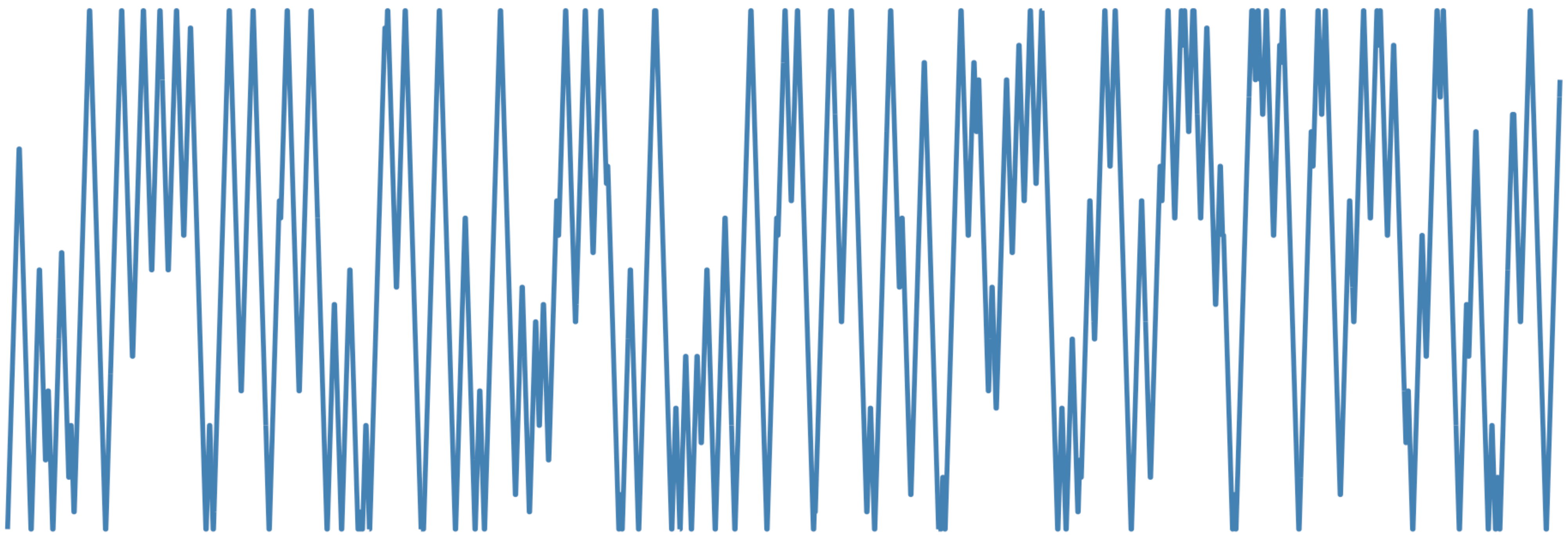
NON-REVERSIBLE PARALLEL TEMPERING ON OPTIMIZED PATHS



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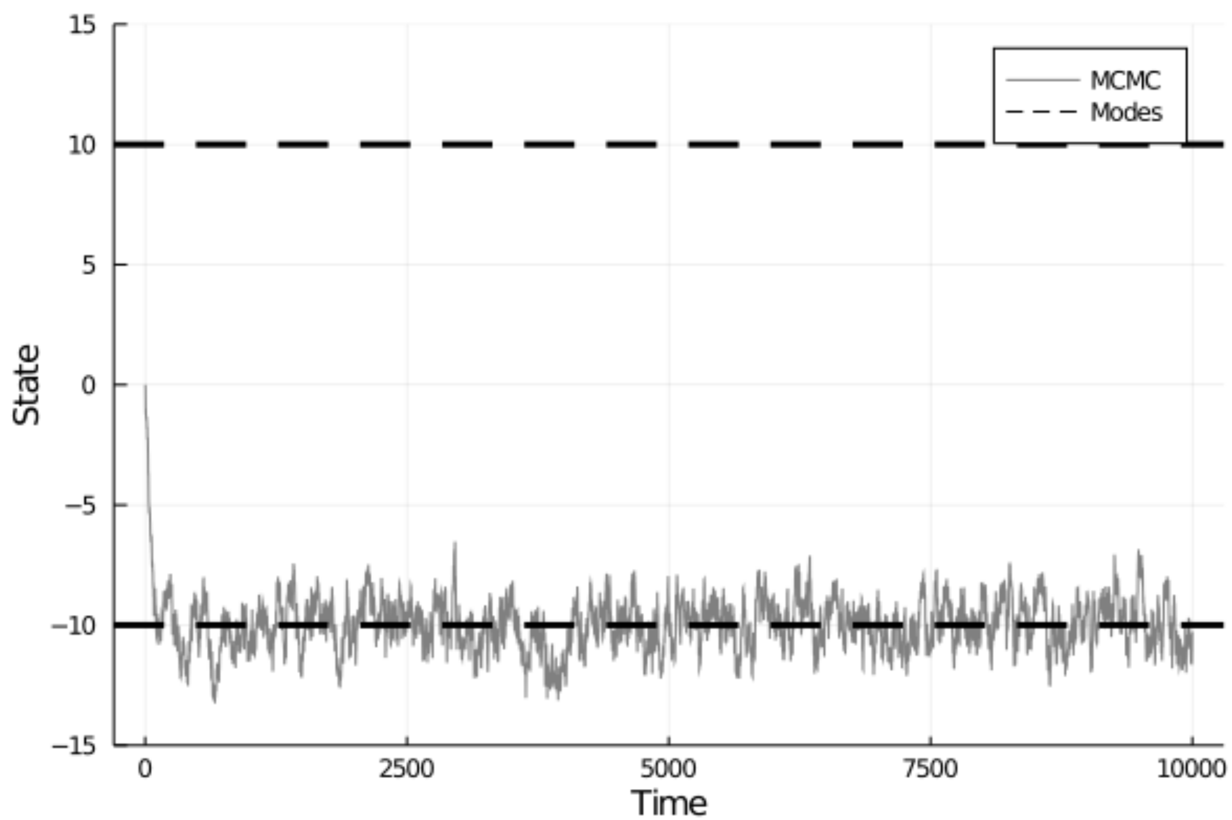
