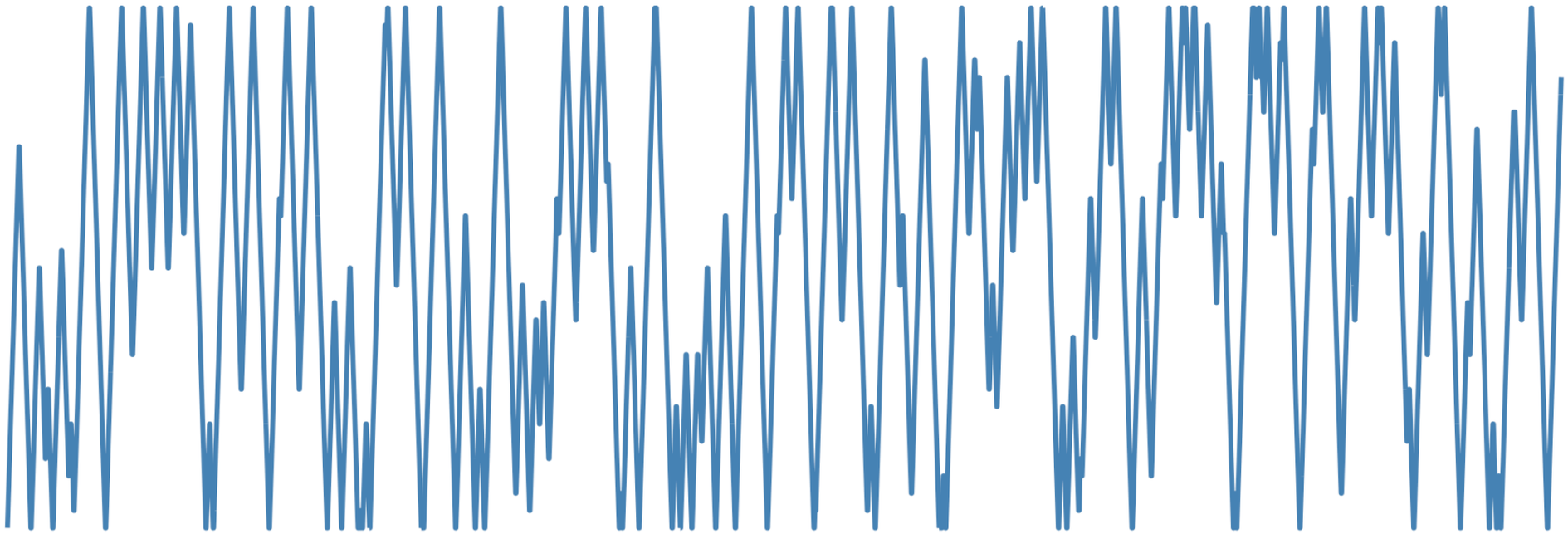
NON-REVERSIBLE PARALLEL TEMPERING



Saifuddin Syed

UNIVERSITY OF OXFORD

MOTIVATION

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- **Problem:** Want to compute expectations

$$\mathbb{E}[f] = \int_{\mathcal{X}} f(x)\pi_1(x)\mathrm{d}x$$

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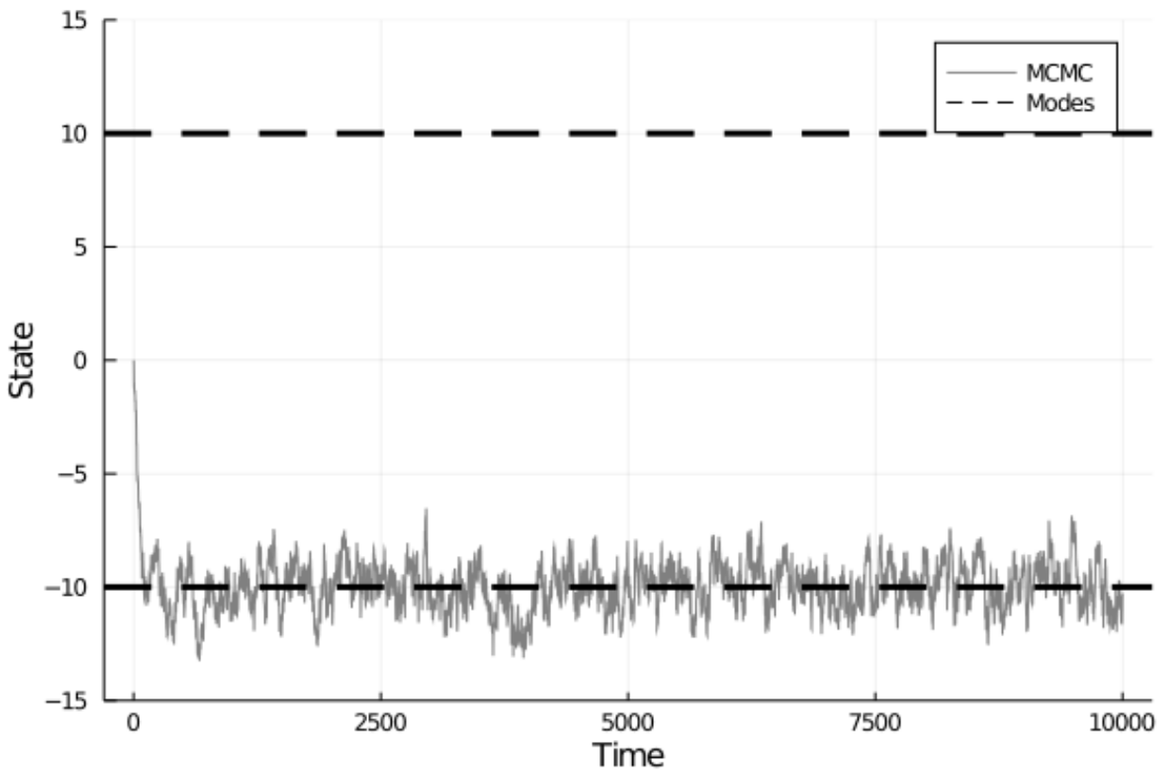
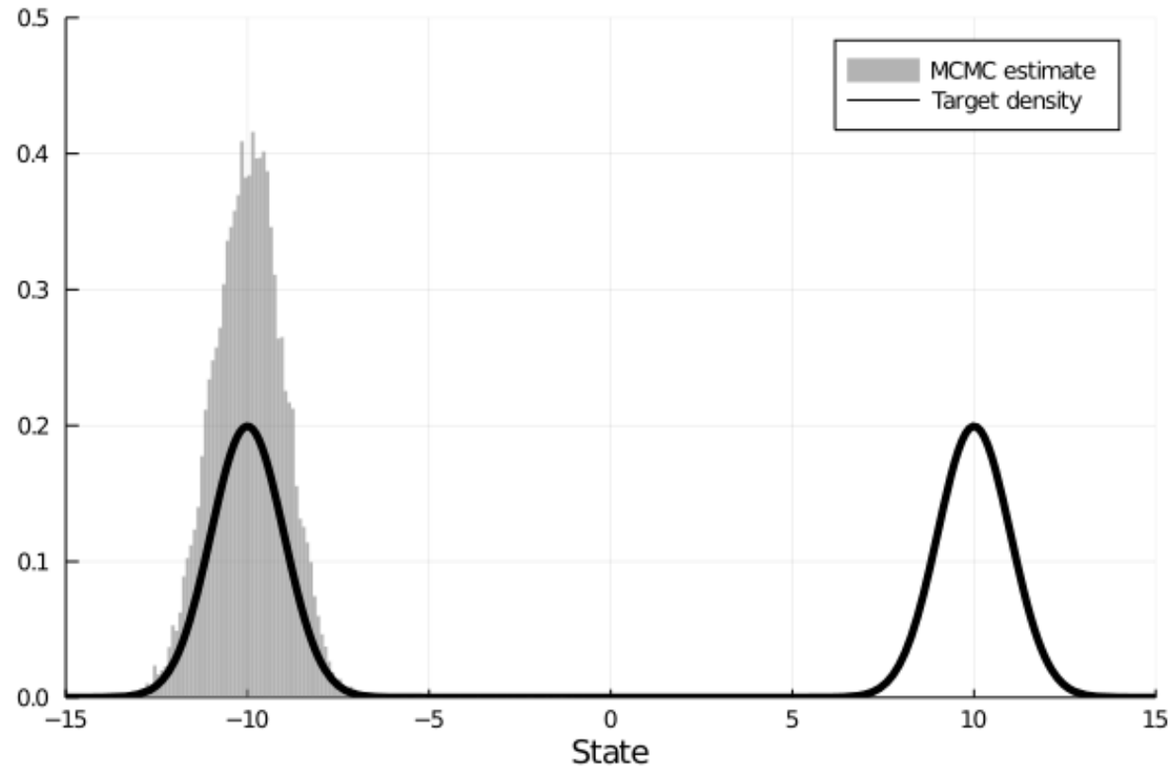
- **Solution:** Numerically approximate expectation using MCMC
- Run Markov chain stationary with respect to target and use ergodic theorem.

$$\mathbb{E}[f] = \lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} f(X_t)$$

MCMC

- **Problem:** MCMC can get stuck :(
  - Chains get trapped in local regions of high probability and mix poorly
  - Worse with high dimensions, discrete spaces, constrained topologies





PARALLEL COMPUTING

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- **Hardware**: Clock speeds stagnant and modern computation is distributed
- **Algorithmic**: Single chain tries to simultaneously efficiently explore & be accurate

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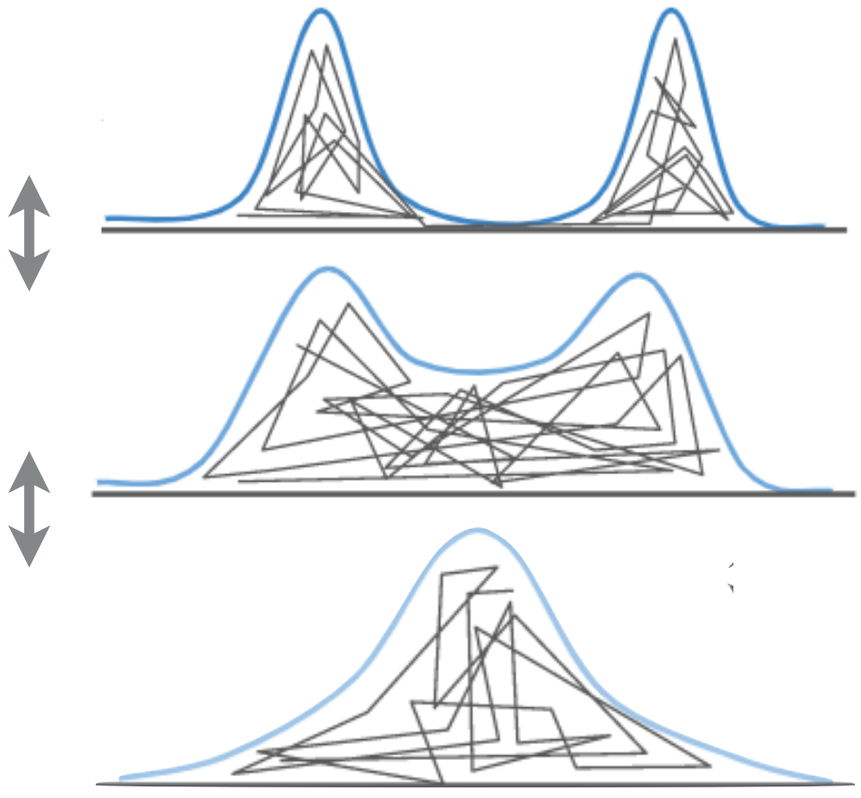
- **A Solution:** Run N additional chains in parallel
  - Delegate exploration to tractable **reference** chain
  - Communicate to **target** through the remaining $N-1$ chains



Chain N
Complex **Target**

Chains $1, \ldots, N-1$

Chain 0
Simple **Reference**
(often i.i.d. samples)

ANNEALING

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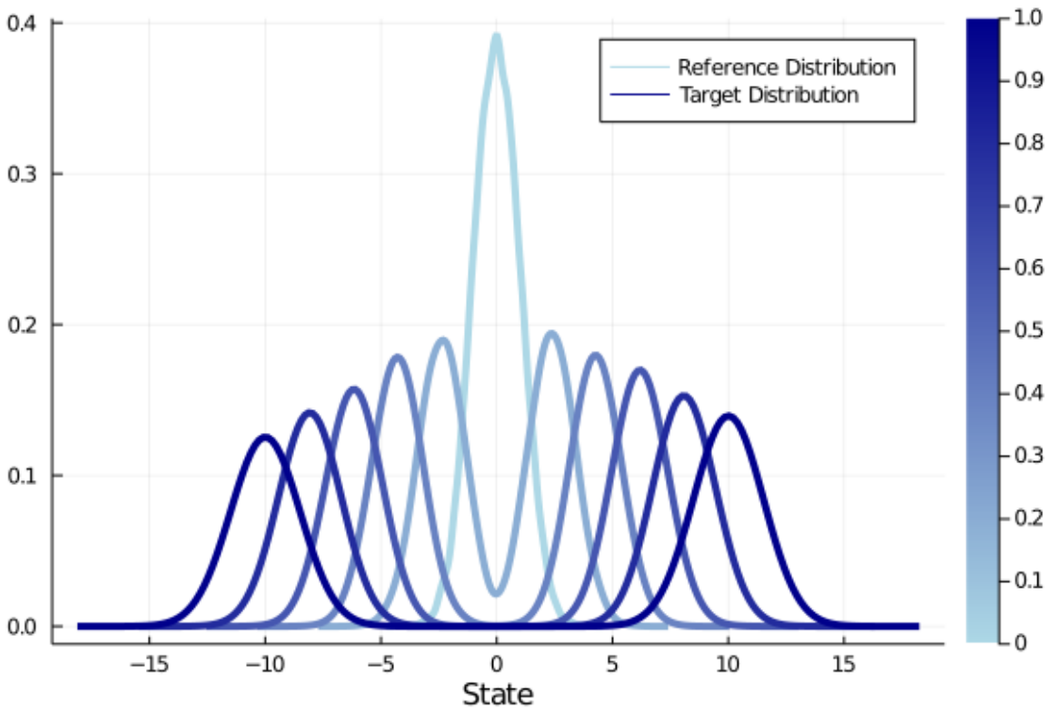

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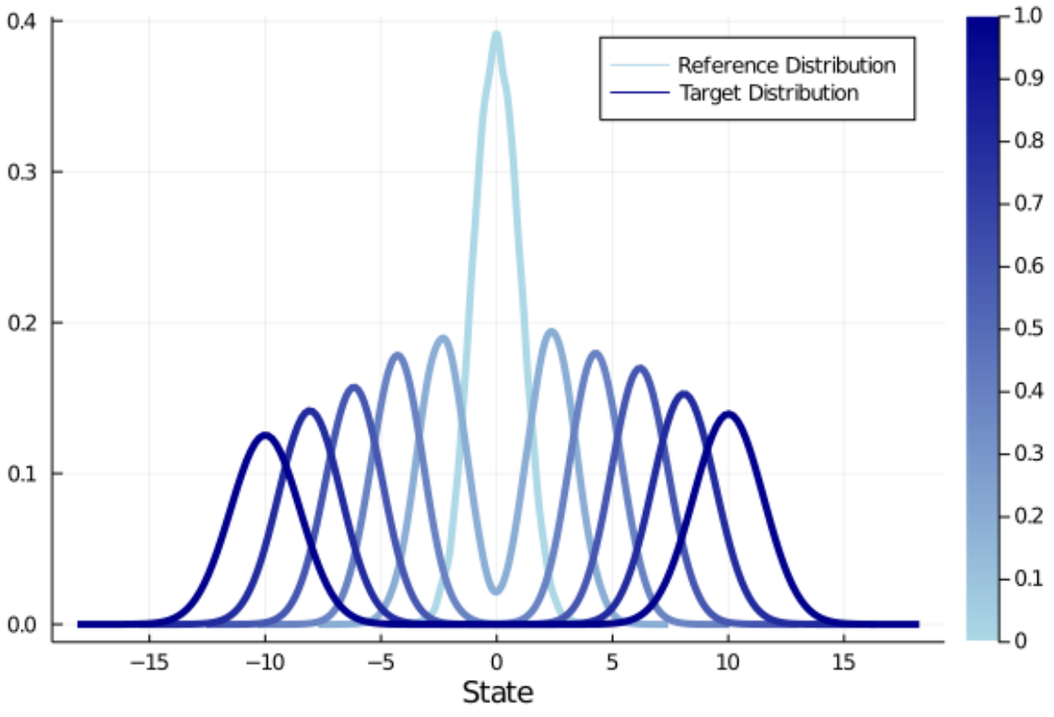

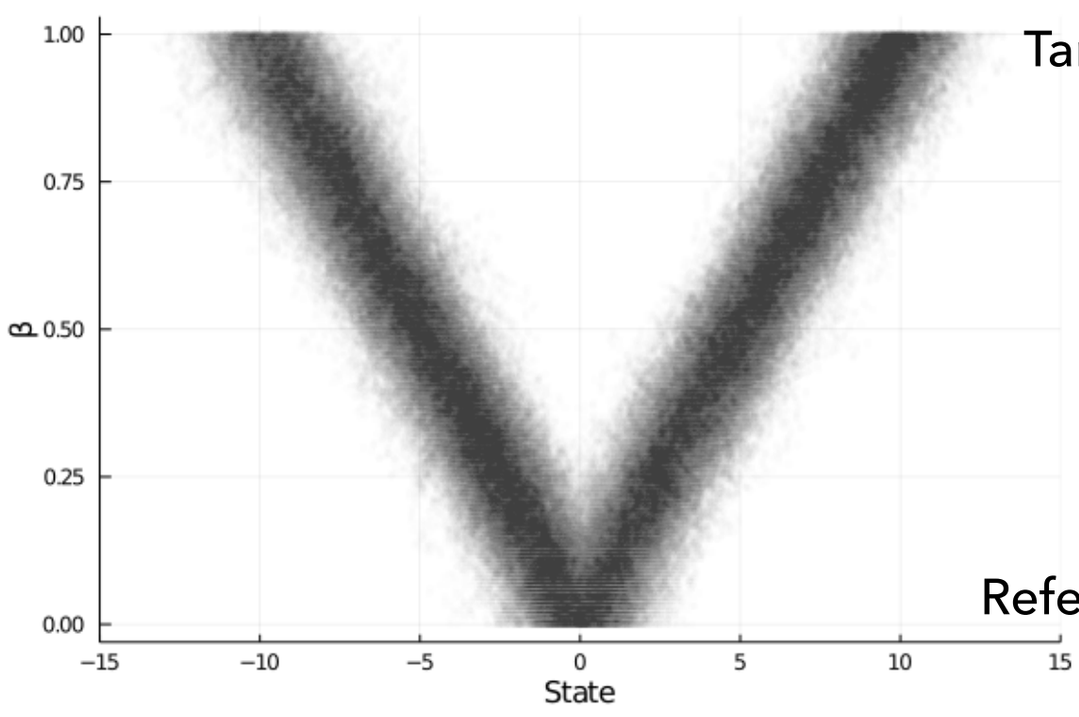

Target

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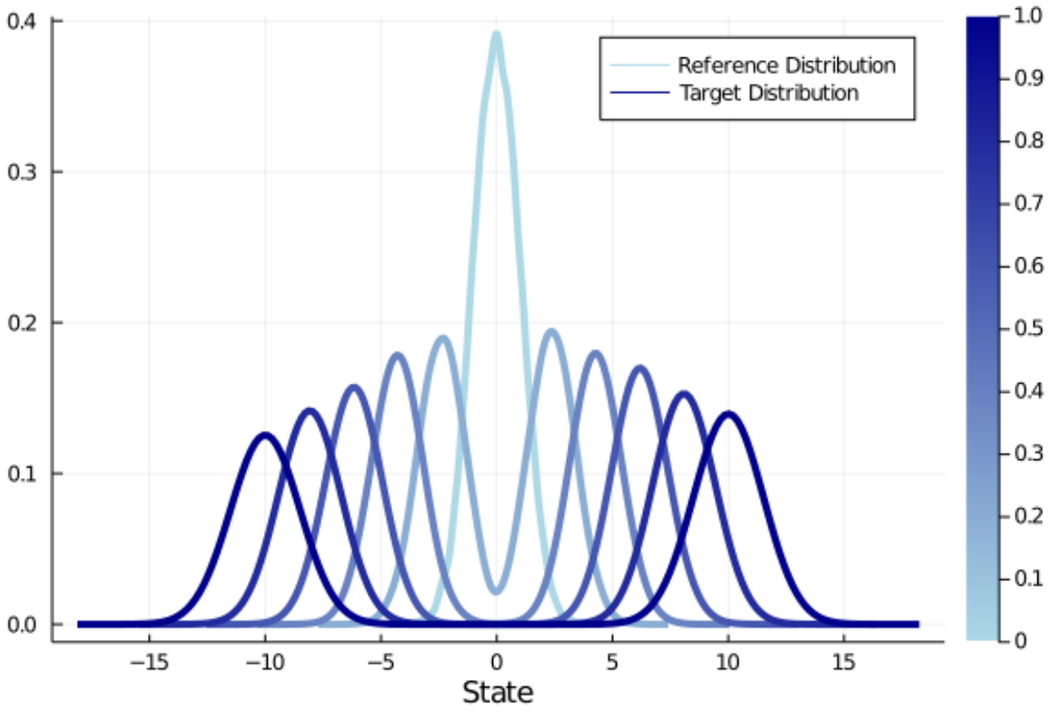

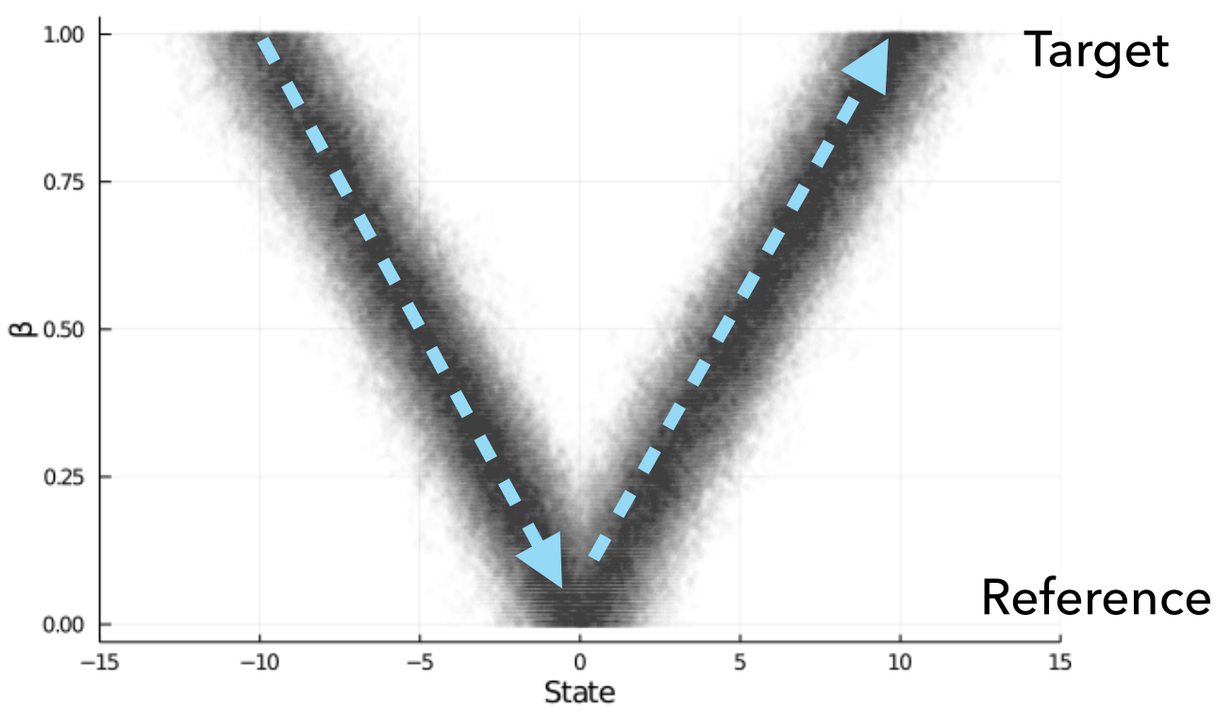

PARALLEL TEMPERING

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- Extend state space $\mathcal{X}^{N+1}$ with join distribution

$$\boldsymbol{\pi}(\mathbf{x}) = \prod_{n=0}^{N} \pi_{\beta_n}(x^n)$$

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2. **Communication:** propose swaps for adjacent component
   - Propose swap components n and $n+1$ for $n \in S_t \subset \{0, \ldots, N-1\}$
   - Accept with probability:

$$\alpha_{n,n+1} = 1 \wedge \frac{\pi_n(x^{n+1})\pi_{n+1}(x^n)}{\pi_n(x^n)\pi_{n+1}(x^{n+1})}$$

