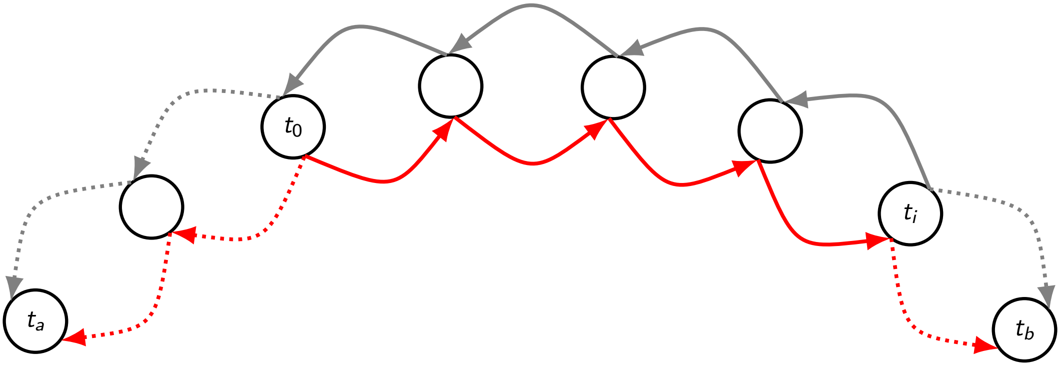

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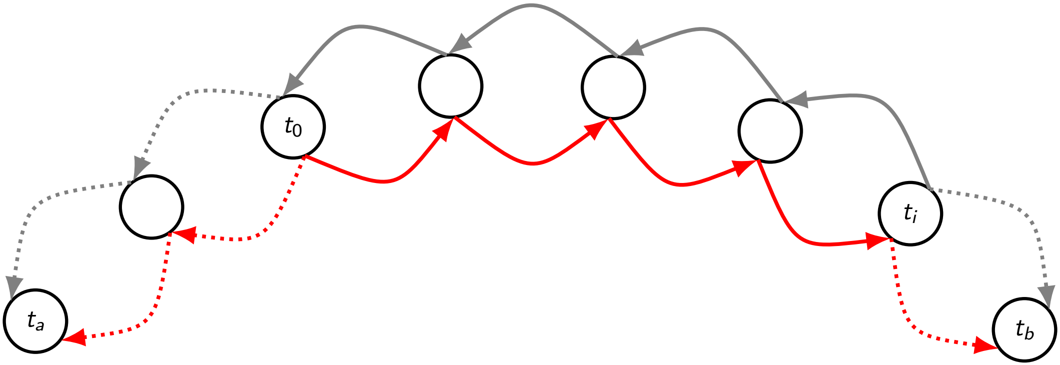

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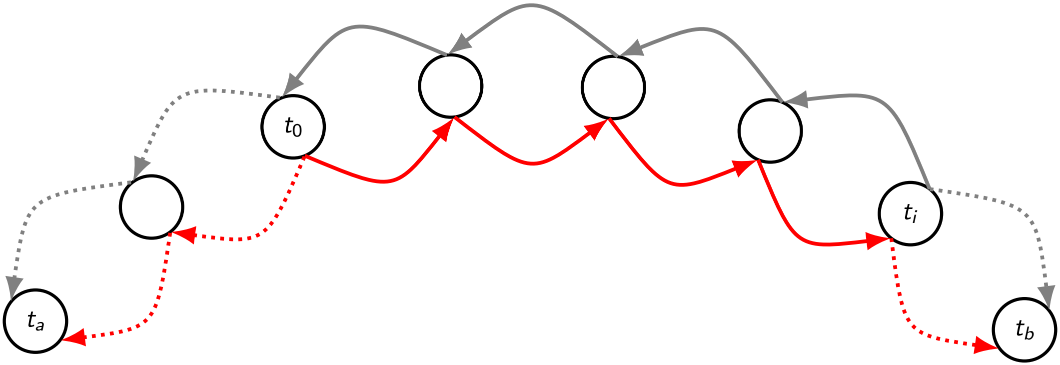

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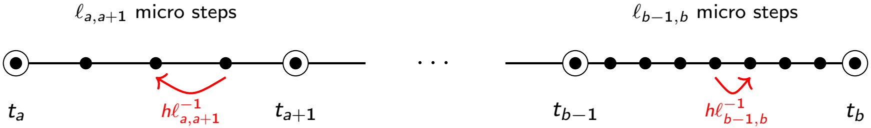
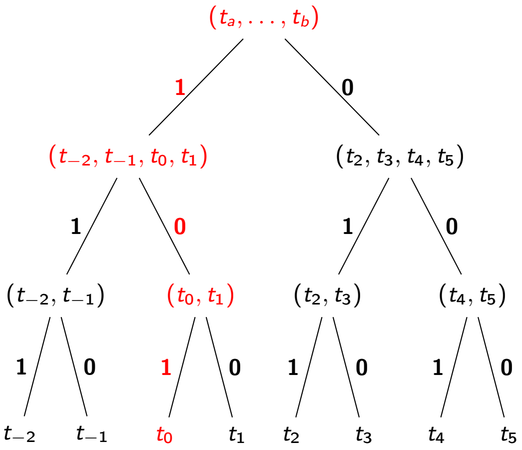