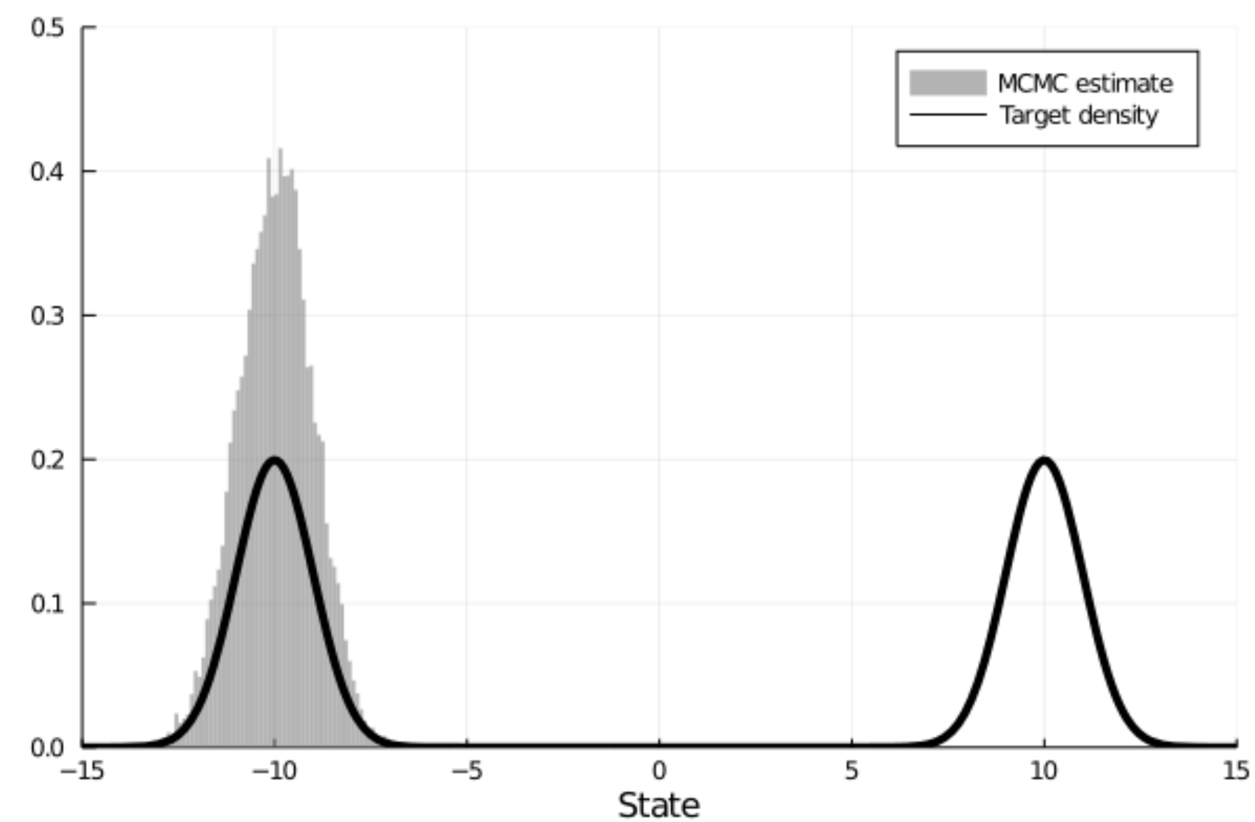
- **Solution:** Numerically approximate expectation using MCMC
- Run Markov chain stationary with respect to target and use ergodic theorem.