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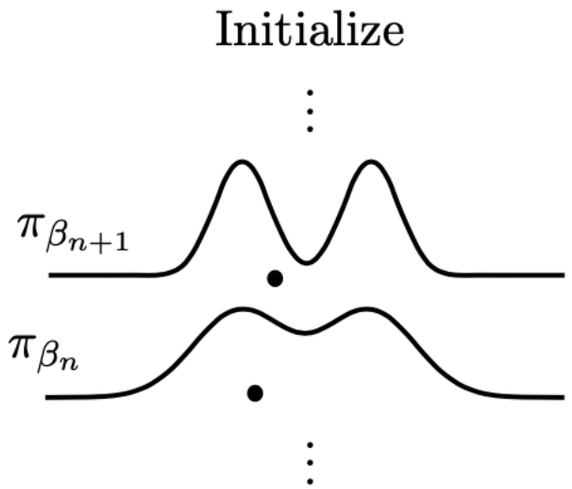

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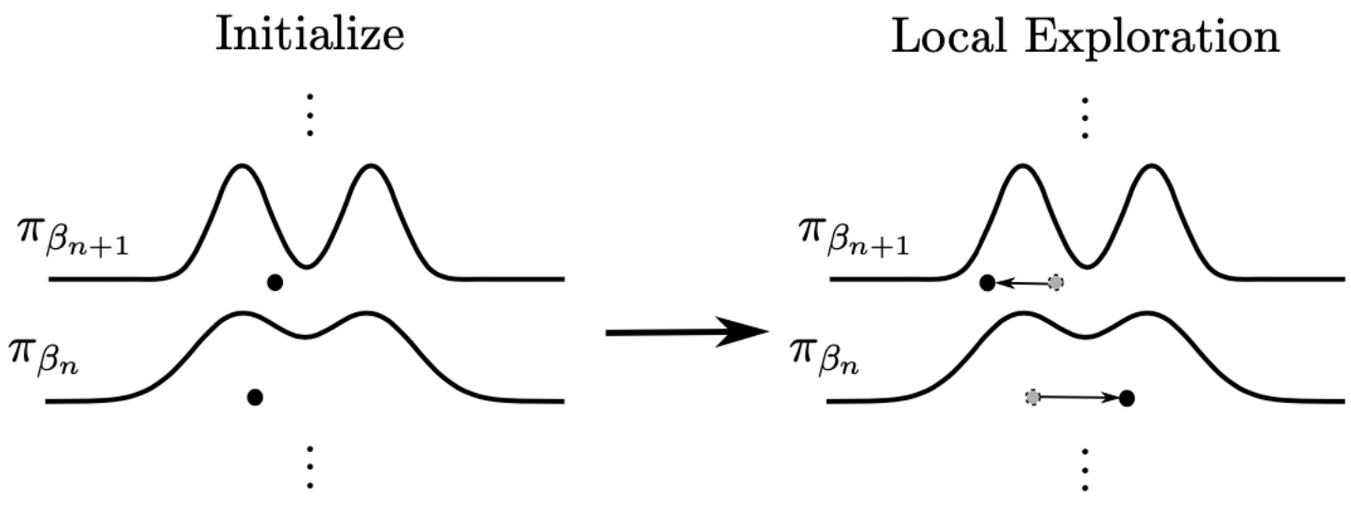

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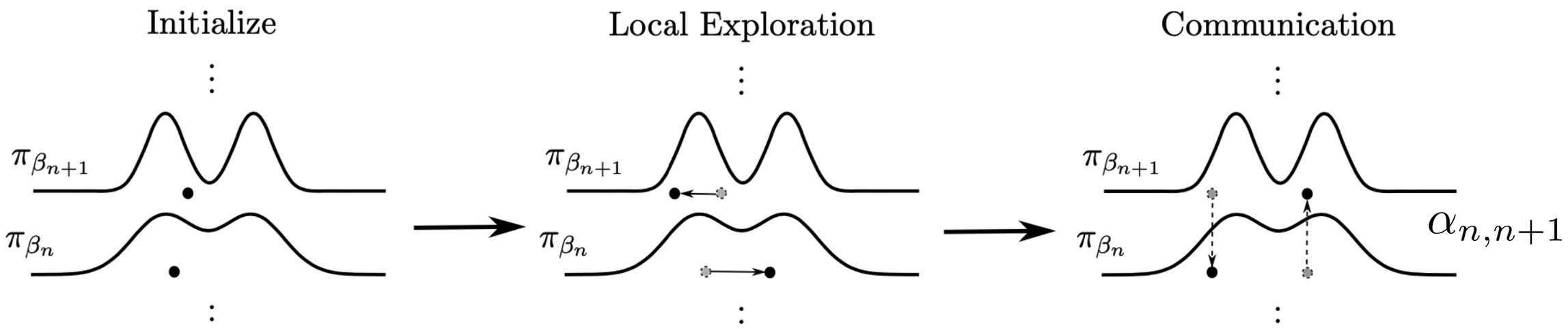

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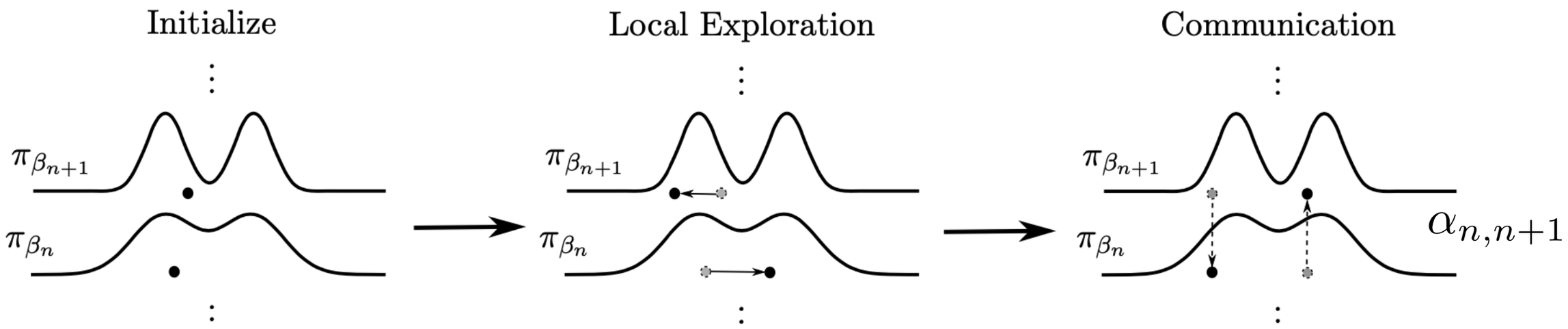

- Acceptance probability:

$$\alpha_{n,n+1} = 1 \wedge \frac{\pi_n(x^{n+1})\pi_{n+1}(x^n)}{\pi_n(x^n)\pi_{n+1}(x^{n+1})}$$

  - Notice swap probability only depends on likelihood ratio of states
  - Agnostic to location of modes

MCMC VS PARALLEL TEMPERING

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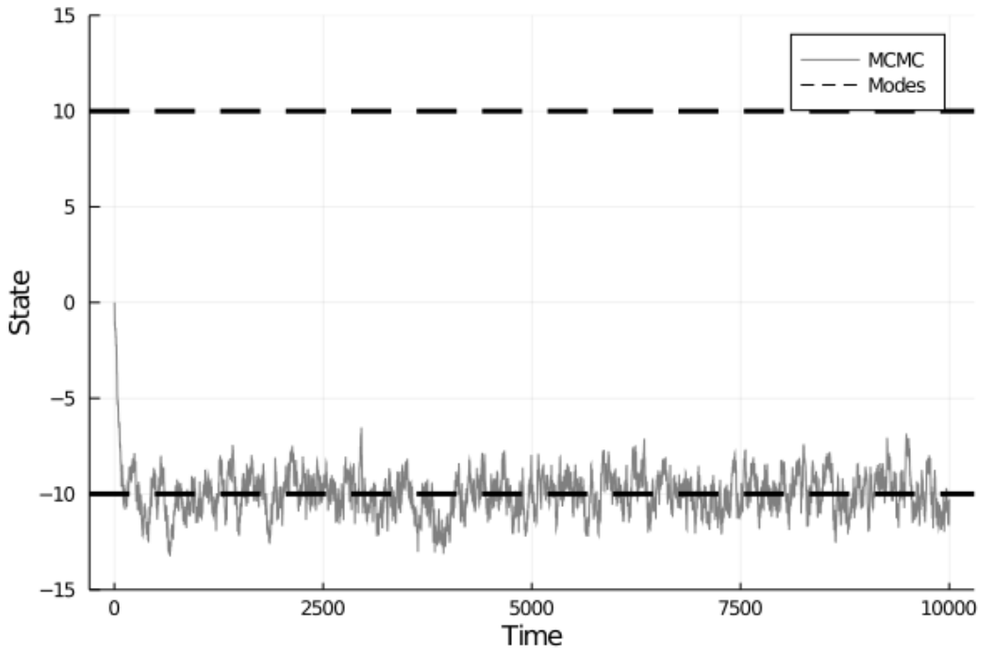
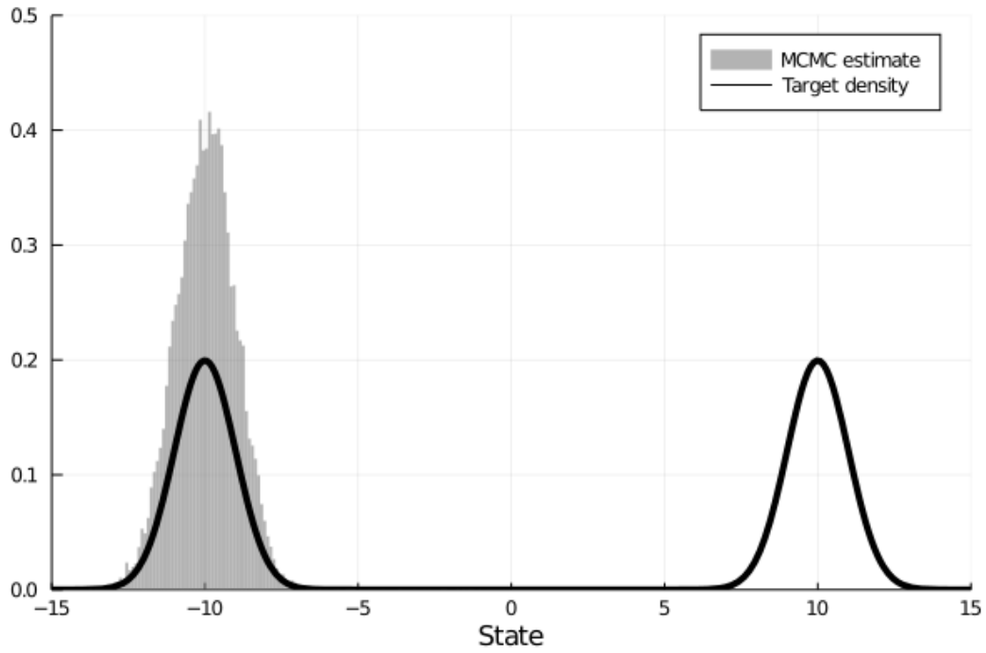
Single chain MCMC





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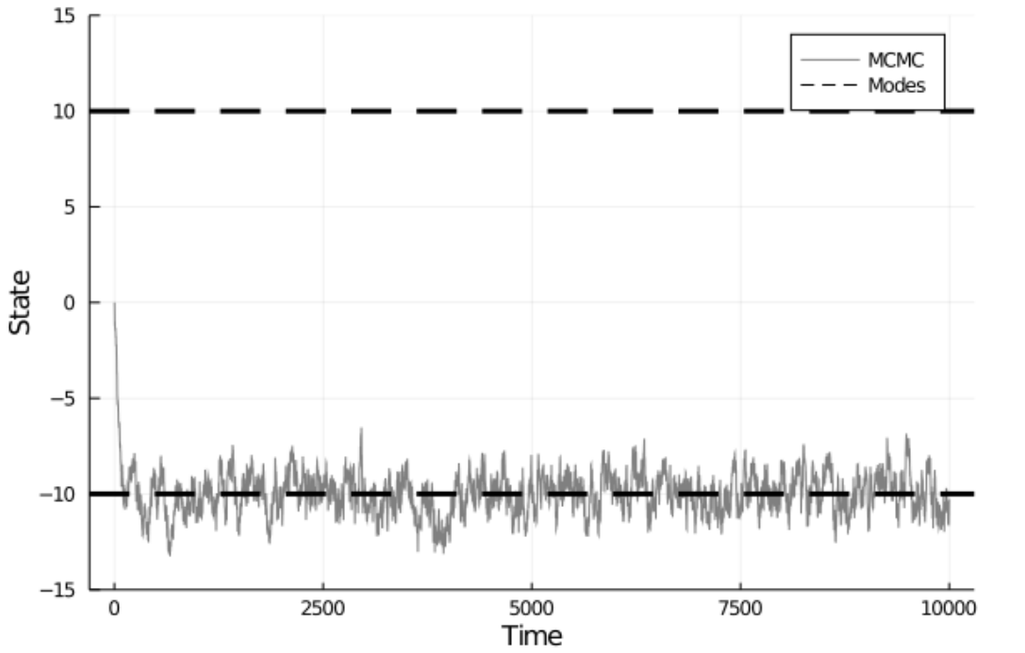
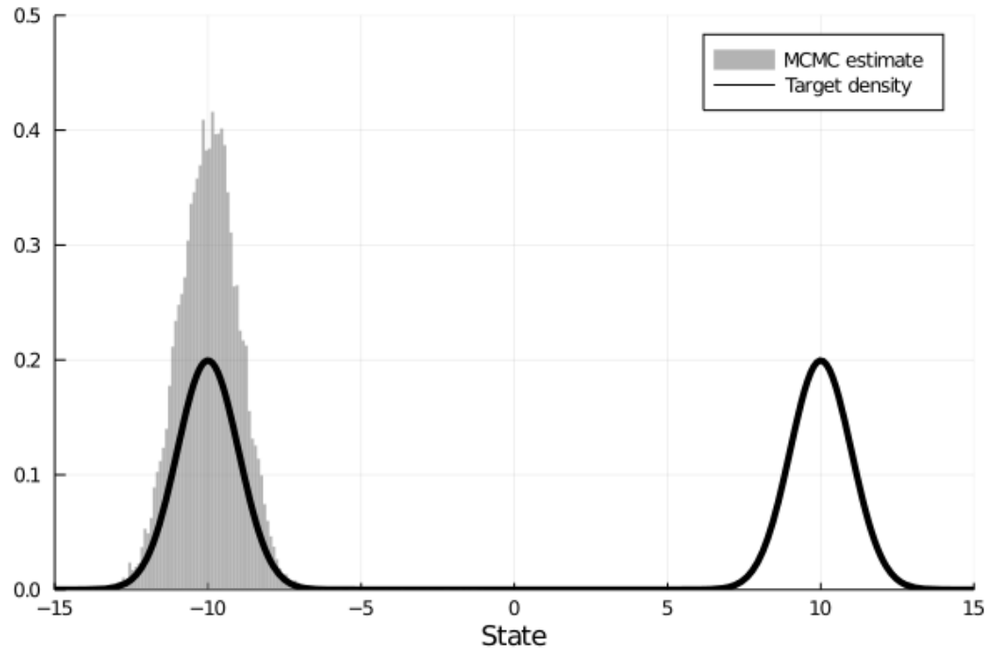
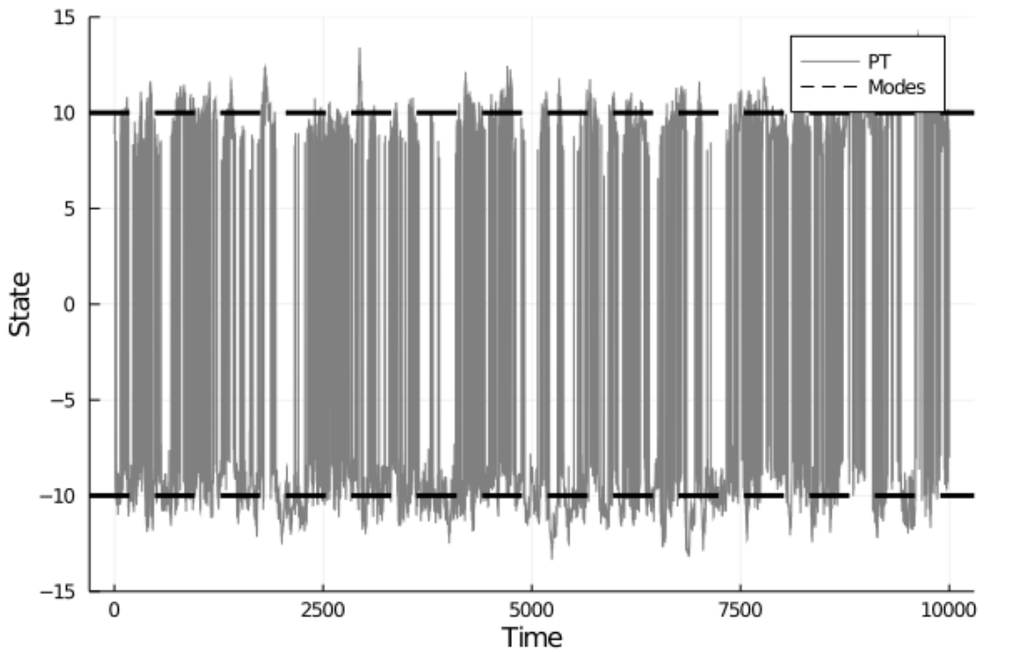
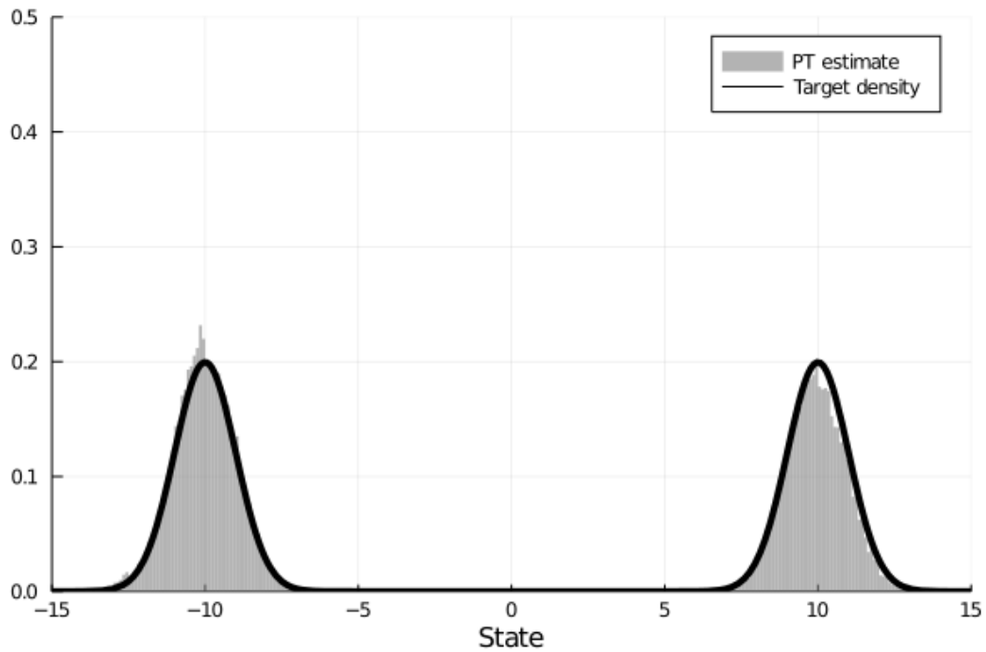




Parallel Tempering (N = 10)





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- How to propose swaps?
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  - Distributed PT and the index process
  - Non-Reversible vs Reversible PT
  - Scaling behavior
  - Tuning non-reversible PT
  - Experiments

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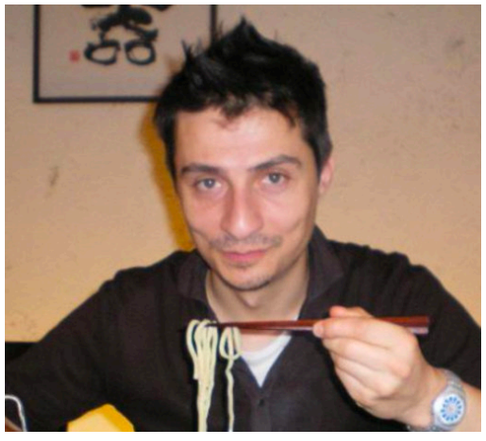
Alexandre Bouchard-Côté

George Deligiannidis



Arnaud Doucet

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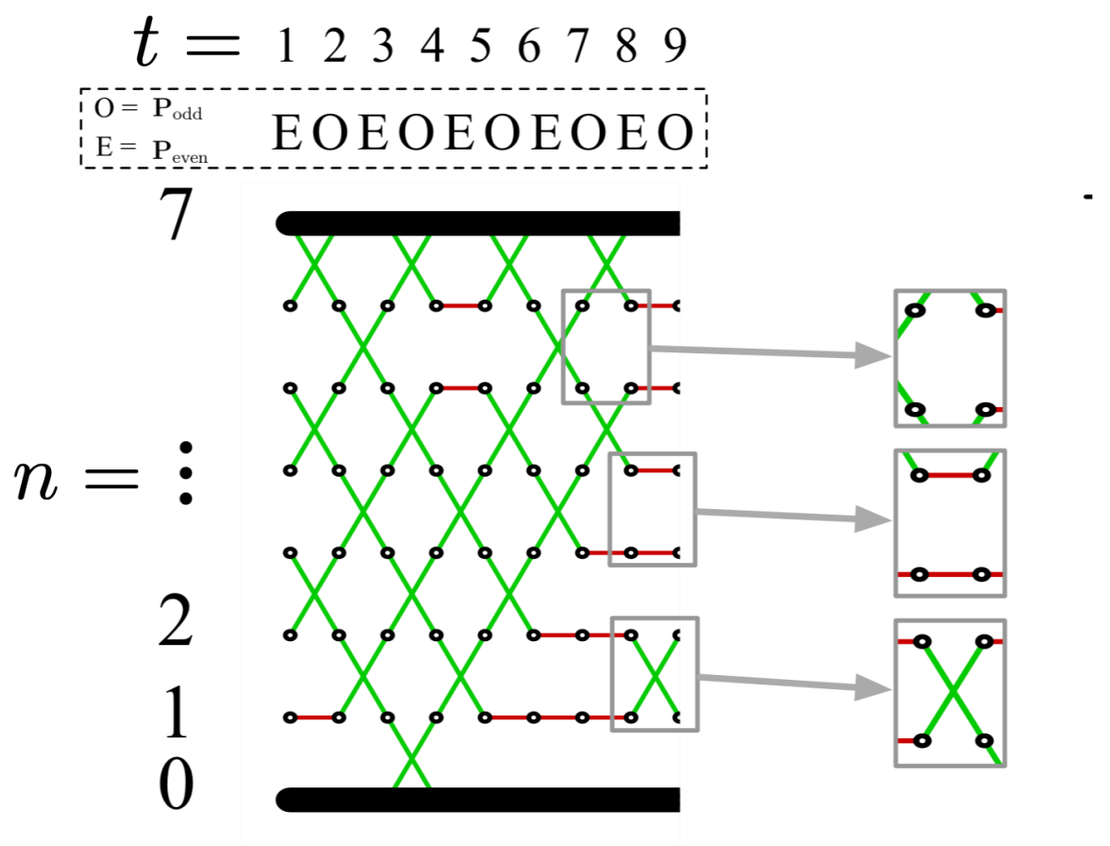