WALNUTS: Doubling Tree and U-turn Condition



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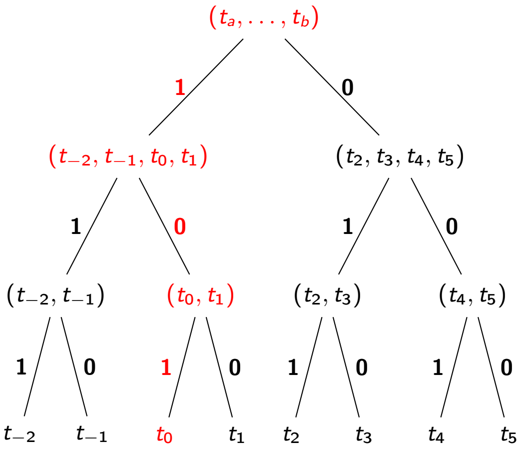

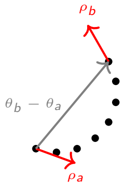

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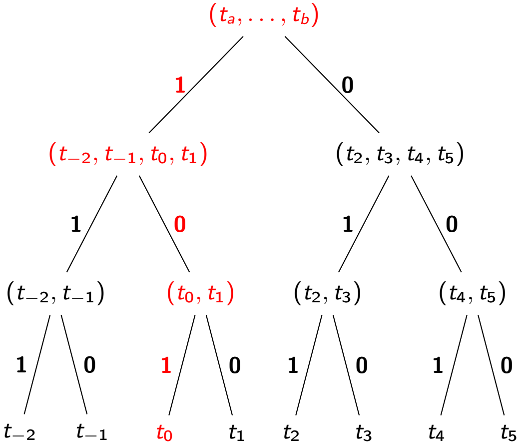

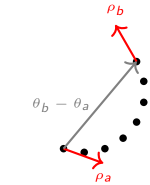

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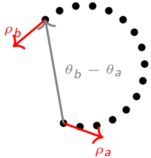

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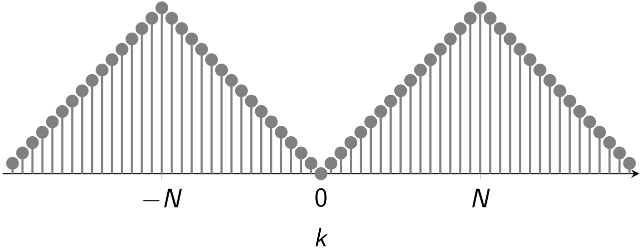
- With uniform weights and orbit lengths, BPS produces a symmetric triangular distribution.



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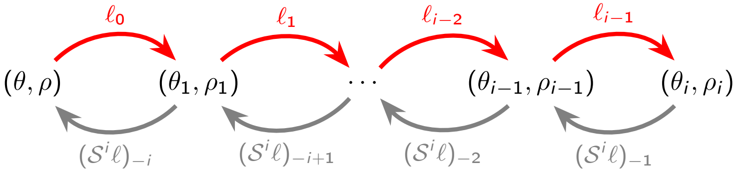

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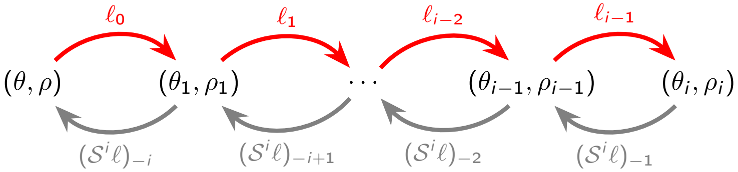

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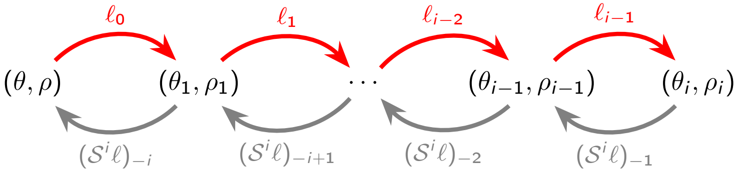

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- **Bottom line:** WALNUTS transition kernel is reversible with respect to the target μ.

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Outlook. Points toward a new class of locally adaptive HMC methods for anisotropic targets.

WALNUTS: Paper and Code

- **Paper:** `arXiv:2506.18746`

- **Code Repository:** `github.com/bob-carpenter/walnuts`

Questions, feedback, or contributions are welcome!