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

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





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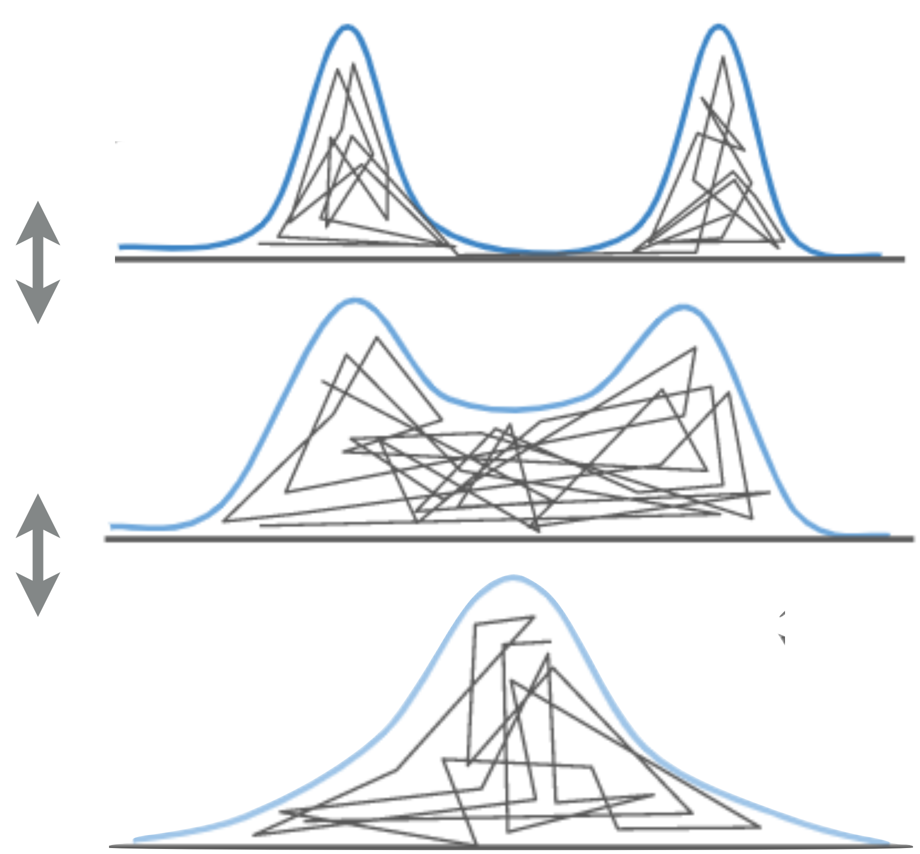
- **A Solution:** Run N additional chains in parallel
  - Delegate exploration to tractable **reference** chain
  - Communicate to **target** through the remaining $N-1$ chains