DISTRIBUTED PT

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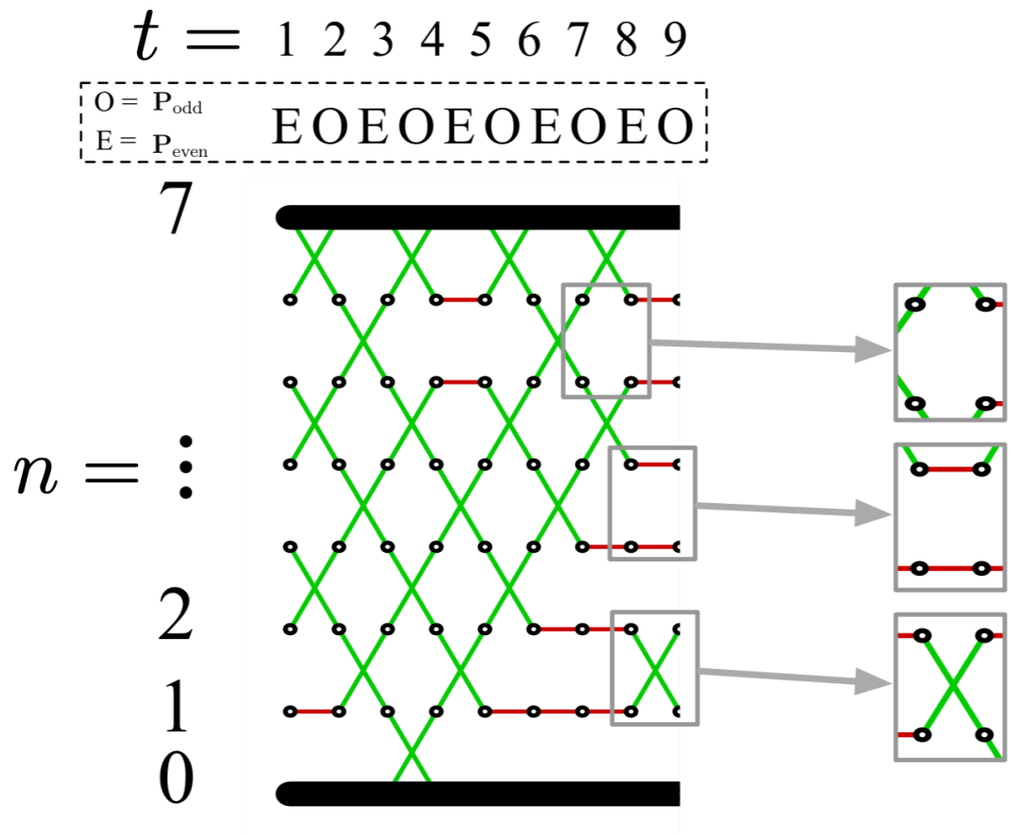
  - More efficient for distributed implementation to swap numbers



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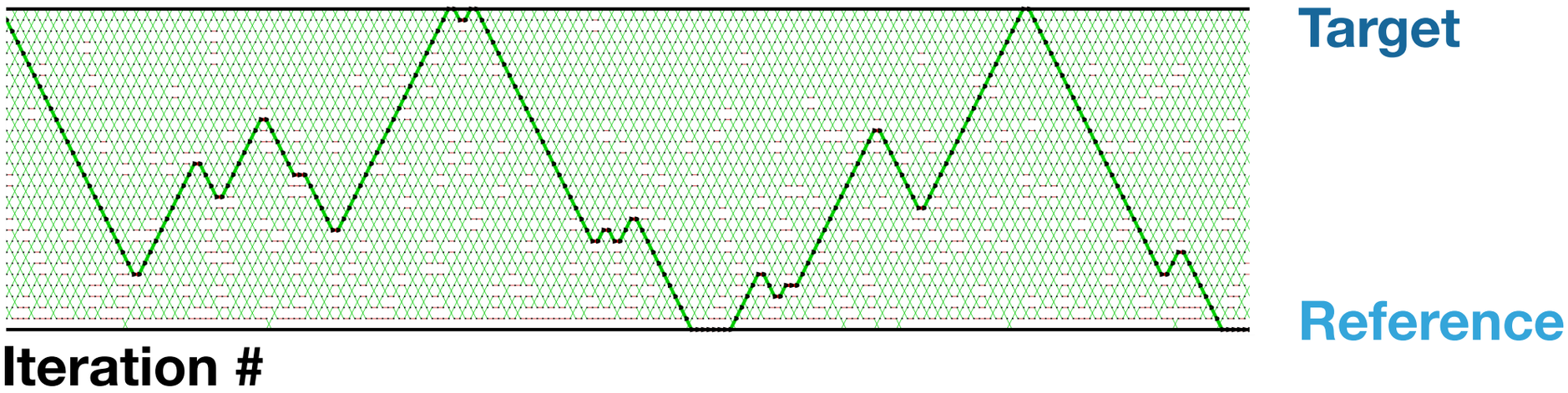

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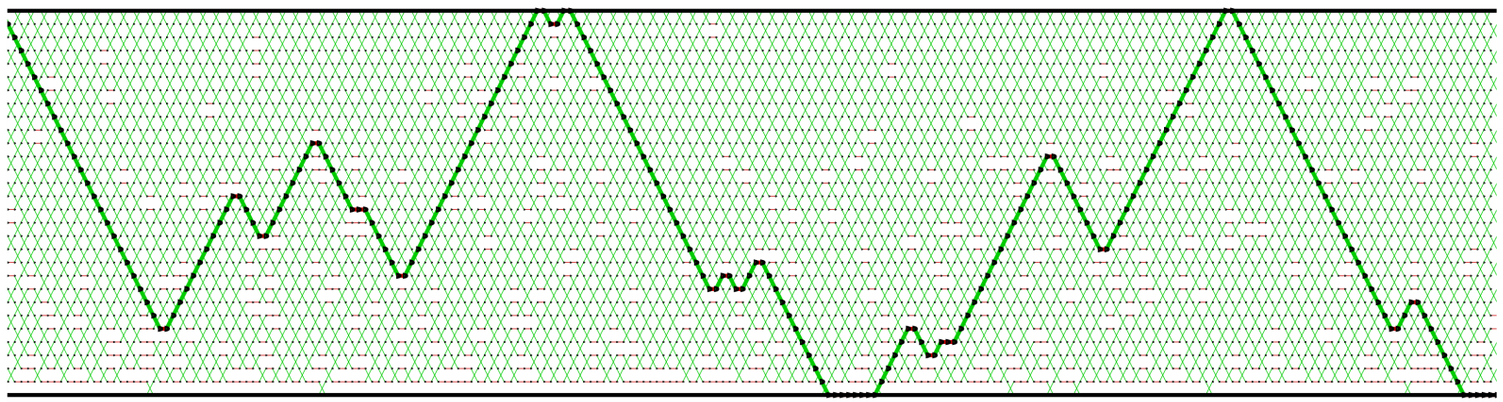

- **Round trip rate** % of iterations with round trip

$$\tau_N = \lim_{t \to \infty} \frac{\mathbb{E}[\text{total round trips by time t}]}{t}$$

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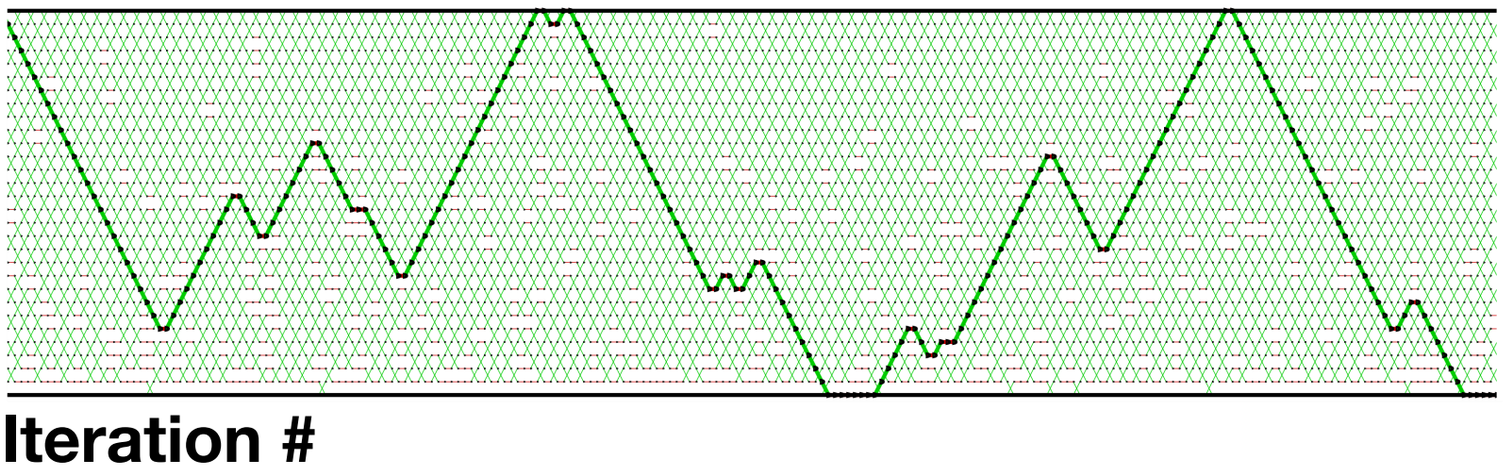

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- Objective is to maximize round trip rate

REVERSIBLE PT

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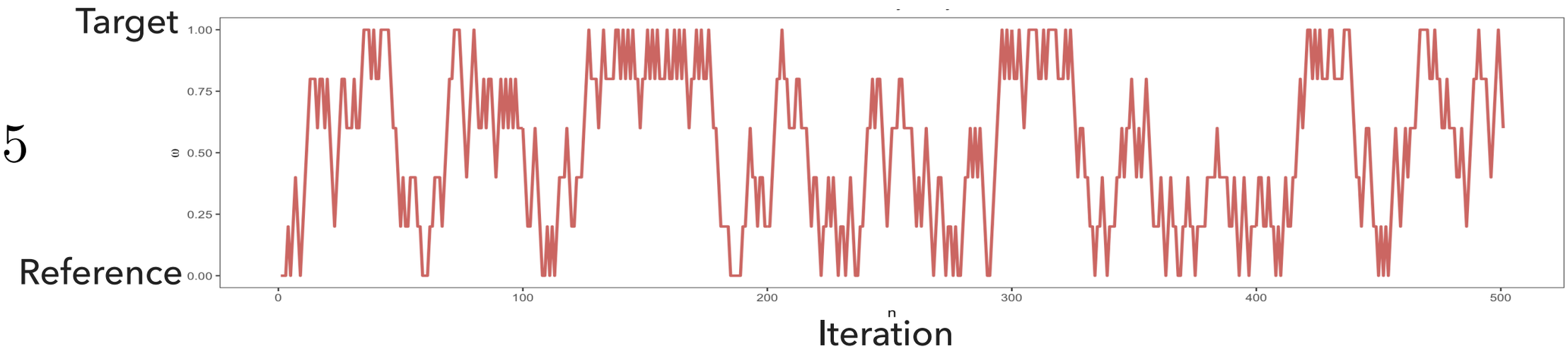
$N = 5$



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- Propose swaps at random in communication phase

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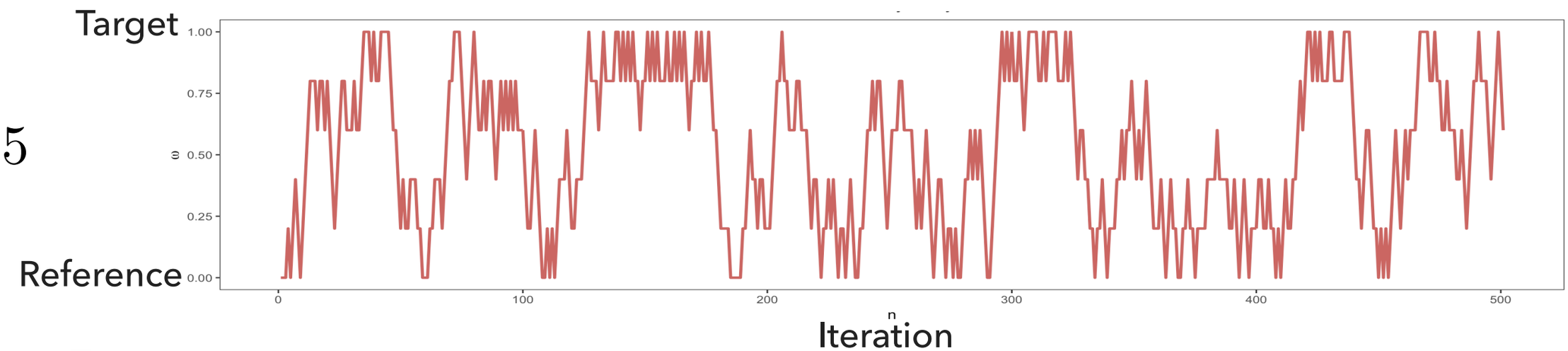

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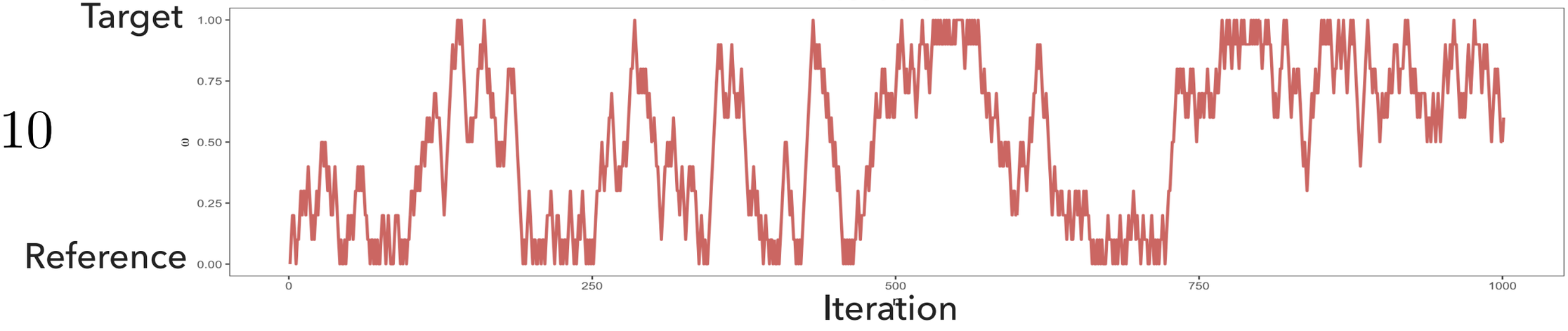

REVERSIBLE PT

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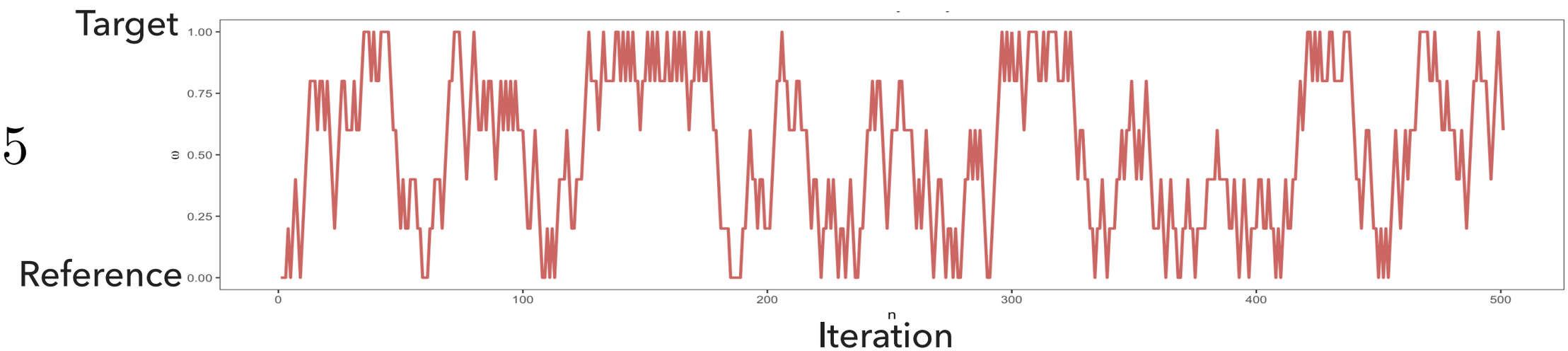

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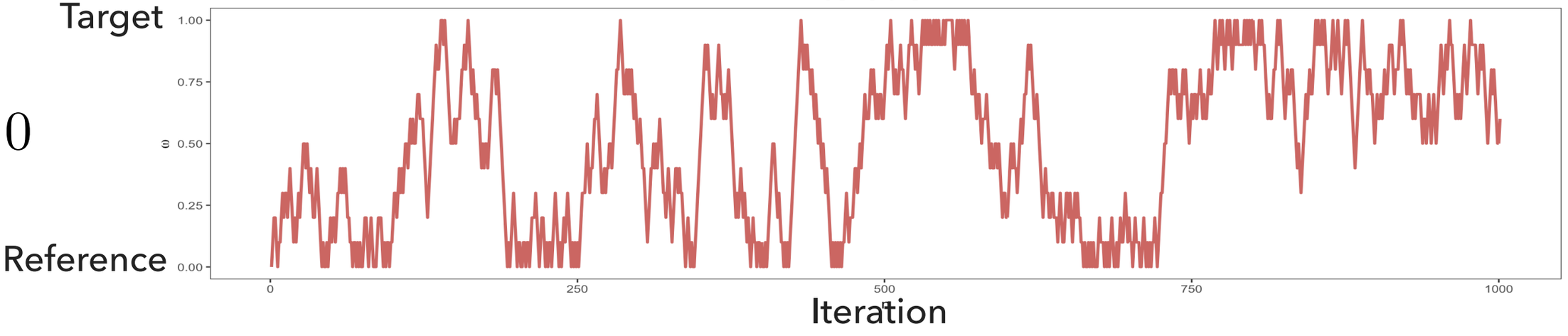

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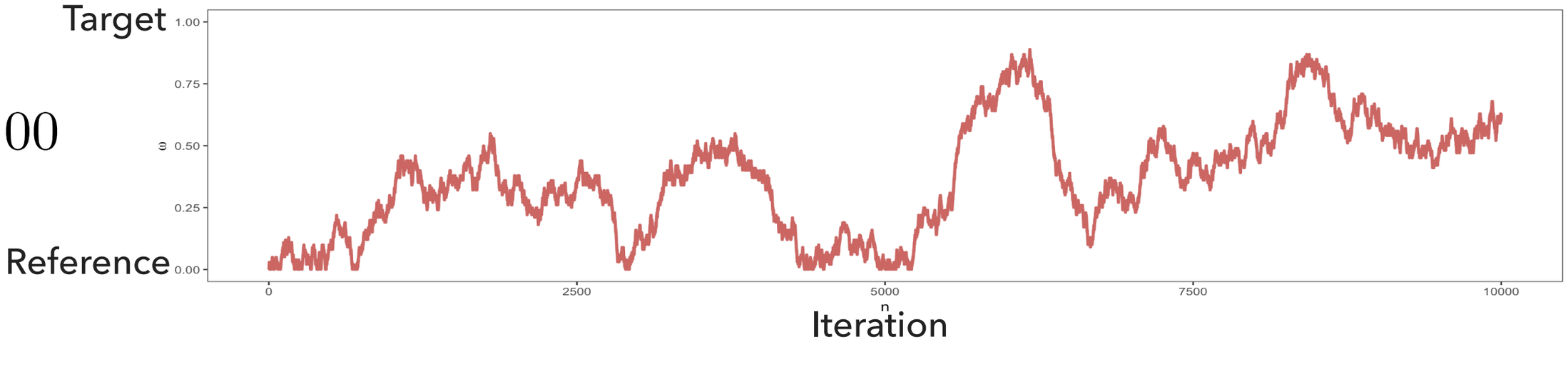

NON-REVERSIBLE PT (OKABE ET AL., 2001)

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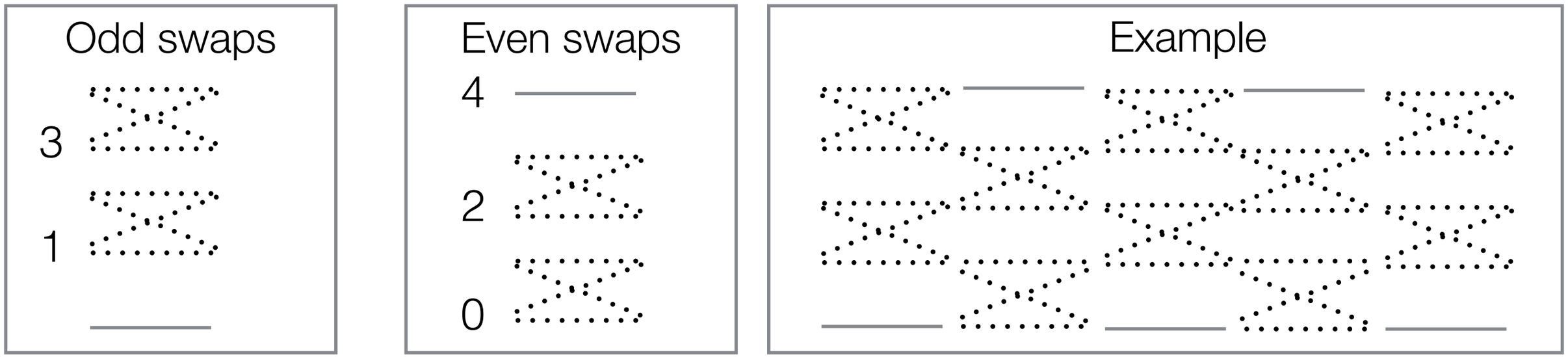

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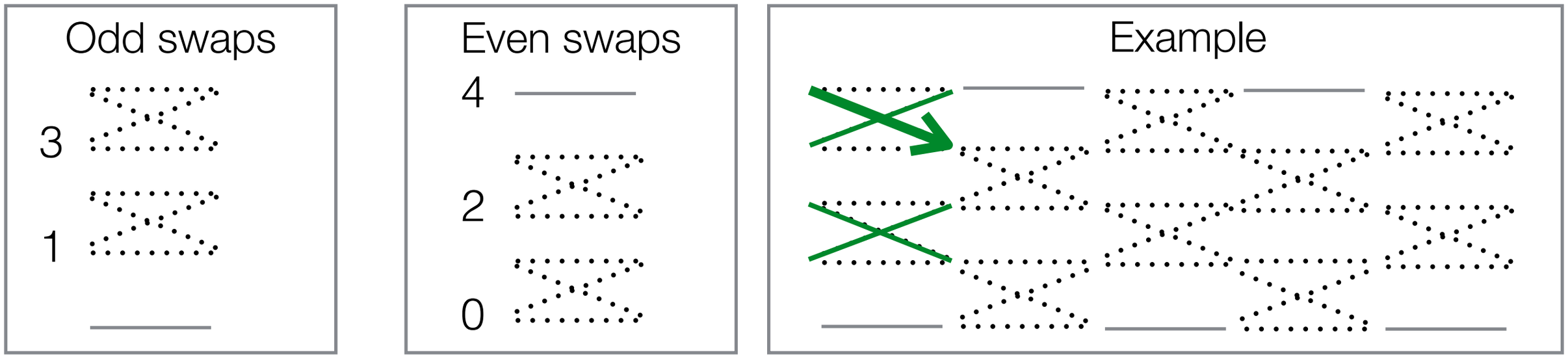

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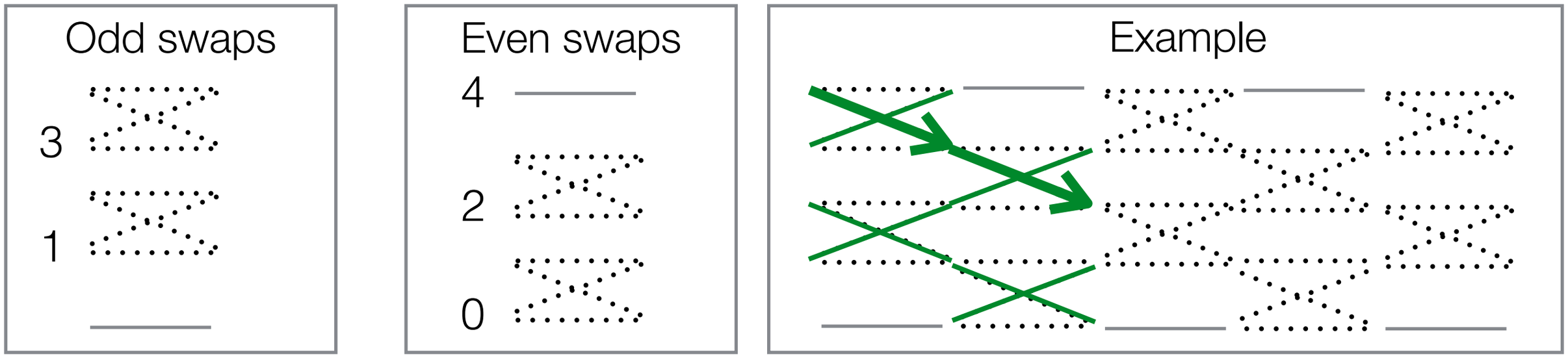

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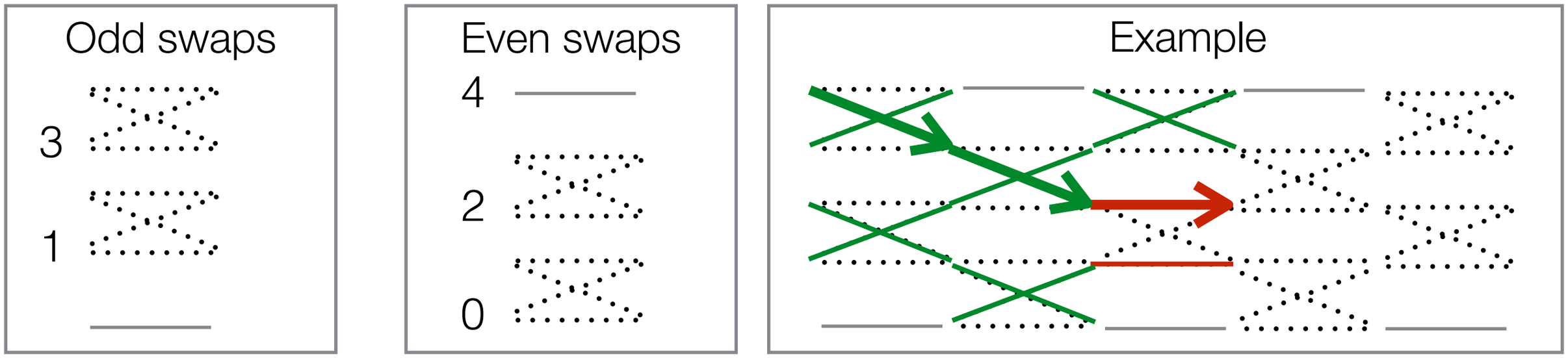

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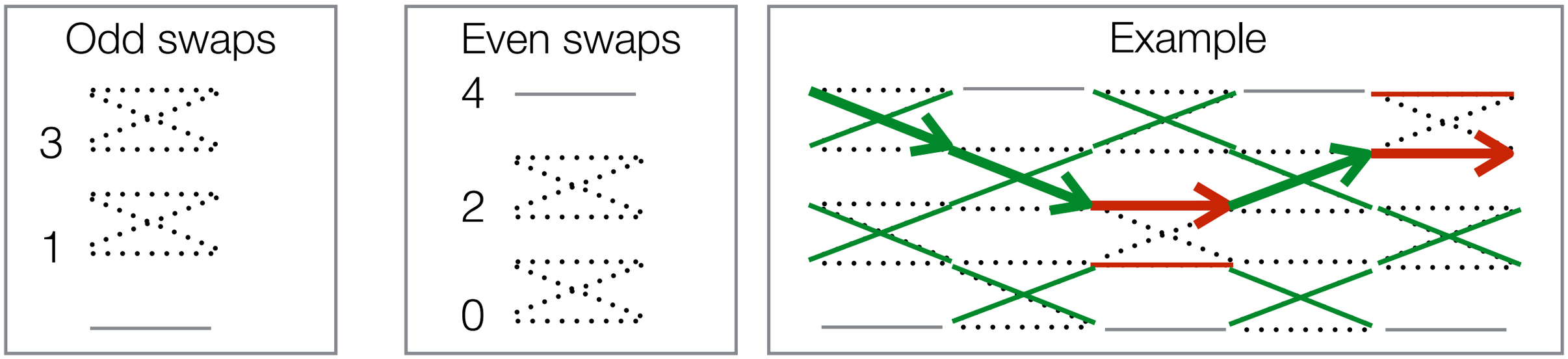

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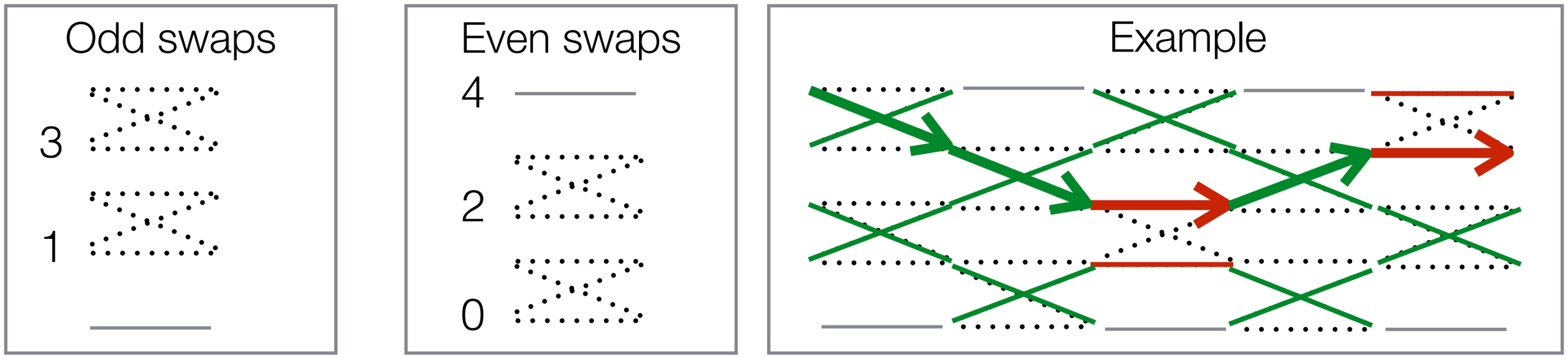

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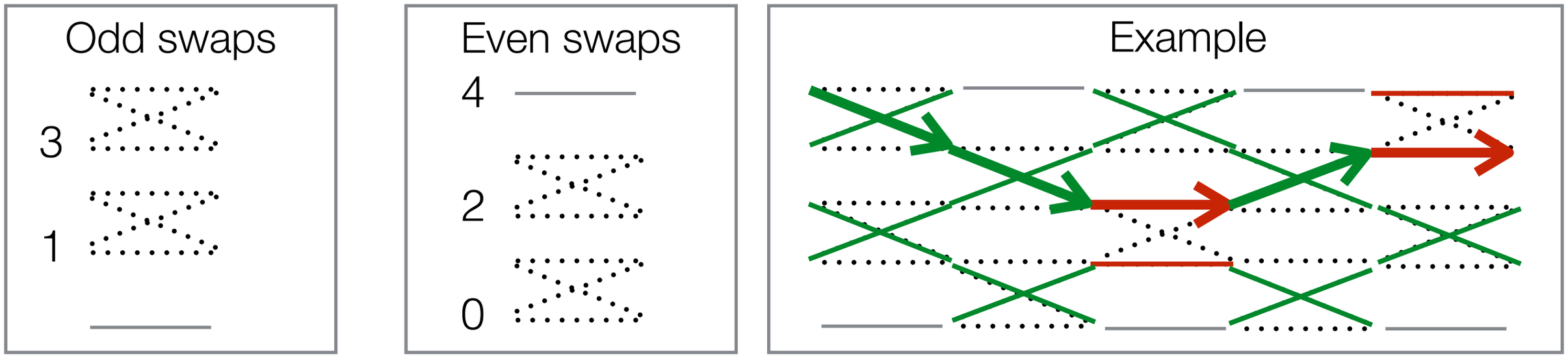

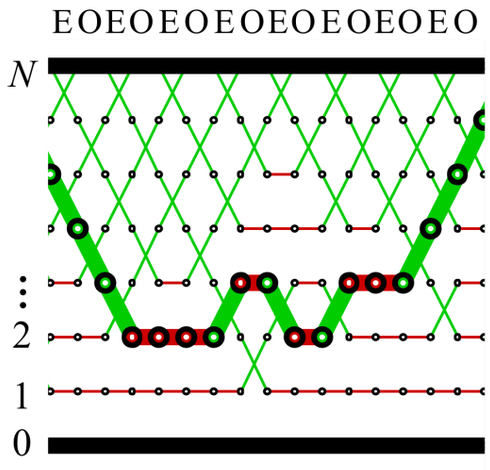

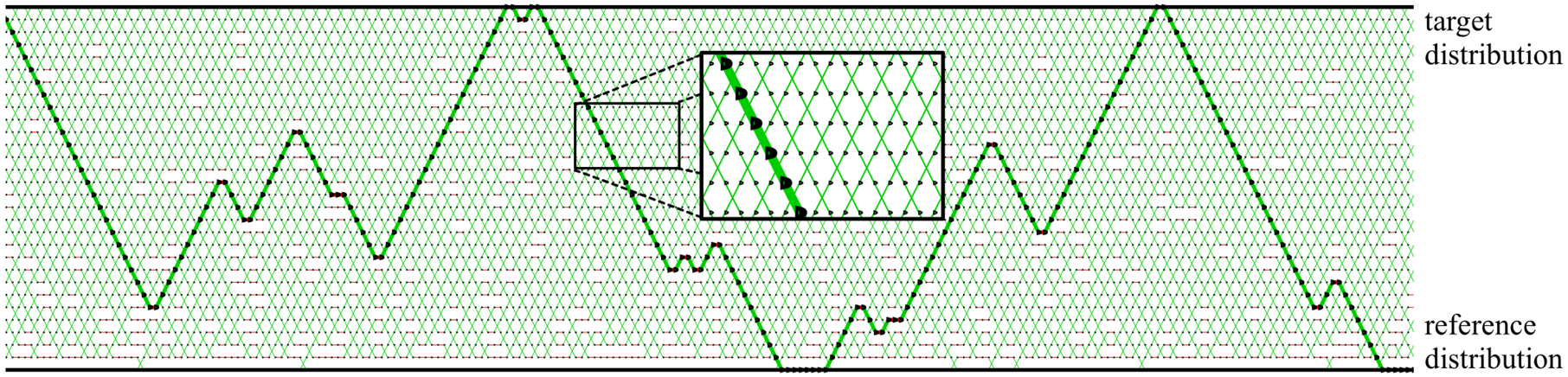

MODEL ASSUMPTIONS

- **(A1) Stationarity:**
  - $\mathbf{X}_t \sim \boldsymbol{\pi}$ for all t

- **(A2) Efficient Local Exploration (ELE):**
  - If $X \sim \pi_\beta$, $X' \sim K_\beta(X, \mathrm{d}x')$ then $V(X)$ and $V(X')$ are independent

$$V(x) = \log \frac{\pi_1(x)}{\pi_0(x)}$$

  - Weaker than assuming X and X' are independent!
  - Sufficient to study communication move independent of (problem specific) local exploration move.
  - Methodology and analysis robust to severe violations in practice

- **(A3) Integrability**
  - $\pi_0(|V|^3), \pi_1(|V|^3) < \infty$

VIODLATION OF ELE

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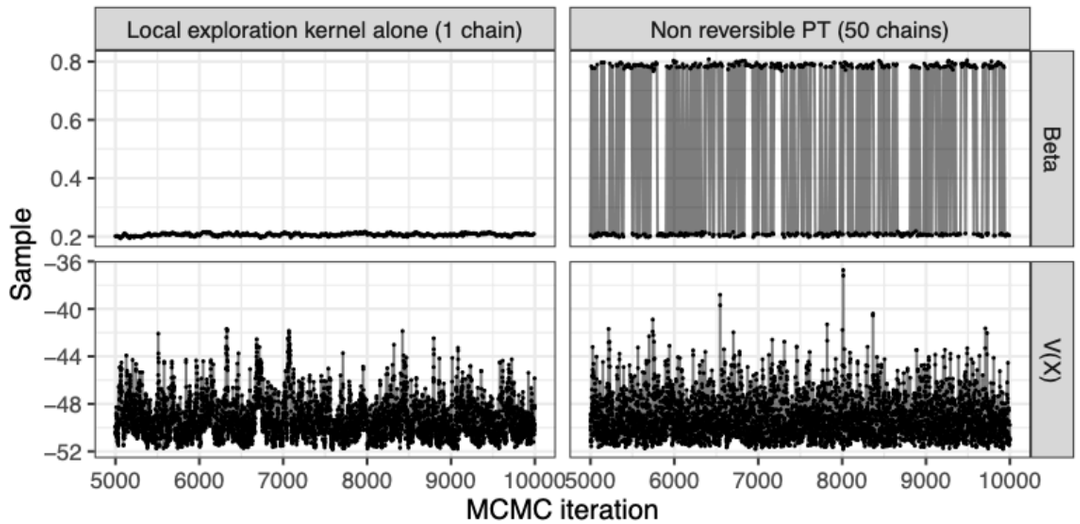
ODE parameter estimation



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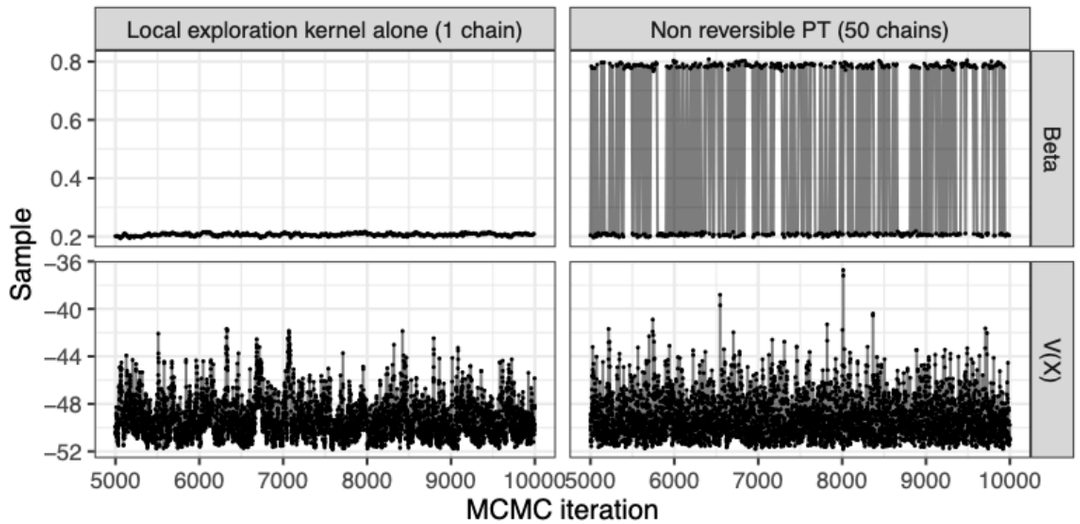
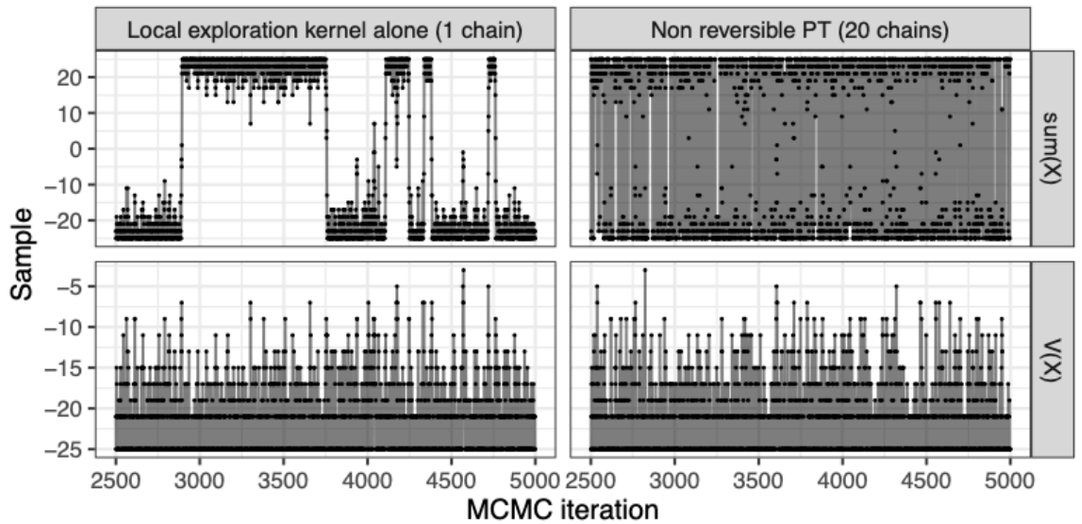
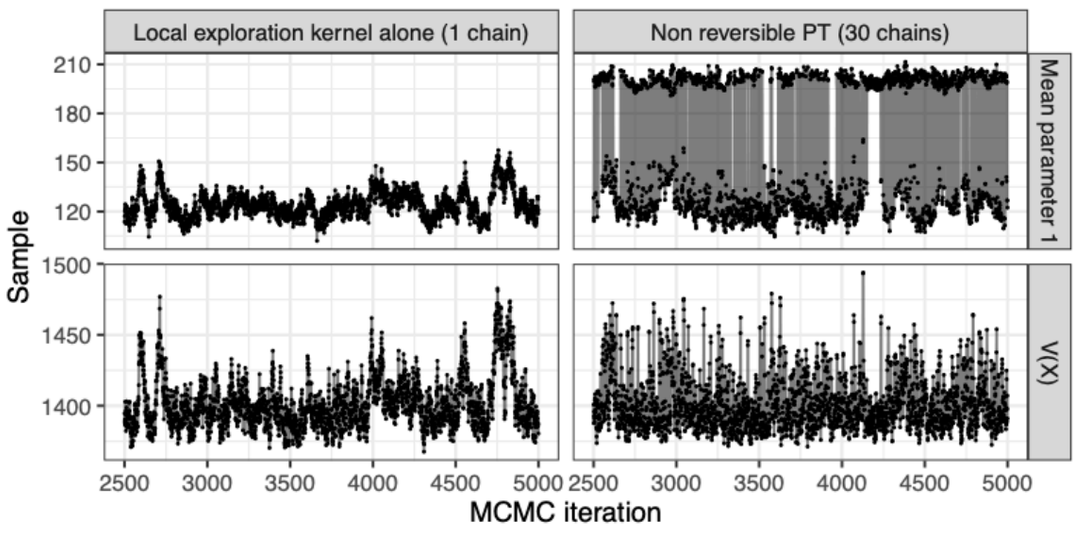


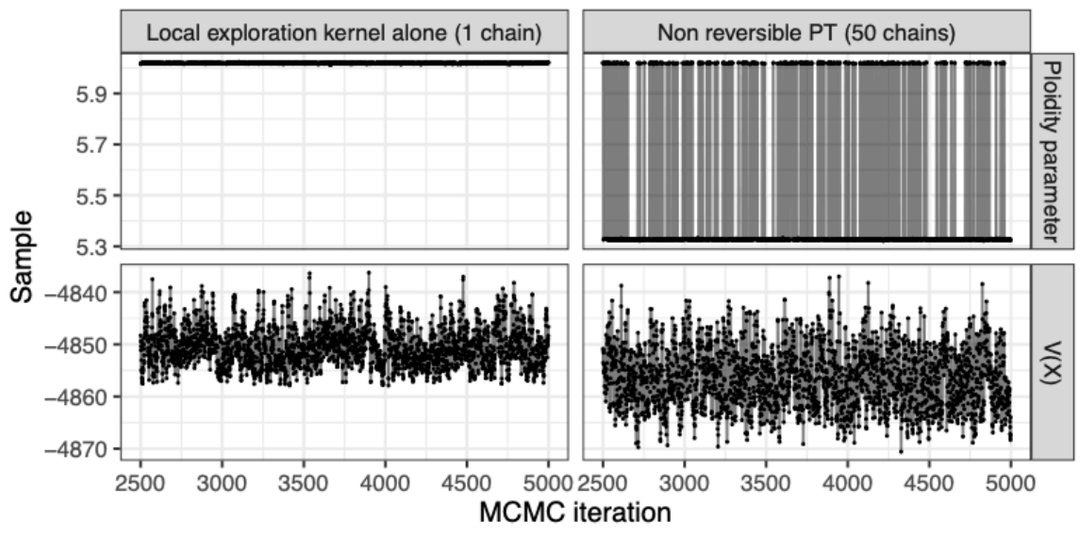
Ising model



Bayesian Mixture Model



Copy-number inference



INDEX PROCESS AS MARKOV CHAIN

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- Makes index process (I_t^m, ε_t^m) a Markov Chain for each machine m.

$$I_{t+1}^m = \begin{cases} I_t^m + \varepsilon_t^m & w.p. \quad s_{n,n+\varepsilon_t^m} \\ I_t^m & w.p. \quad 1 - s_{n,n+\varepsilon_t^m} \end{cases}$$

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- By key-renewal theorem:

$$\tau(\mathcal{B}_N) = \lim_{t \to \infty} \frac{1}{t} \mathbb{E}[\text{Total round trips by time } t]$$

$$= \frac{N+1}{\mathbb{E}[\text{round trip time per machine}]}$$

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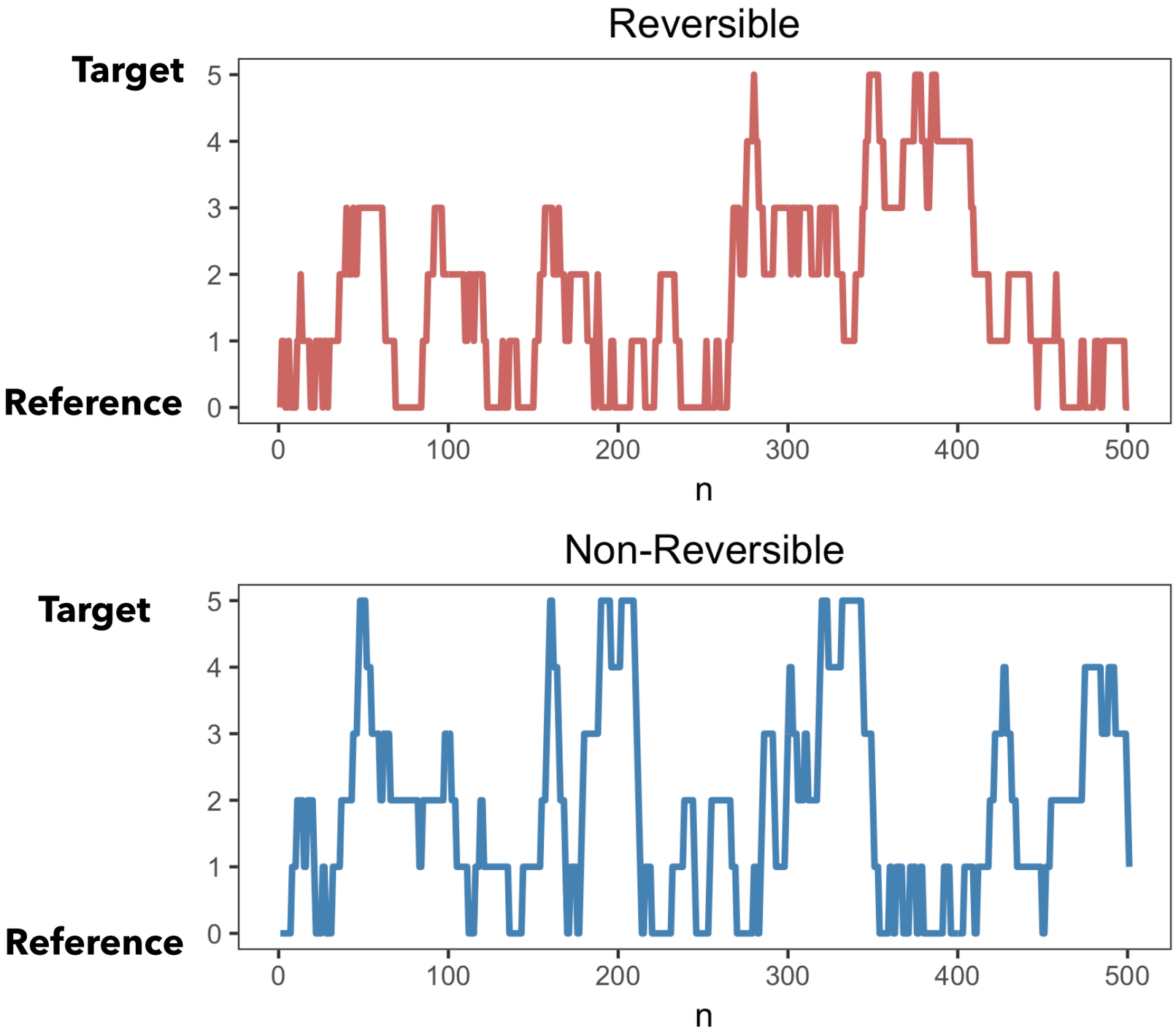
SAMPLE TRAJECTORIES