Chain N
Complex **Target**

Chains $1, \ldots, N-1$

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

ANNEALING

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$$\pi_n = \pi_{\beta_n}$$

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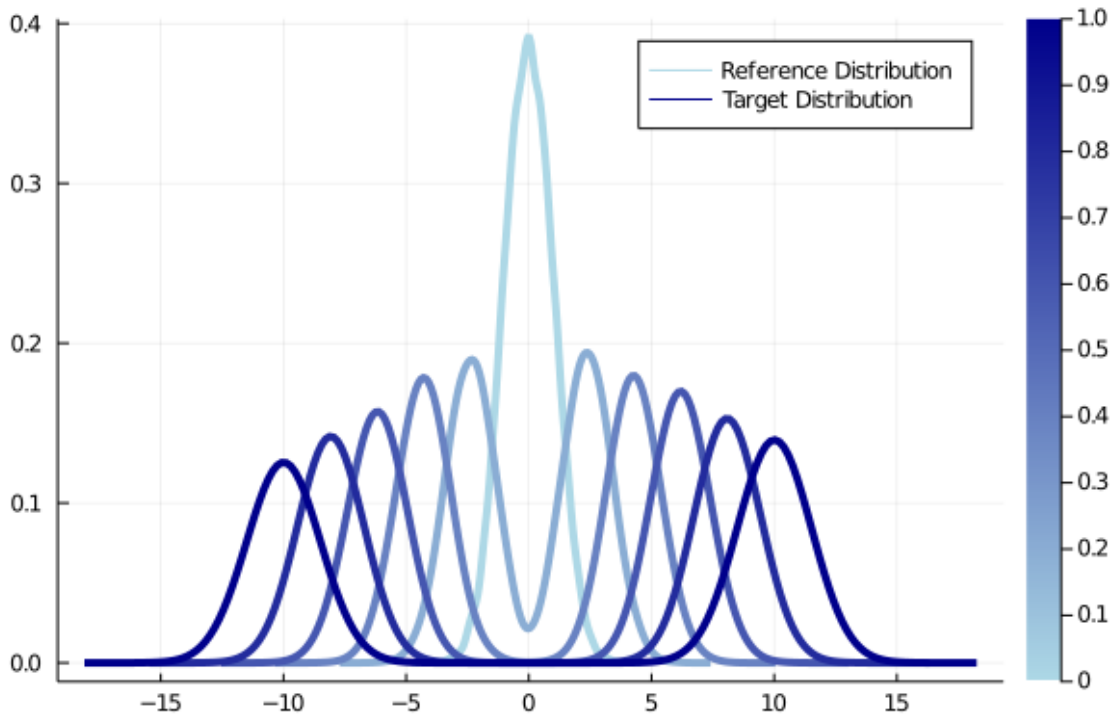
$$\pi_{\beta_0}, \ldots, \pi_{\beta_N}$$