$$N = 5$$

 # Round Trips



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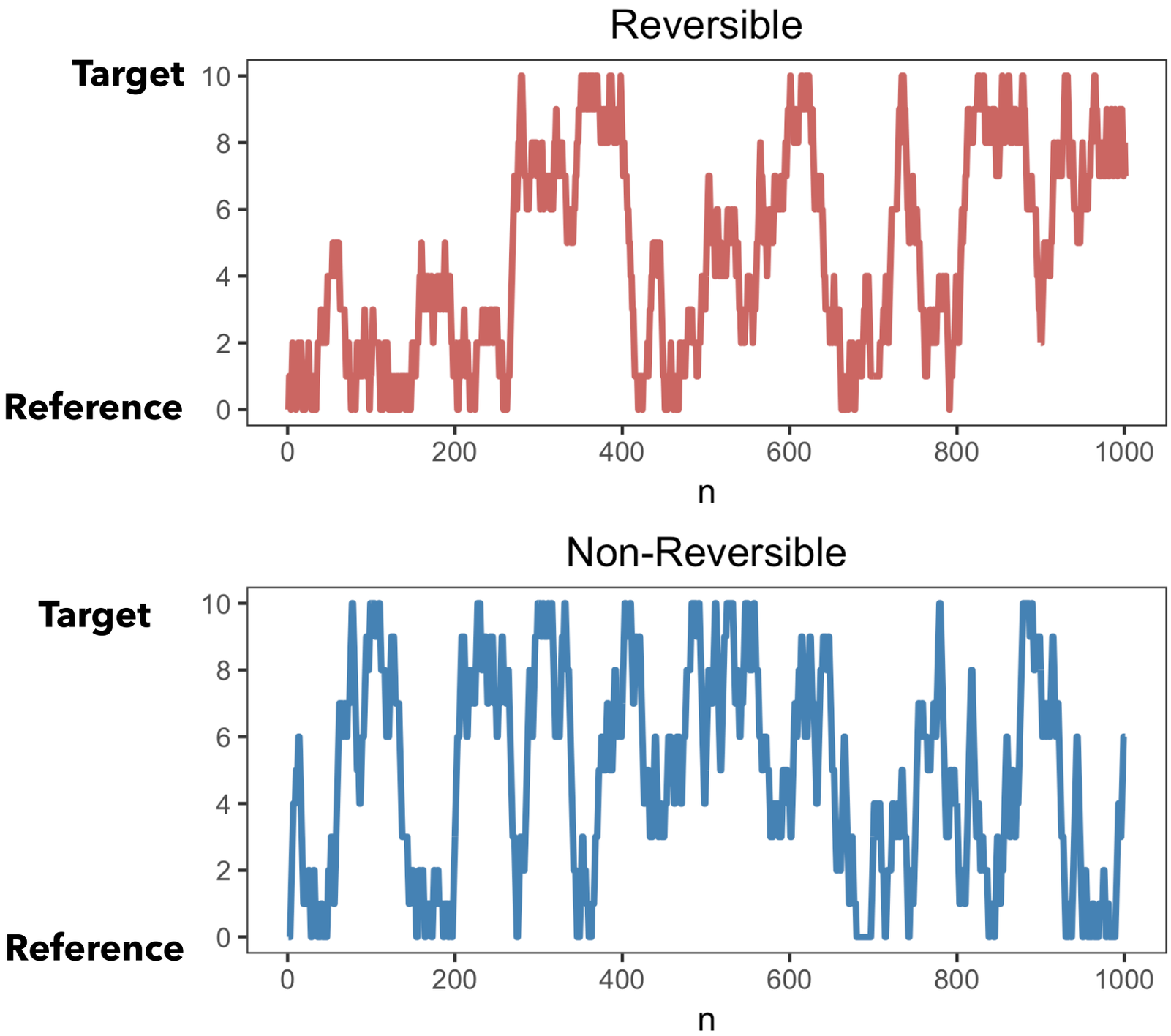
SAMPLE TRAJECTORIES

$$N = 10$$

 # Round Trips



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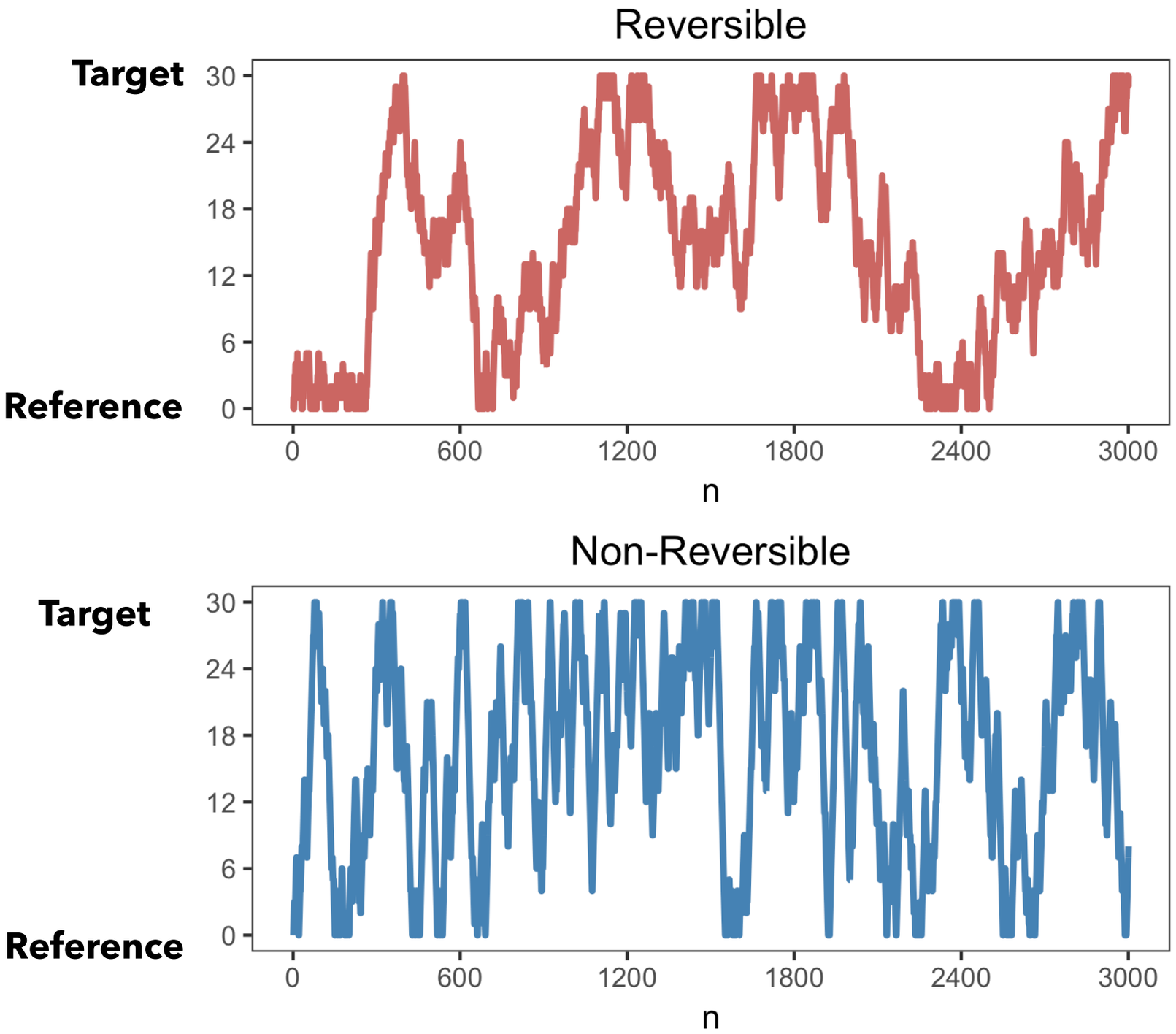
SAMPLE TRAJECTORIES

$$N = 30$$

 # Round Trips



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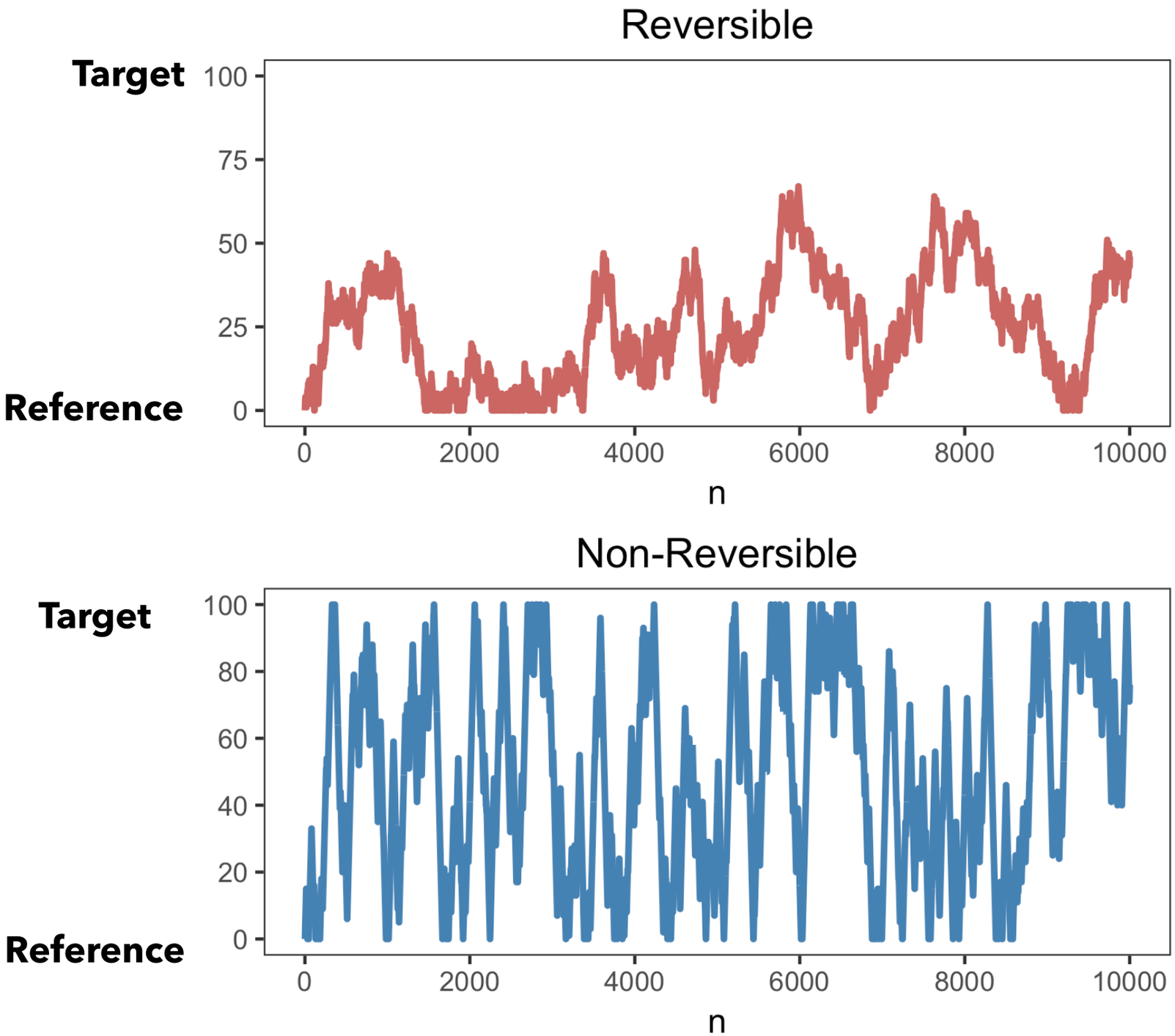
SAMPLE TRAJECTORIES

$$N = 100$$

 # Round Trips



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SCALING LIMIT (REVERSIBLE)

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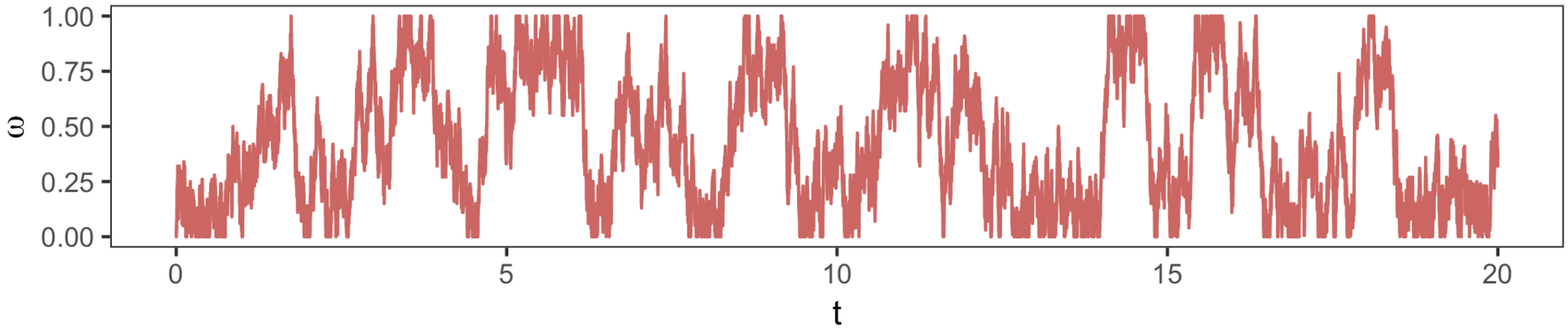

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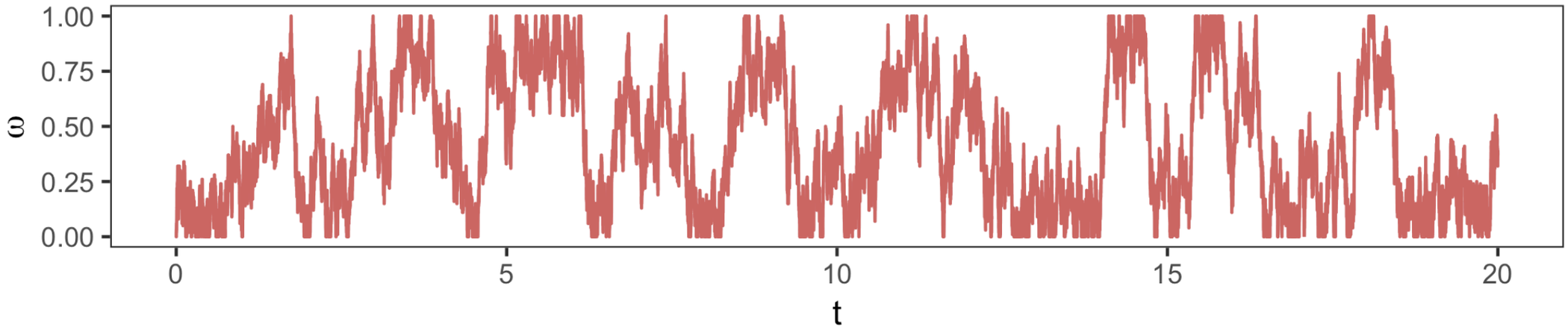

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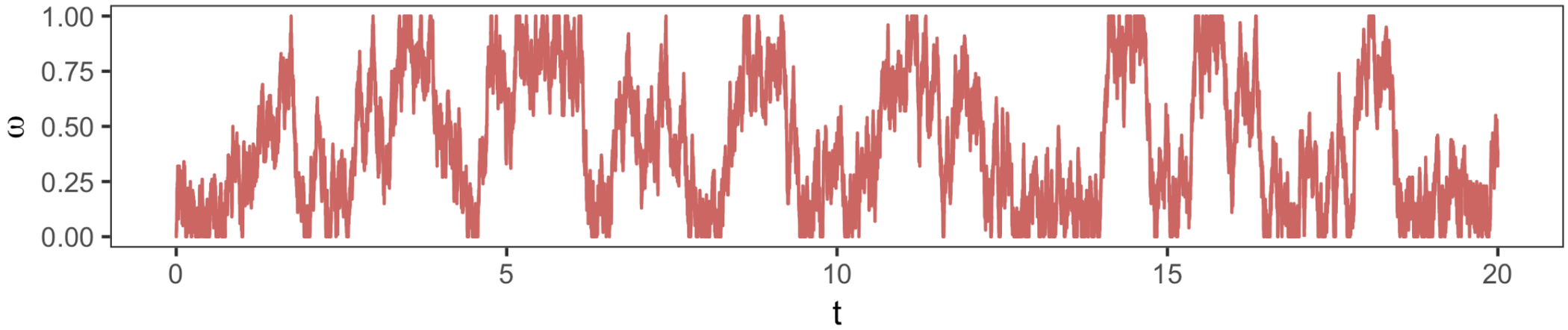

- As N grows large, noise from diffusivity dominates
- When N is large, modifying reference, target, or path leads to marginal gains

SCALING LIMIT (NON-REVERSIBLE)

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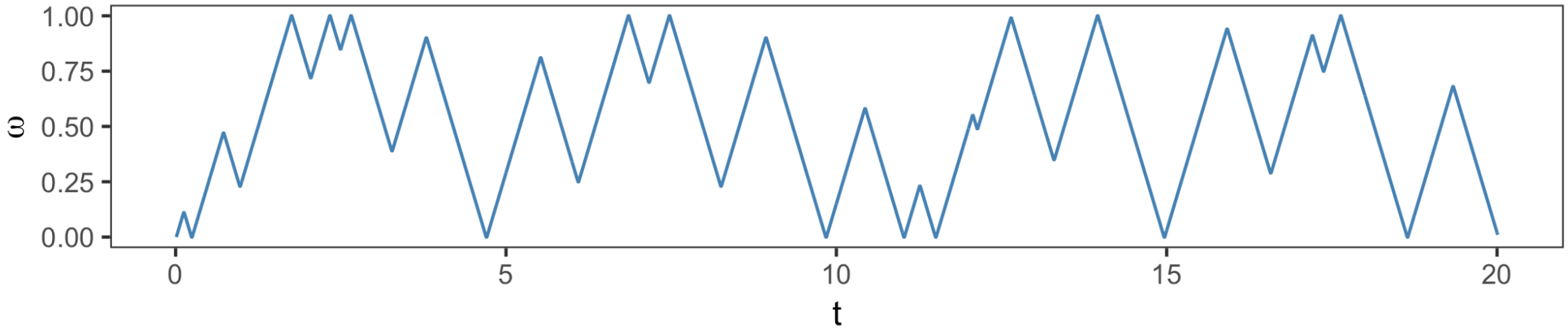

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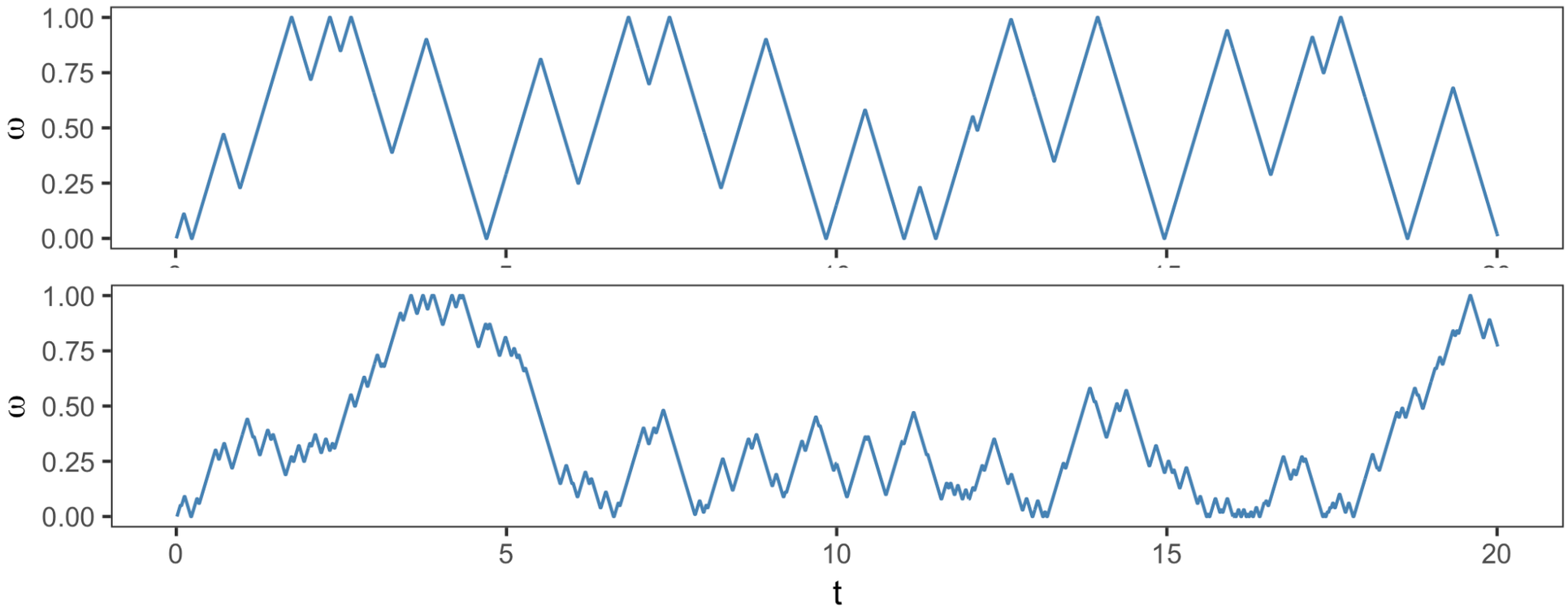

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SCALING LIMIT (NON-REVERSIBLE)

Theorem: Scaling the index by N and time by N, the scaled index process for non-reversible PT converge to piecewise deterministic Markov process depending on the annealing path through Λ

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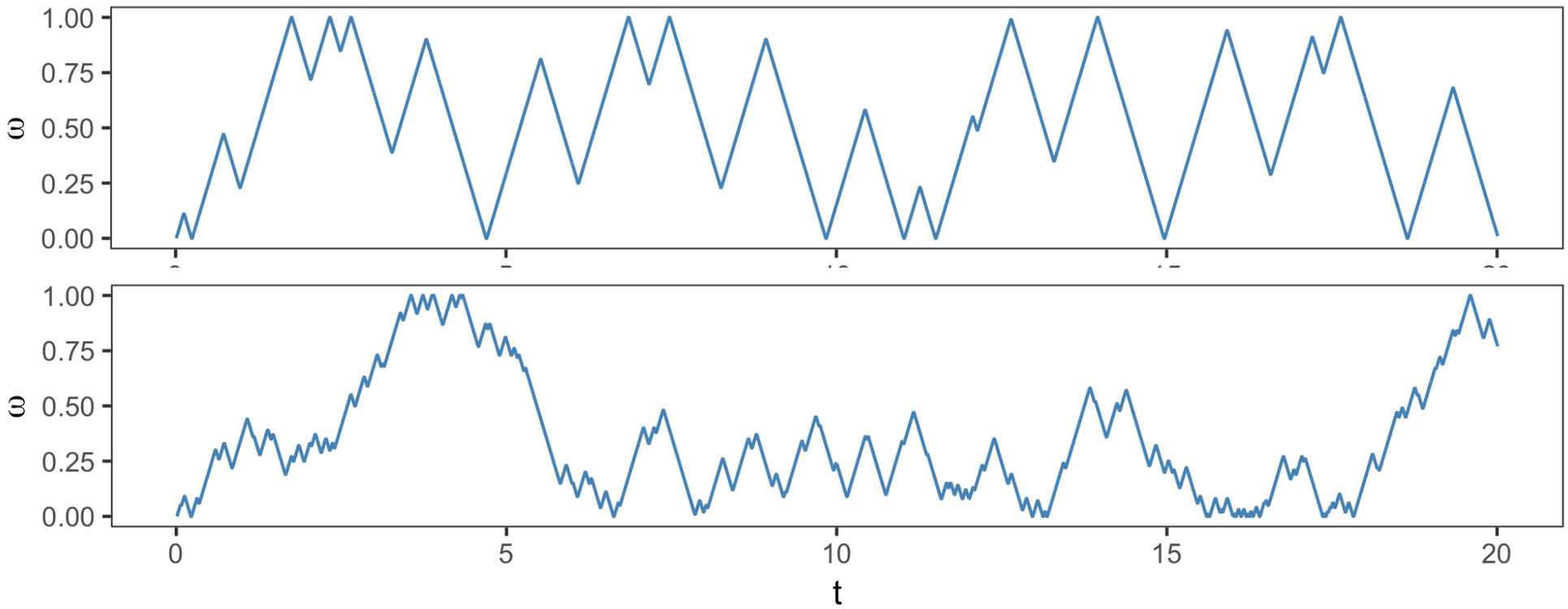

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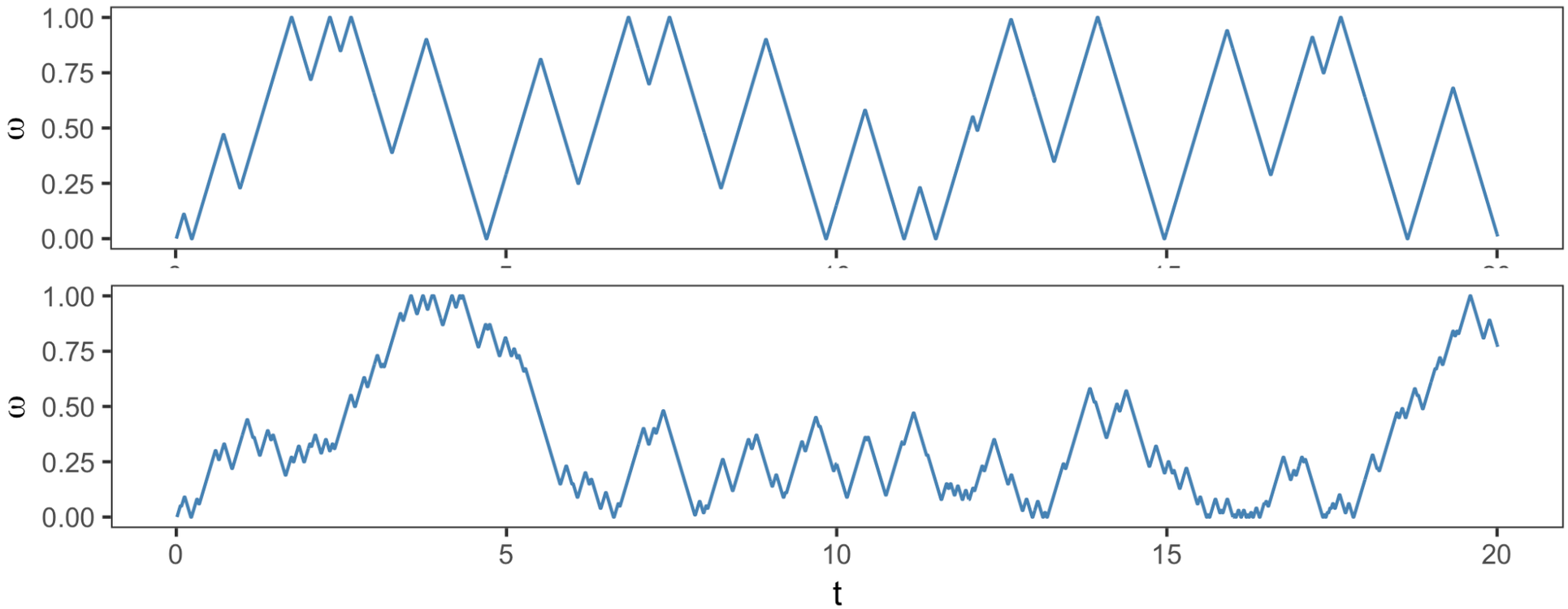

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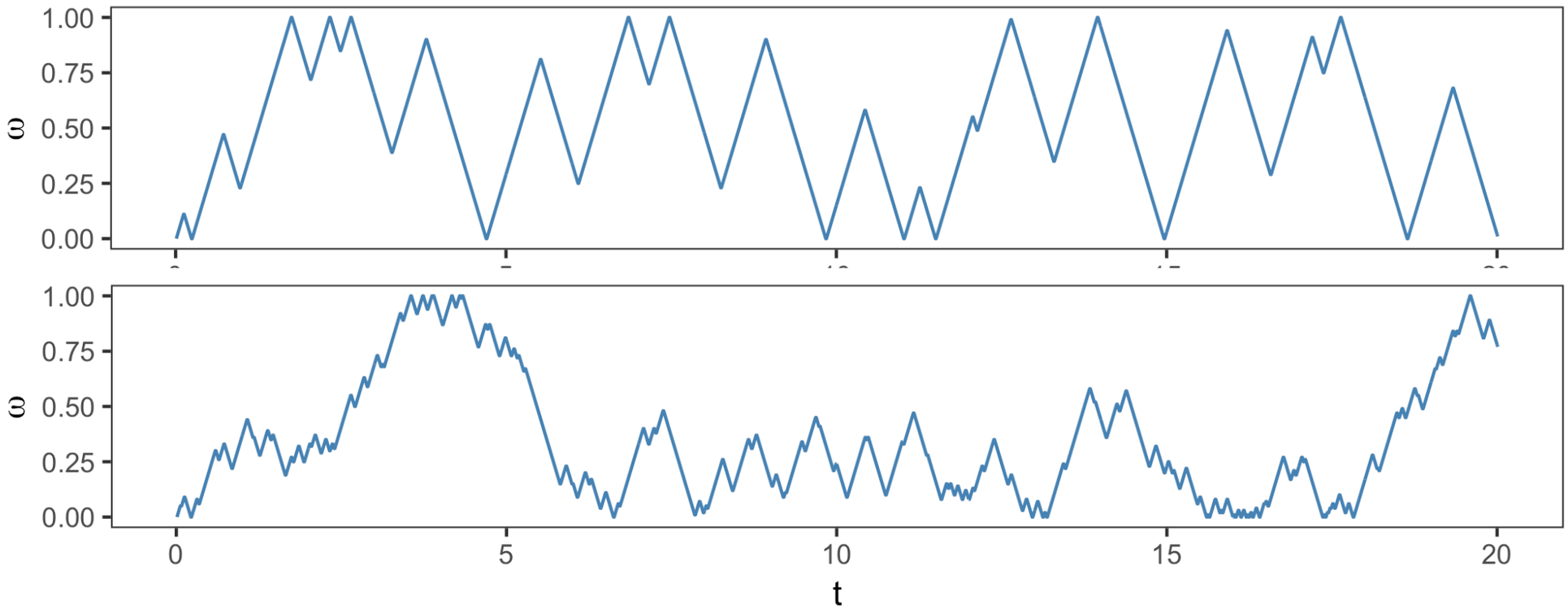

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- Fundamentally different behaviour compared to **reversible PT**
- As N increases, NRPT stabilizes.
- Asymptotic behaviour of NRPT depends on the annealing path through communication barrier.

COMMUNICATION BARRIER

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- **Global communication barrier:**

$$\Lambda = \int_0^1 \lambda(\beta) \mathrm{d}\beta$$

Cumulative rejection rate along path

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$$r_n^* = \frac{\Lambda}{N}$$

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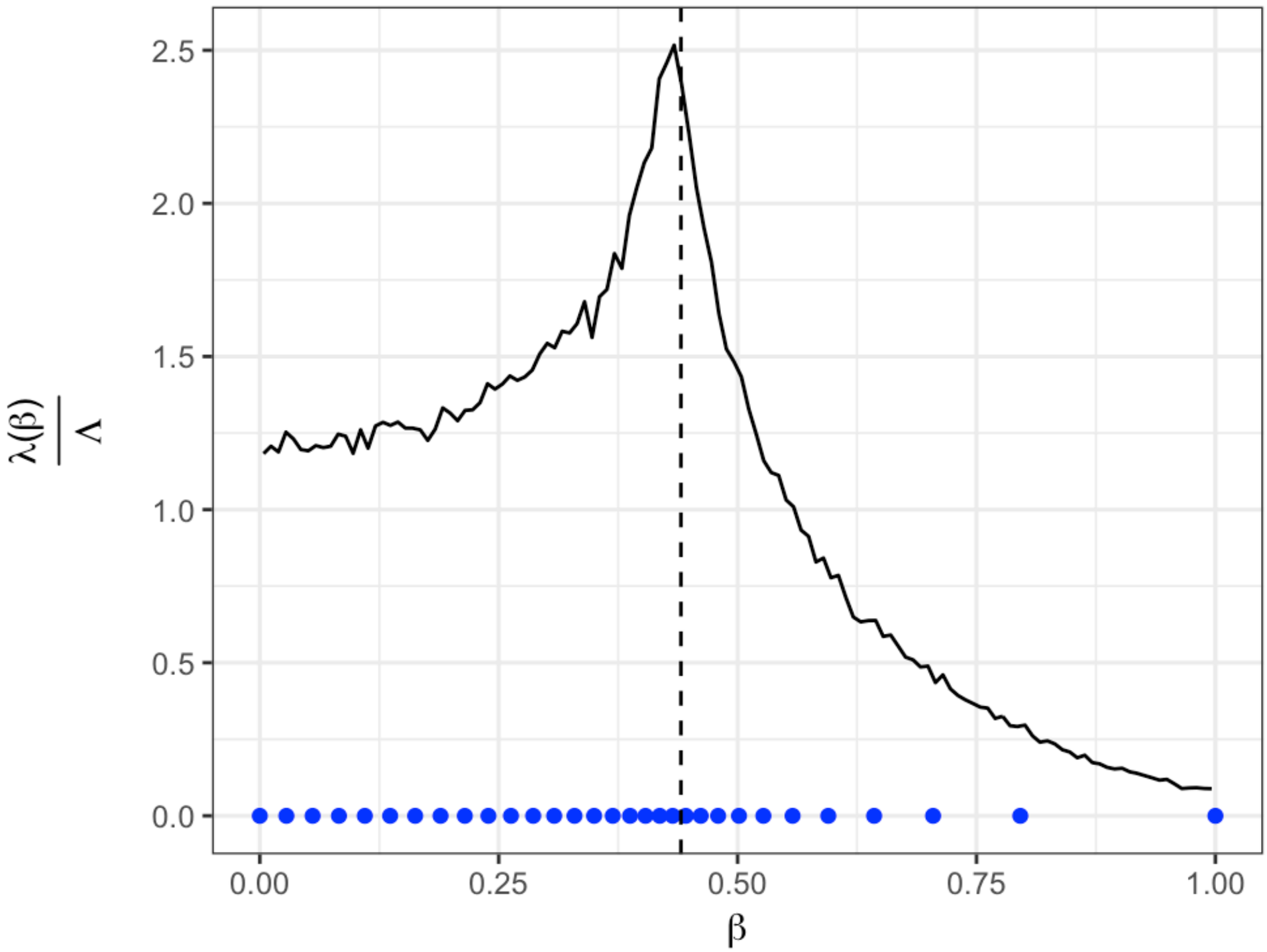
- Theorem implies:

$$\int_{\beta_{n-1}}^{\beta_n} \lambda(\beta)\mathrm{d}\beta = \frac{\Lambda}{N}$$

EXAMPLE ISING MODEL



COMPUTE SCHEDULE

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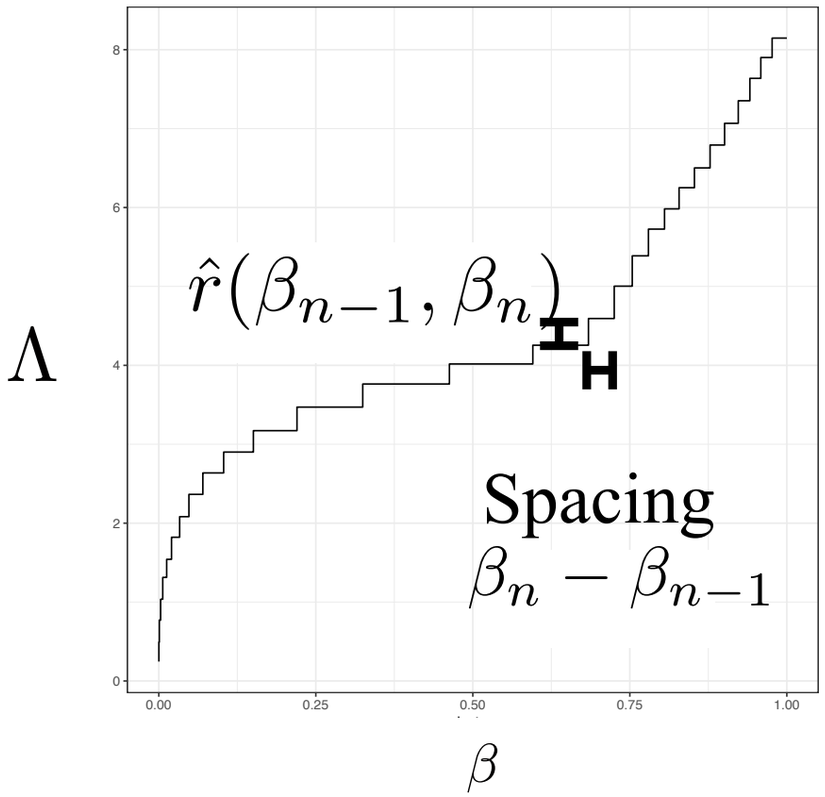

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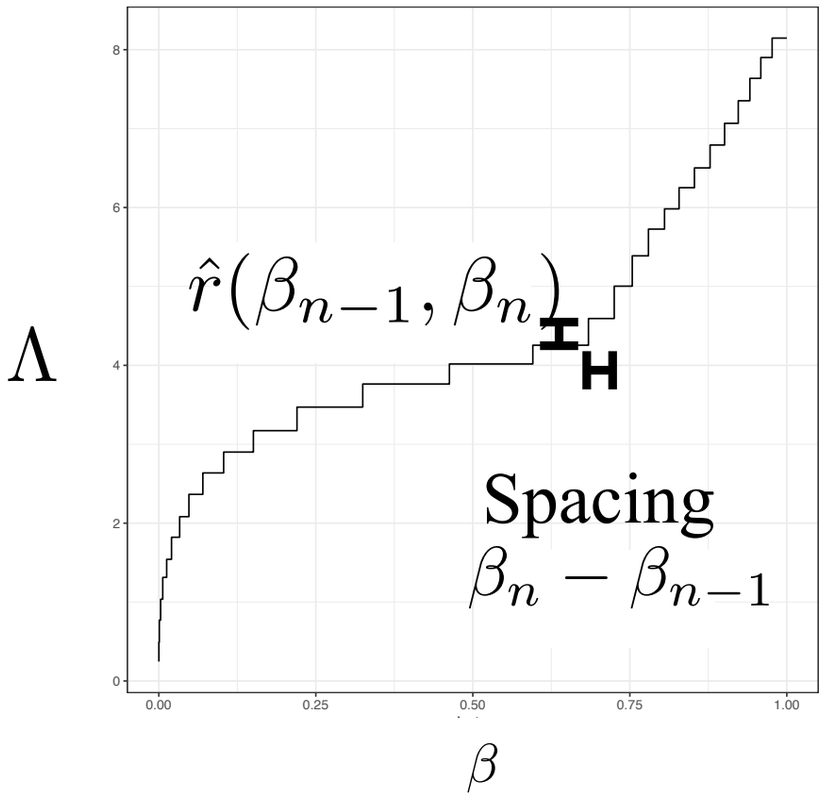

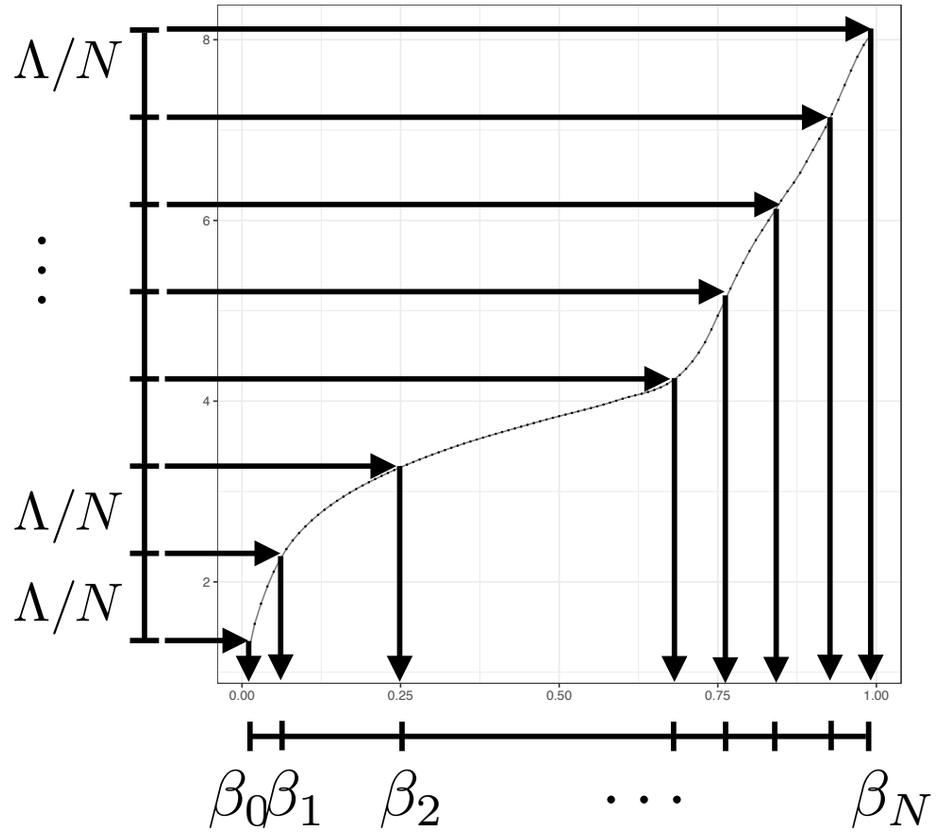

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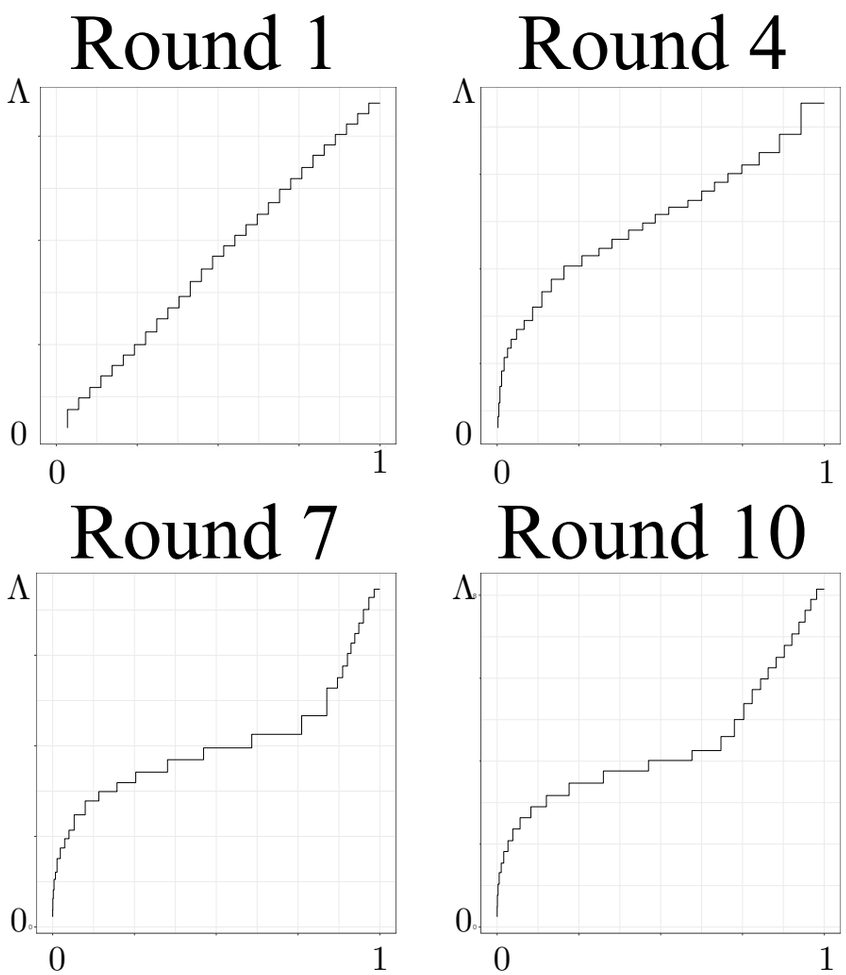
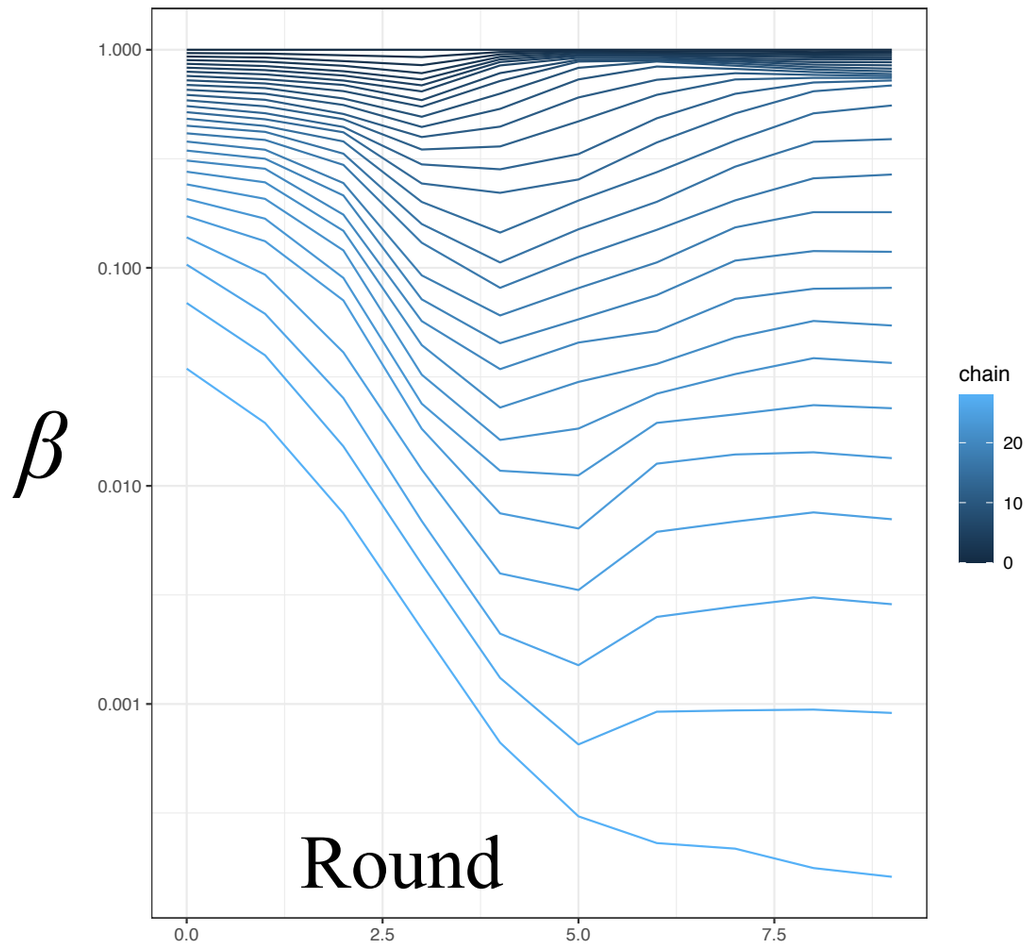
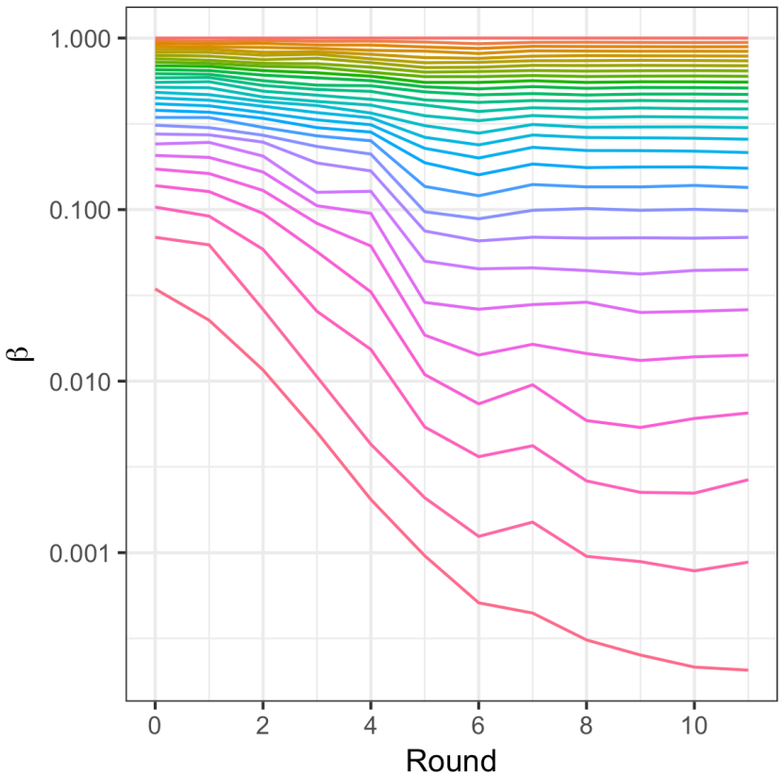
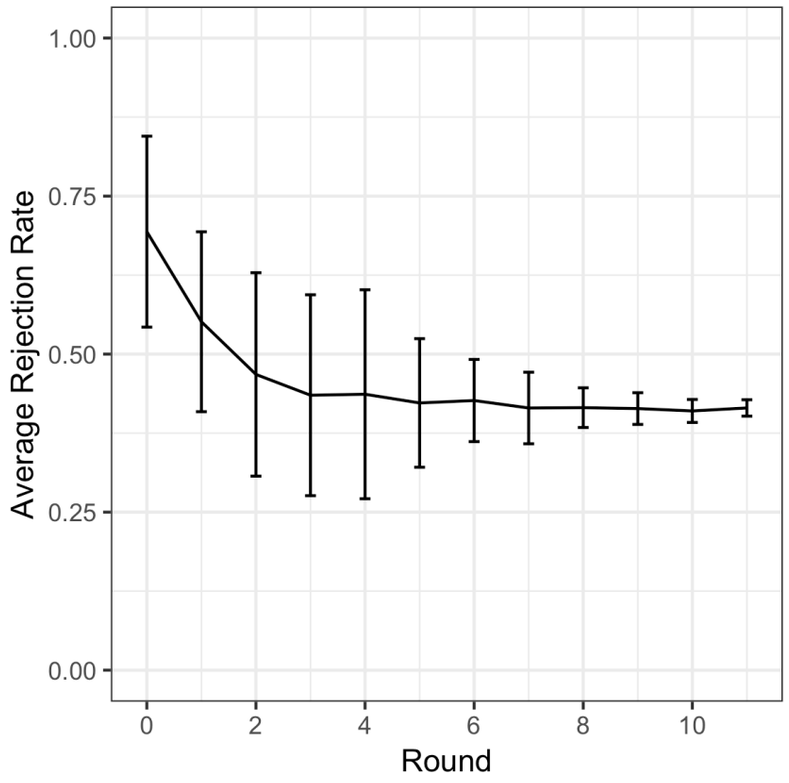
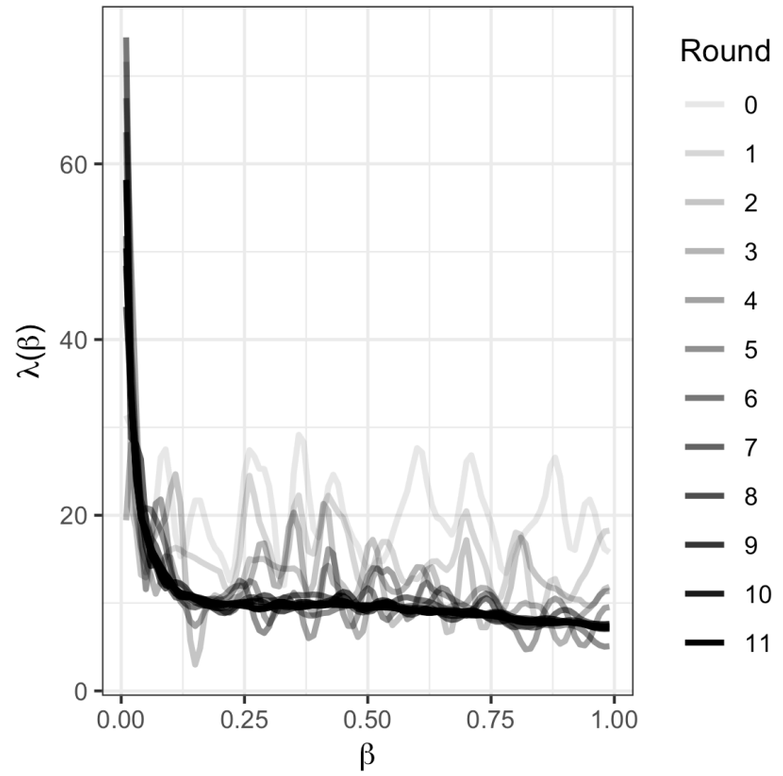