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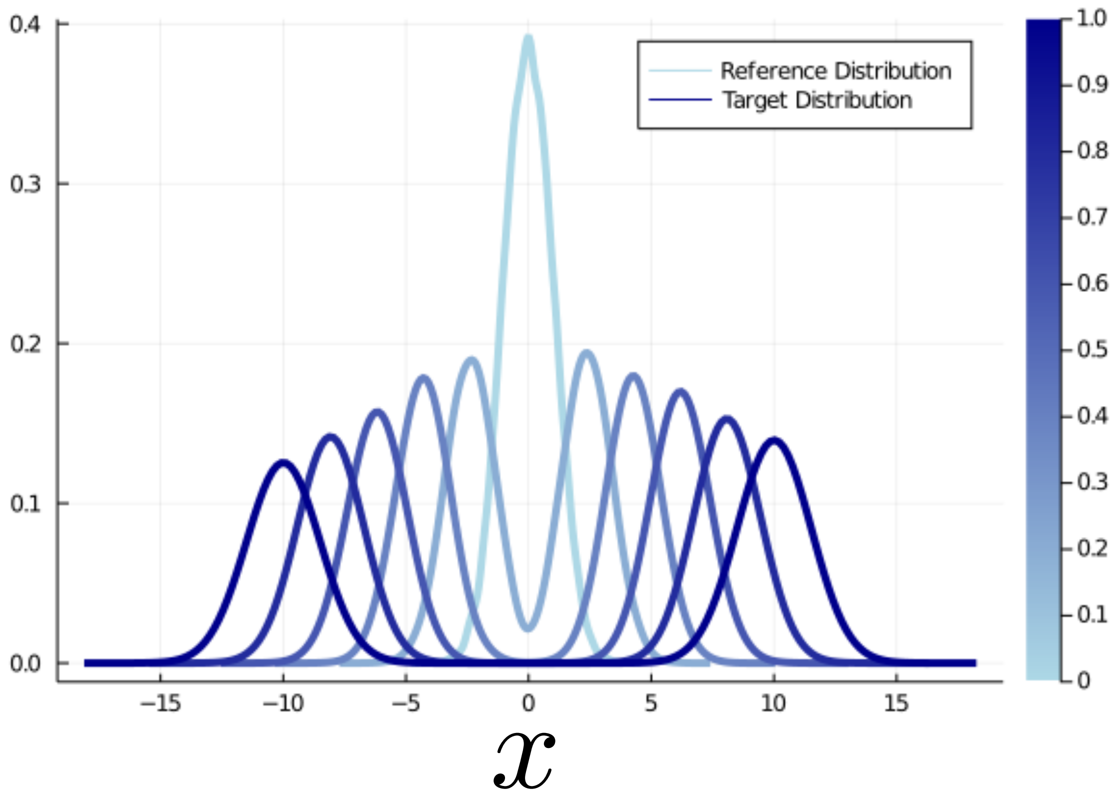

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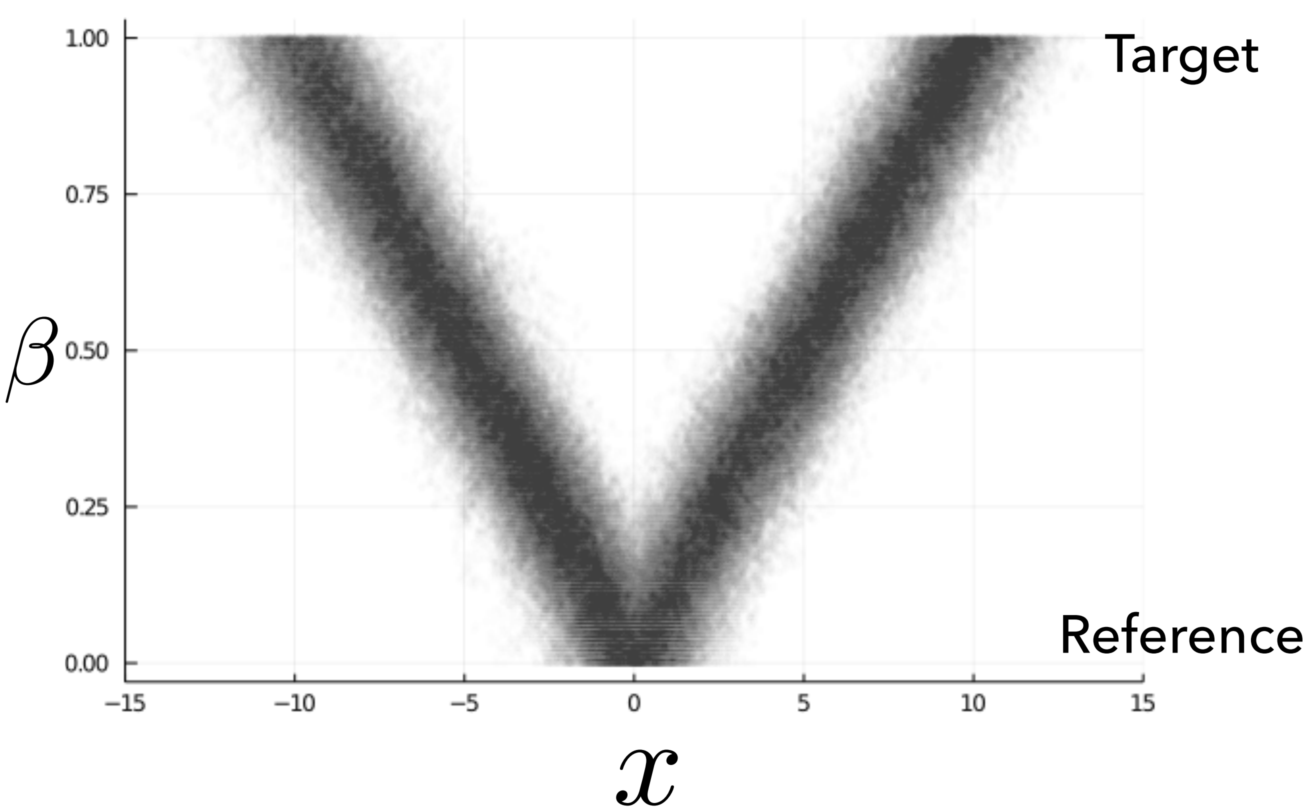

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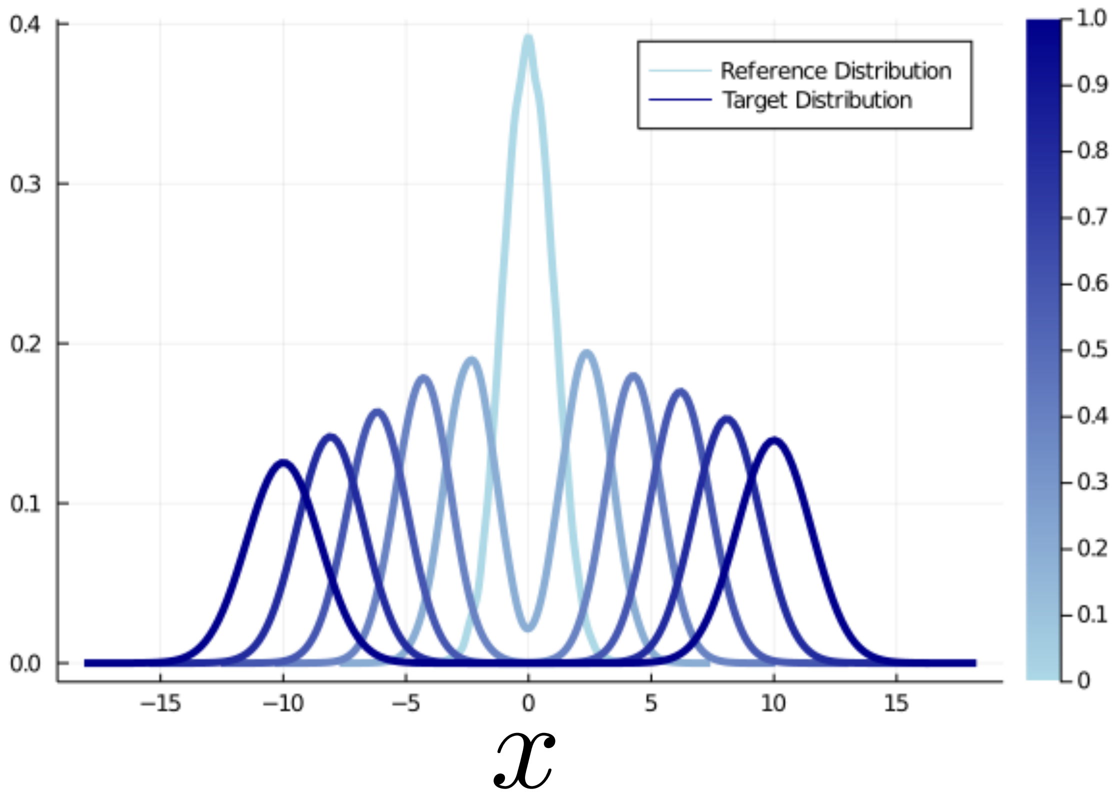