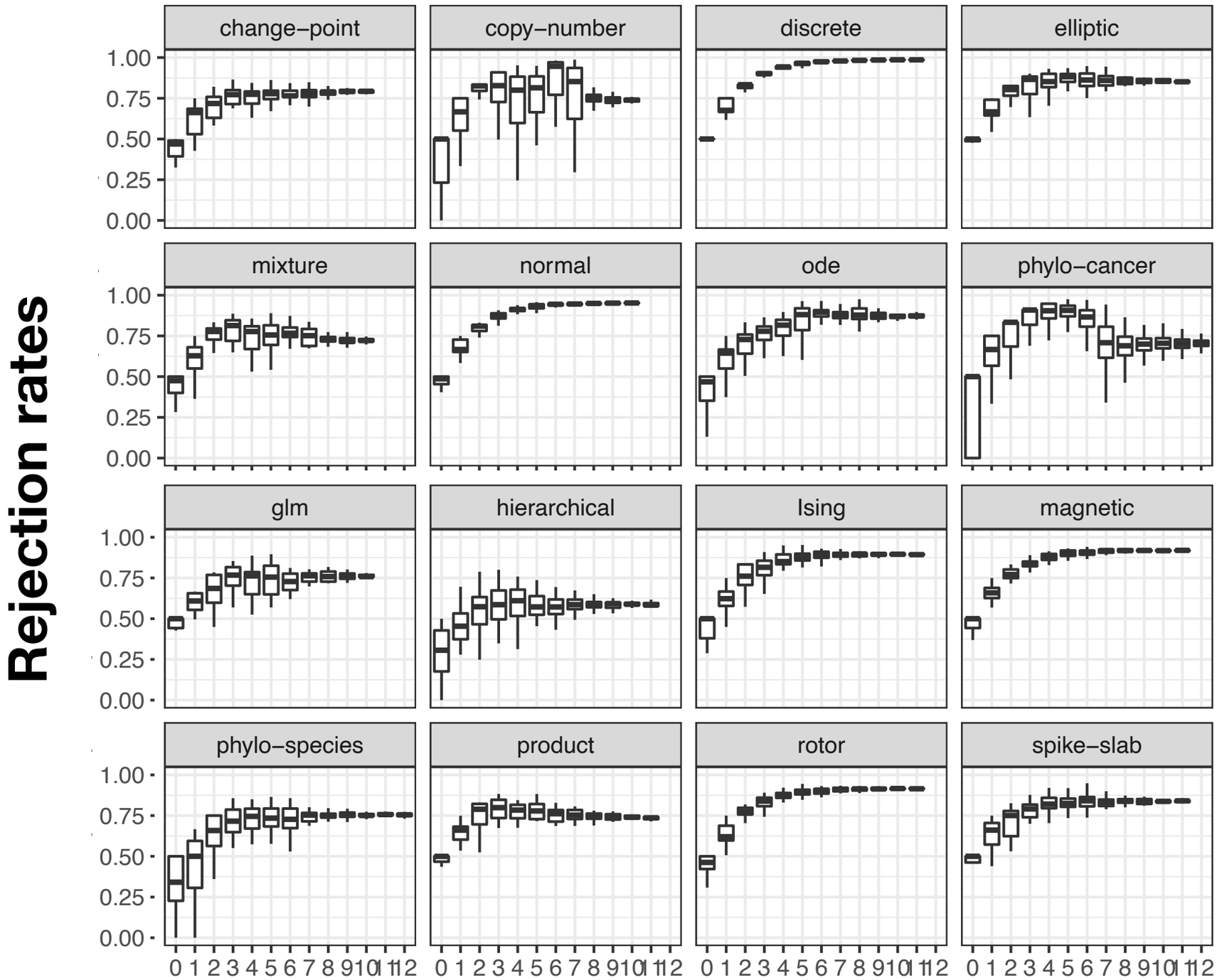
HIERARCHICAL BAYESIAN MODEL (D = 369)





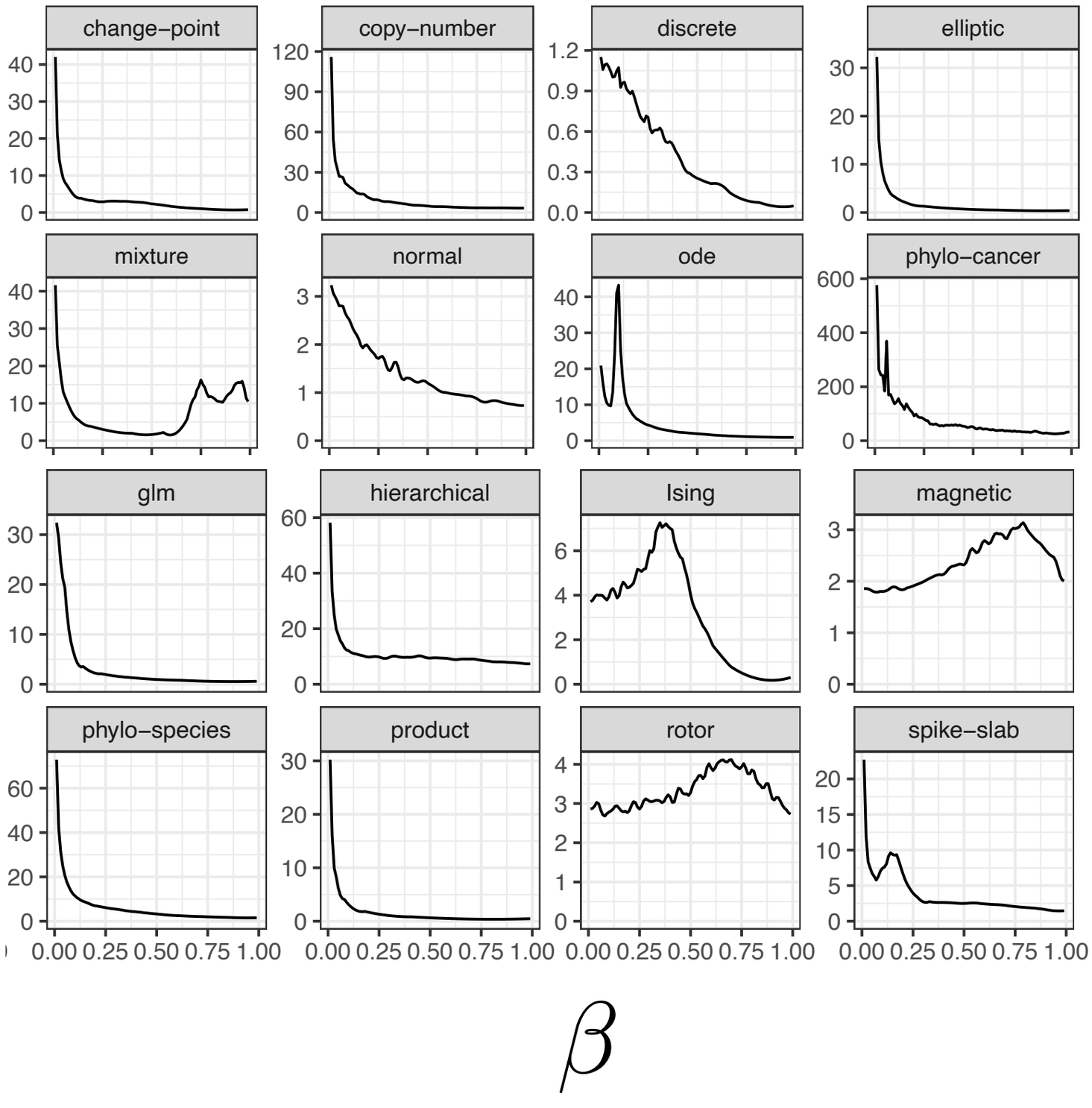


NRPT IN PRACTICE



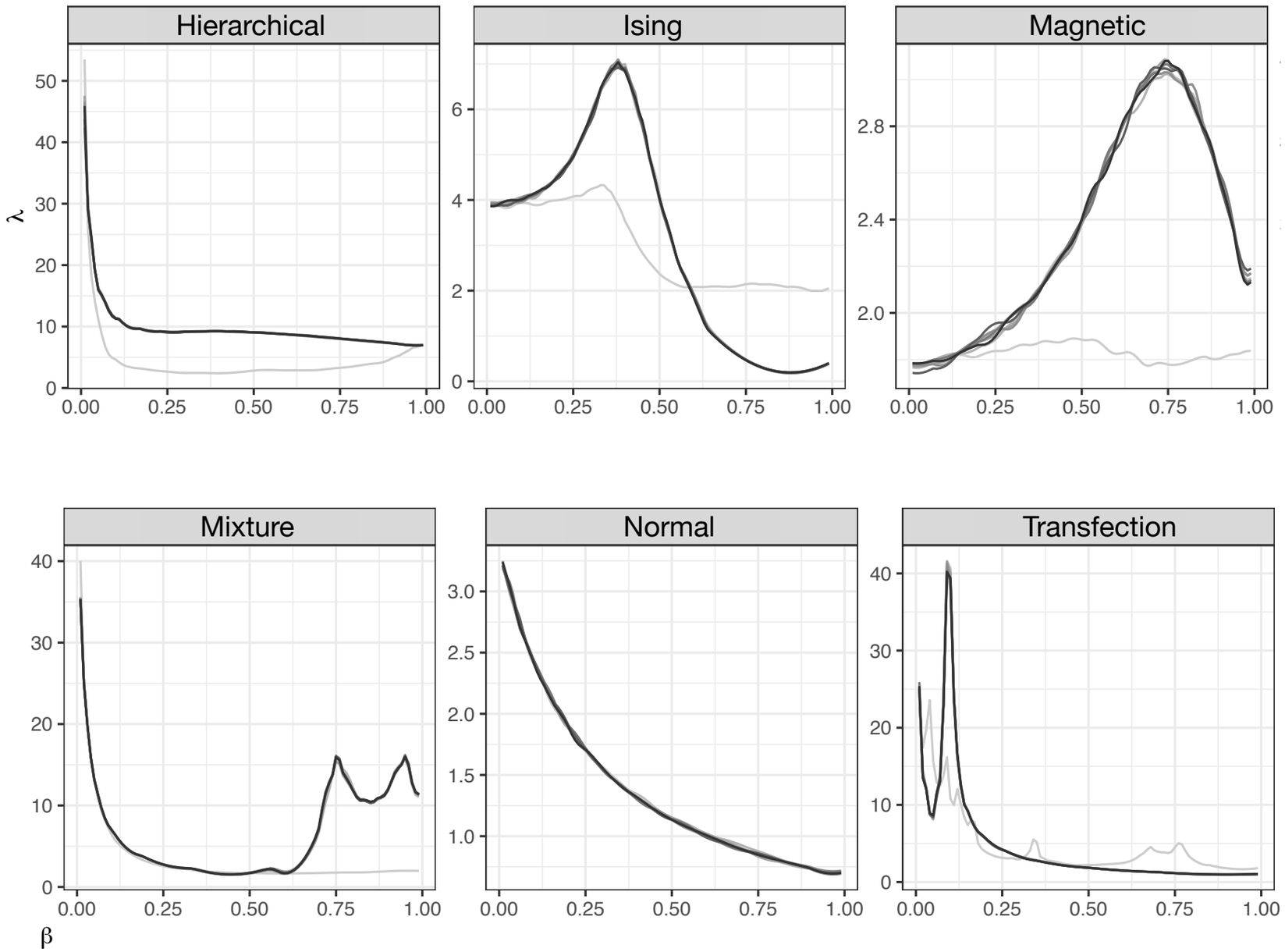
LOCAL COMMUNICATION BARRIER

$\lambda(\beta)$



β

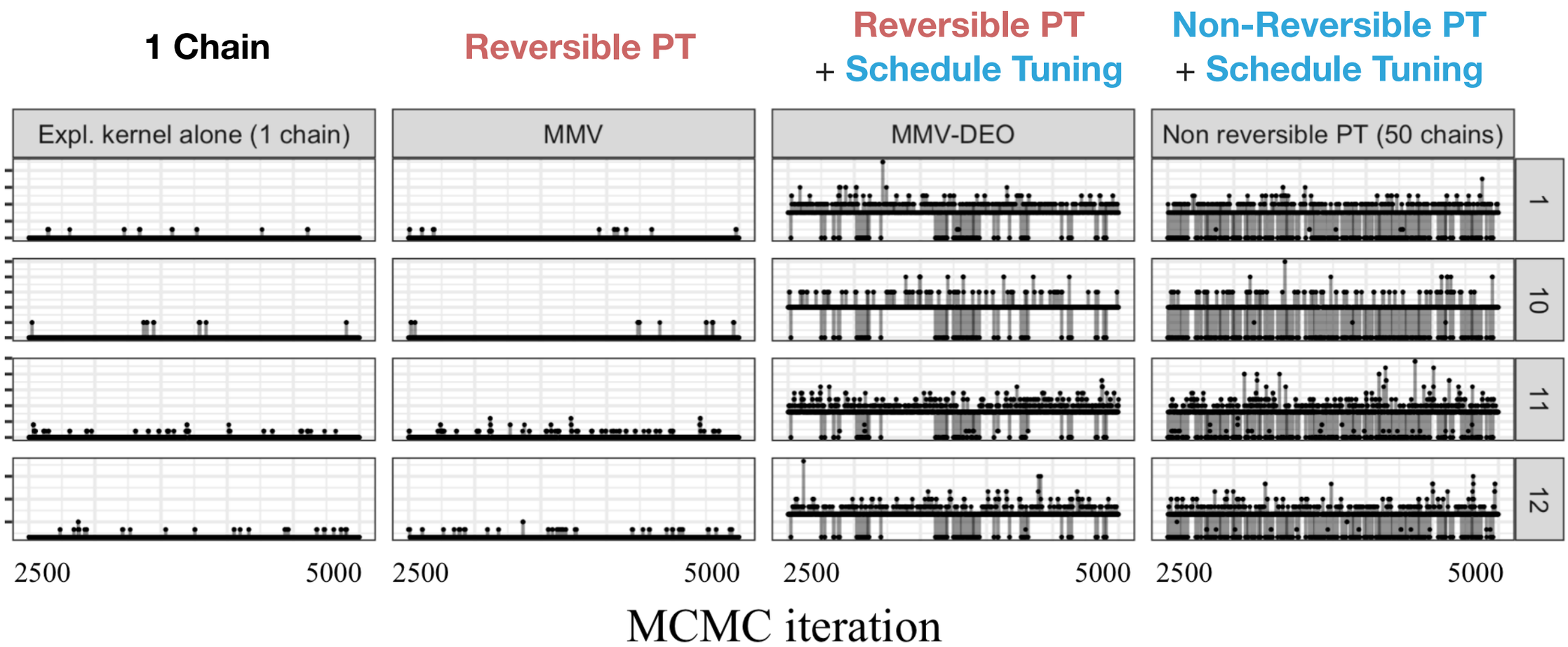
TUNING ROBUST TO ELE VIOLATION



Variables updated per local exploration move

- 0
- 0.5
- 1
- 2
- 4
- 8
- 16
- 32

EXAMPLE: COPY NUMBER INFERENCE (D = 30)



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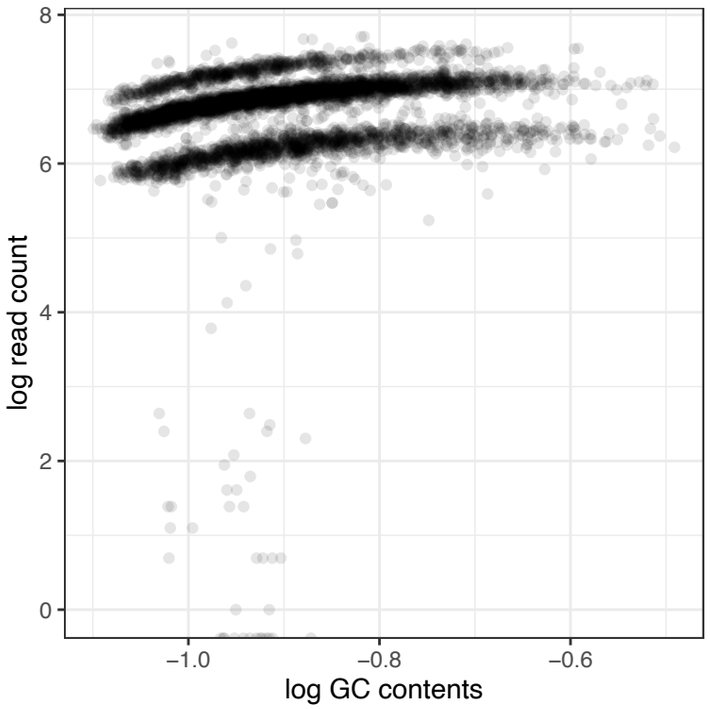
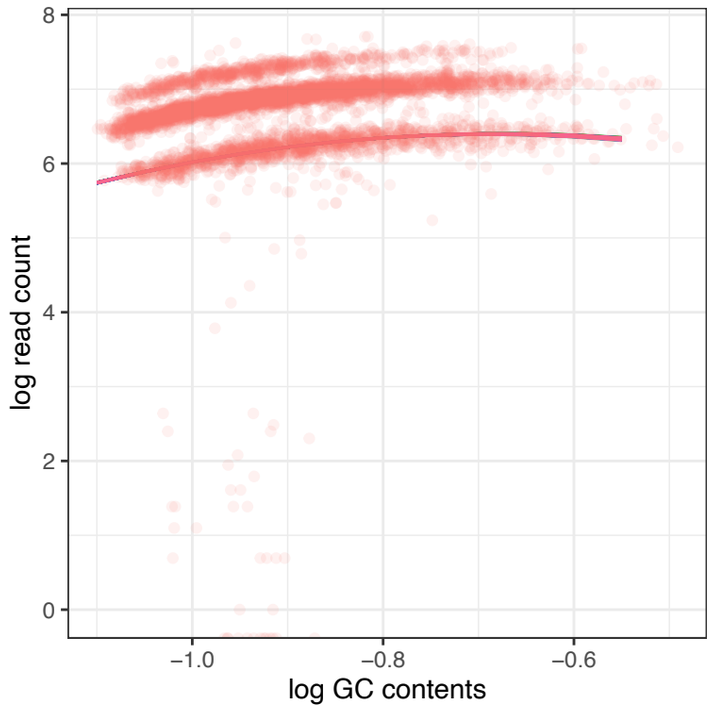
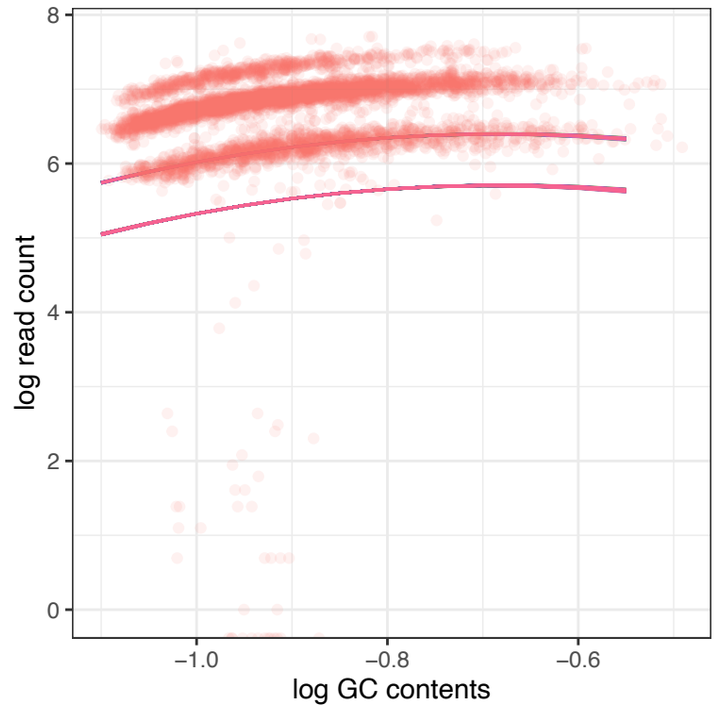
Data



1 Chain

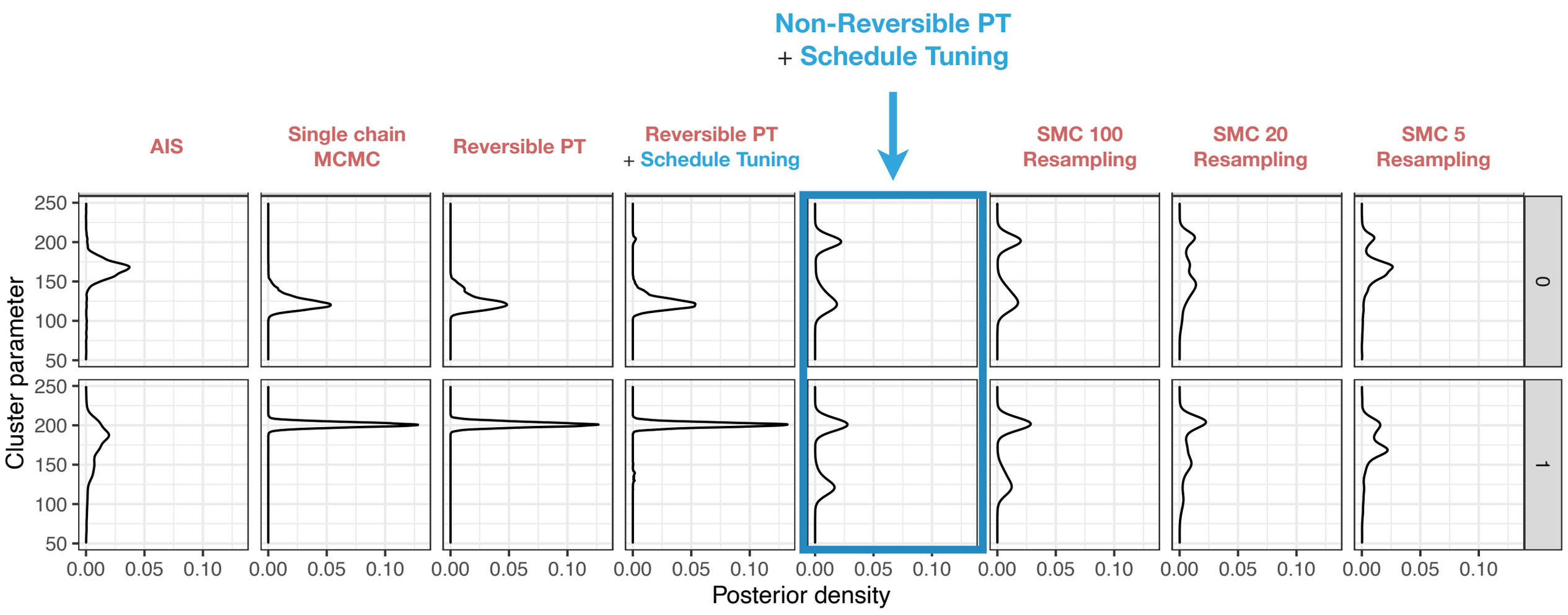


Non-Reversible PT



COMPARISON TO STATE OF THE ART

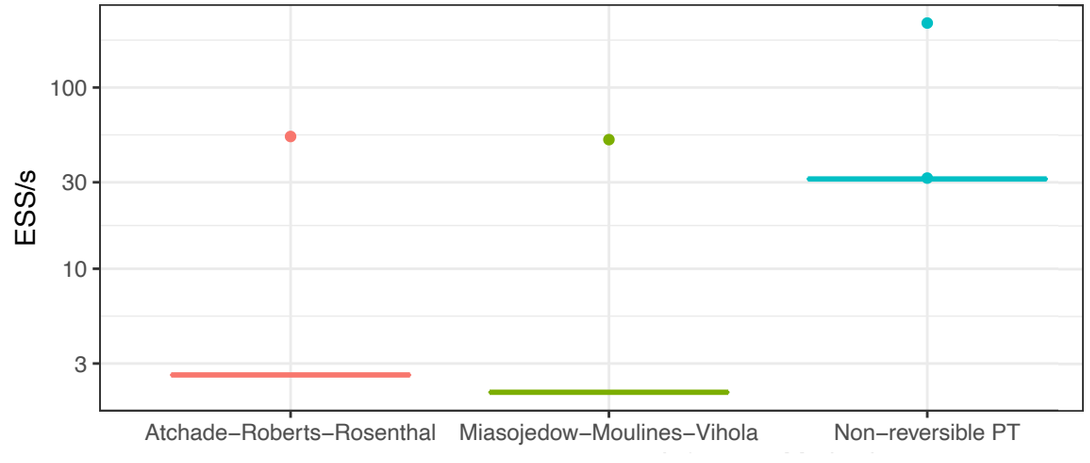
Bayesian Mixture Model (d = 155)



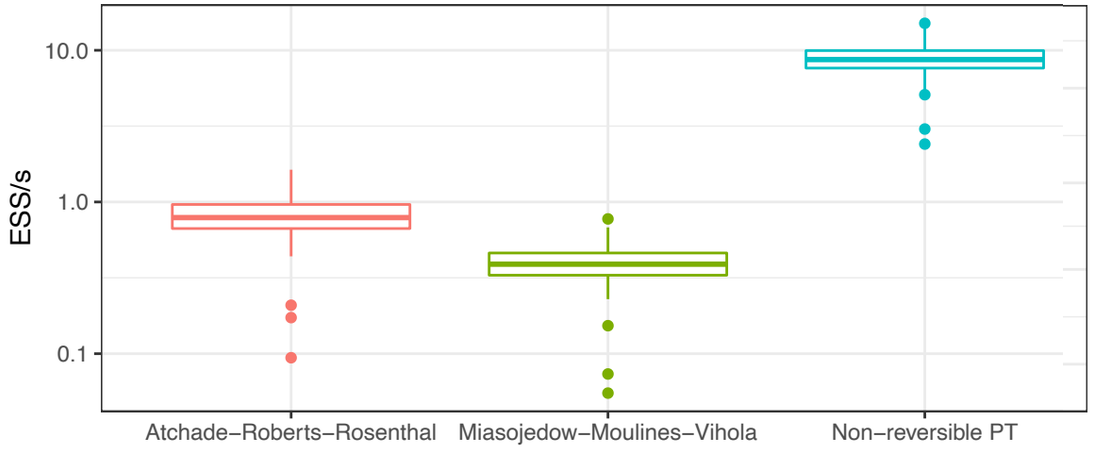
ESS COMPARED TO REVERSIBLE PT

Spike–and–Slab (RMS Titanic passengers dataset)

Ising



Hierarchical model (rocket launches dataset 1957–2017)



Wright–Fisher SDE

State of the art for Reversible PT (Miasojedow, et al. 2013)

Non-Reversible PT

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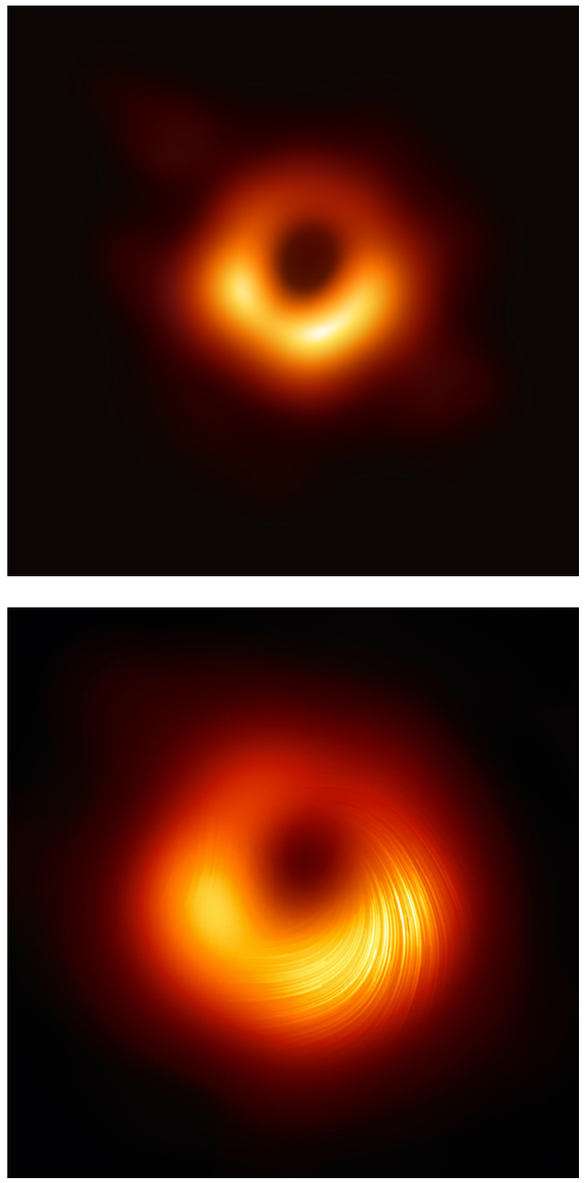

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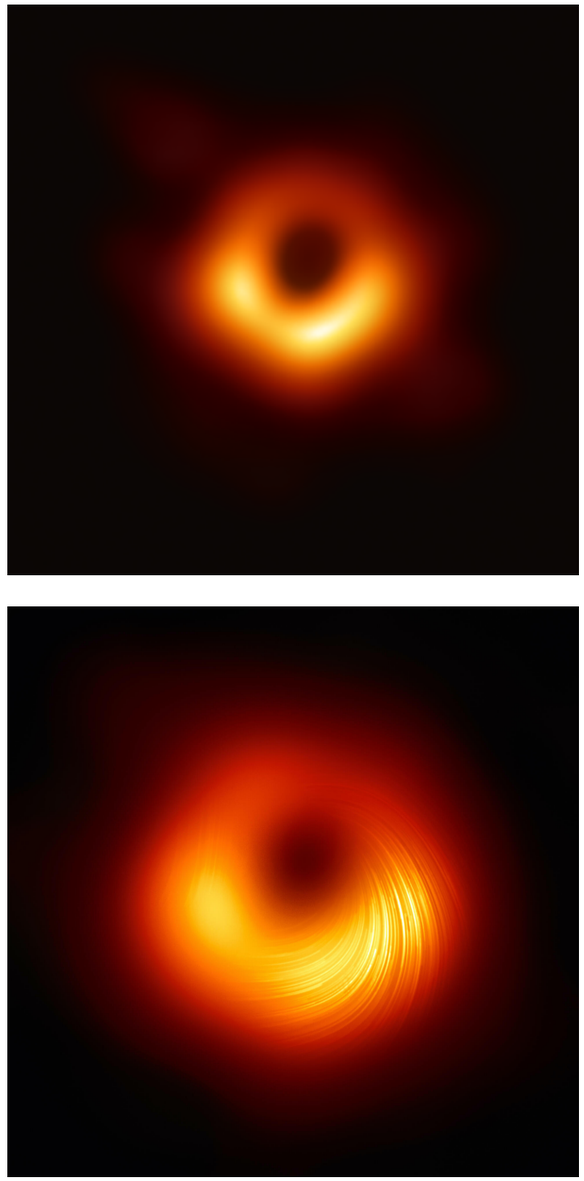

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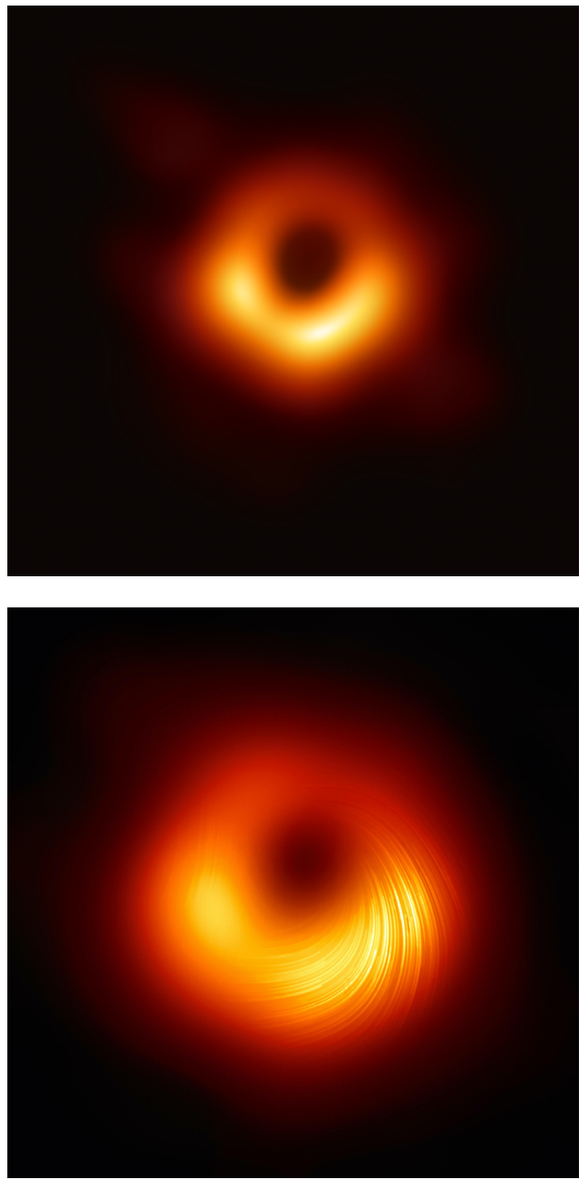

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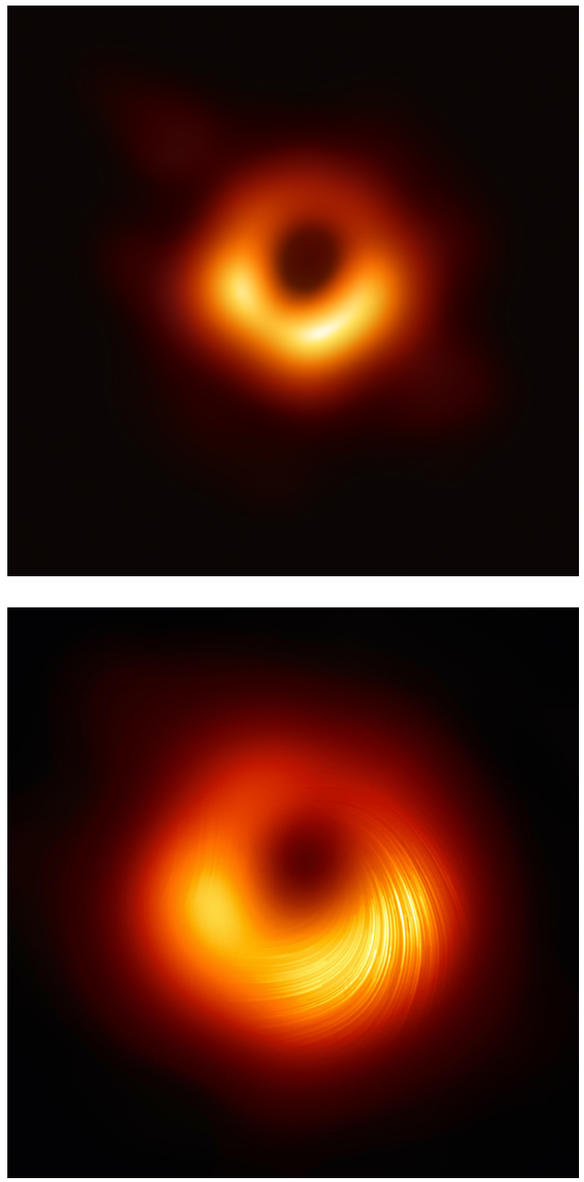

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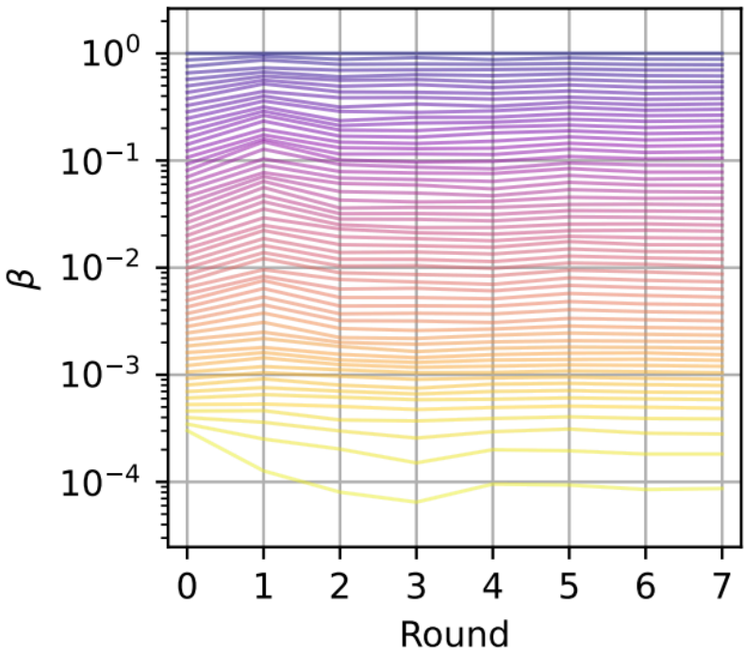
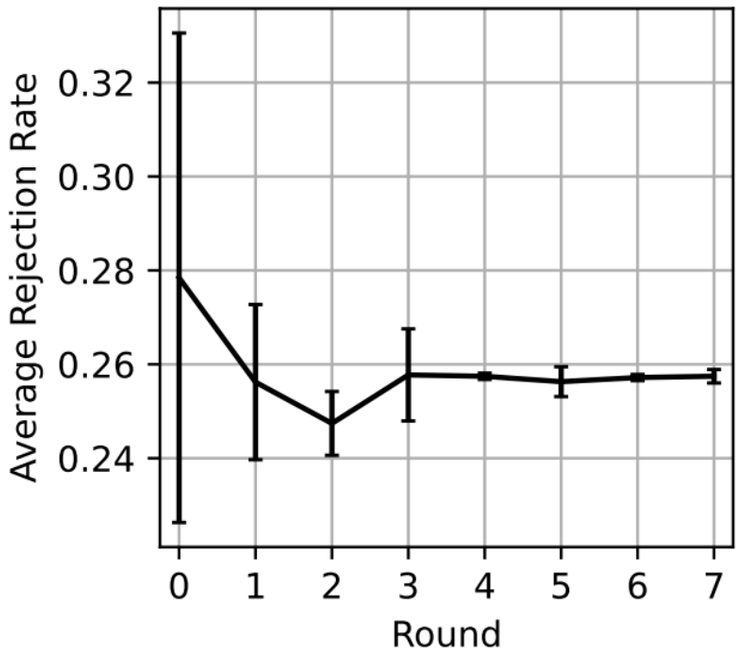
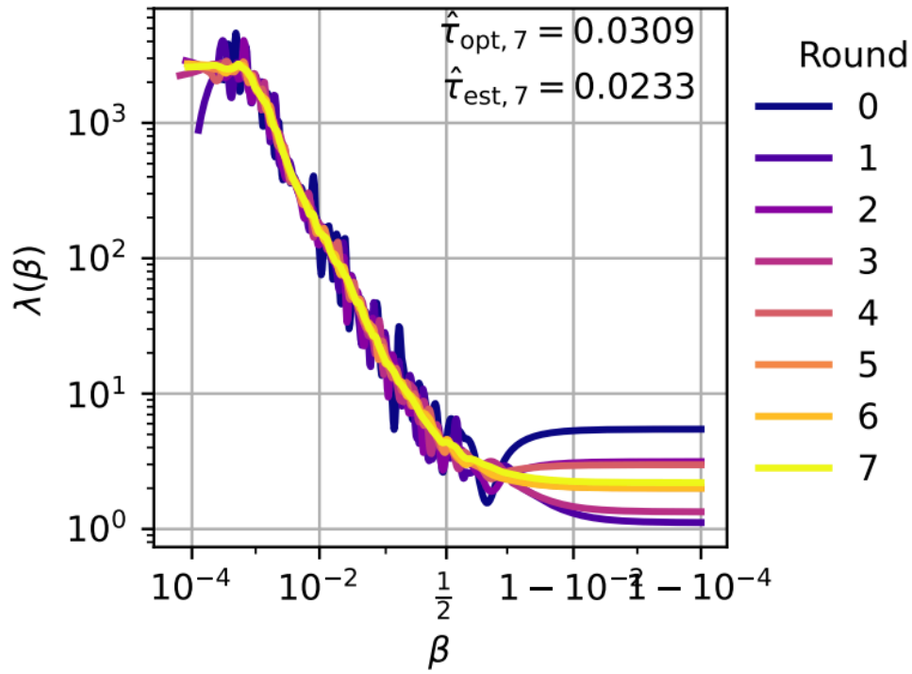
- NRPT useful inference engine for PPL (eg. Blang, Themis, turing.jl, tensorflow probability)

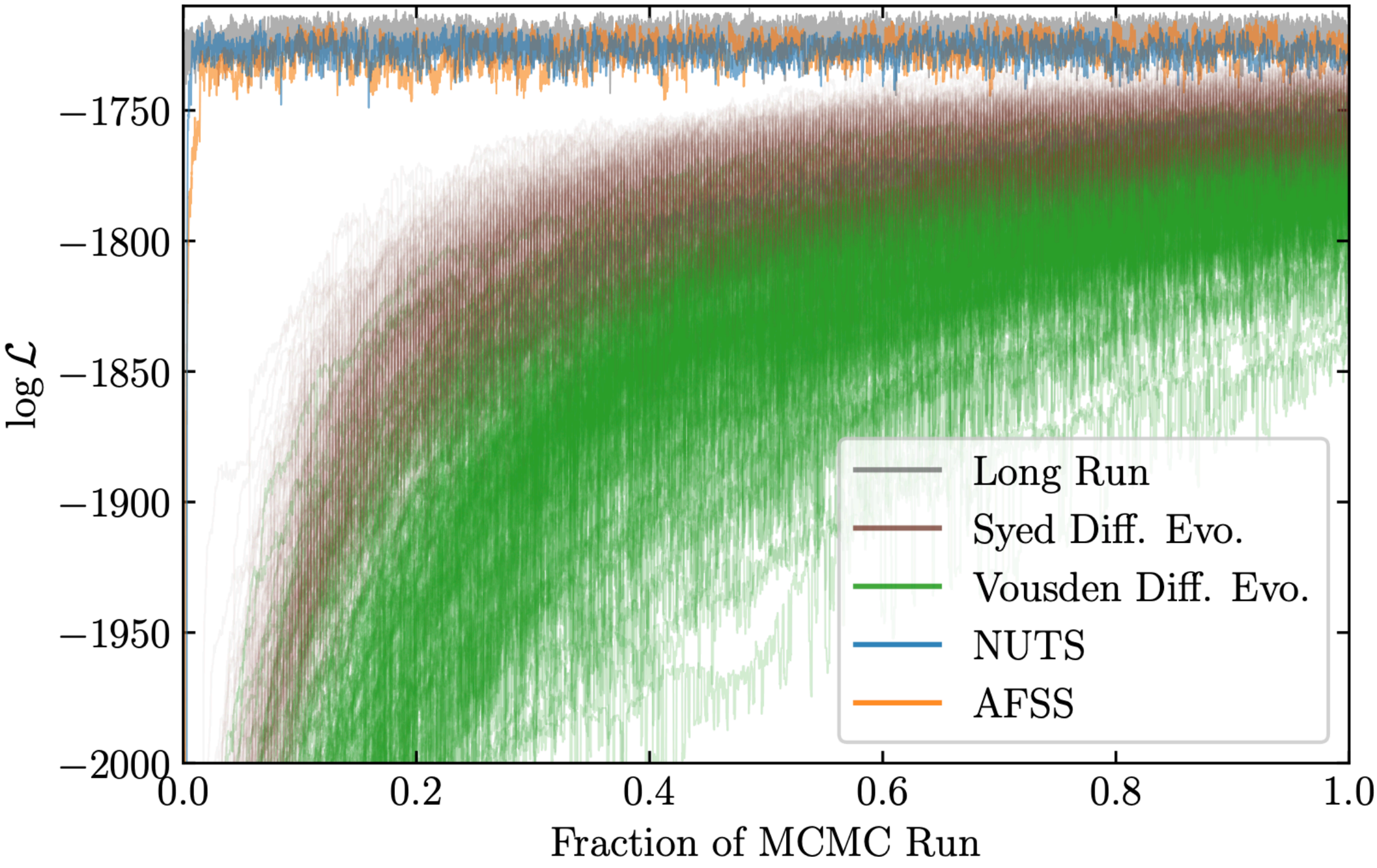
APPLICATIONS OF NRPT







BENCHMARK (TIEDE, 2021)



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