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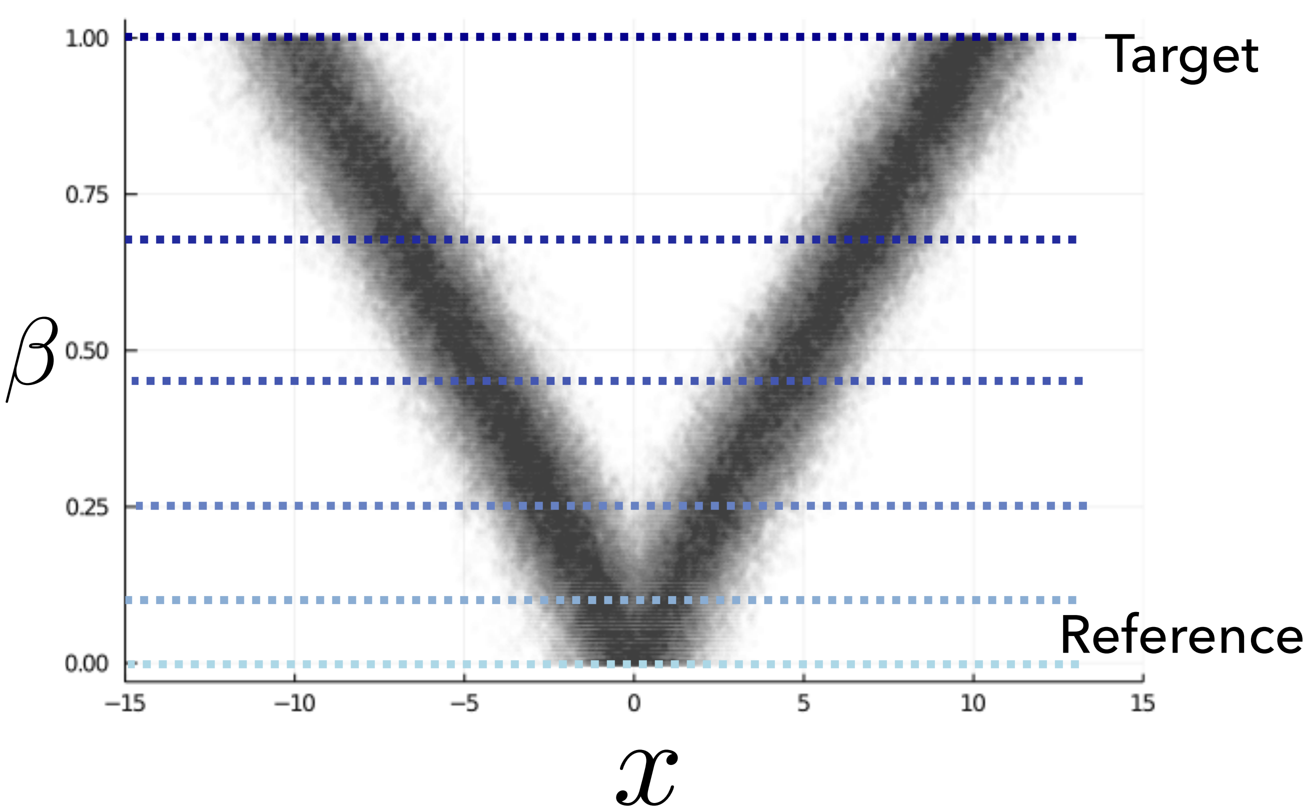

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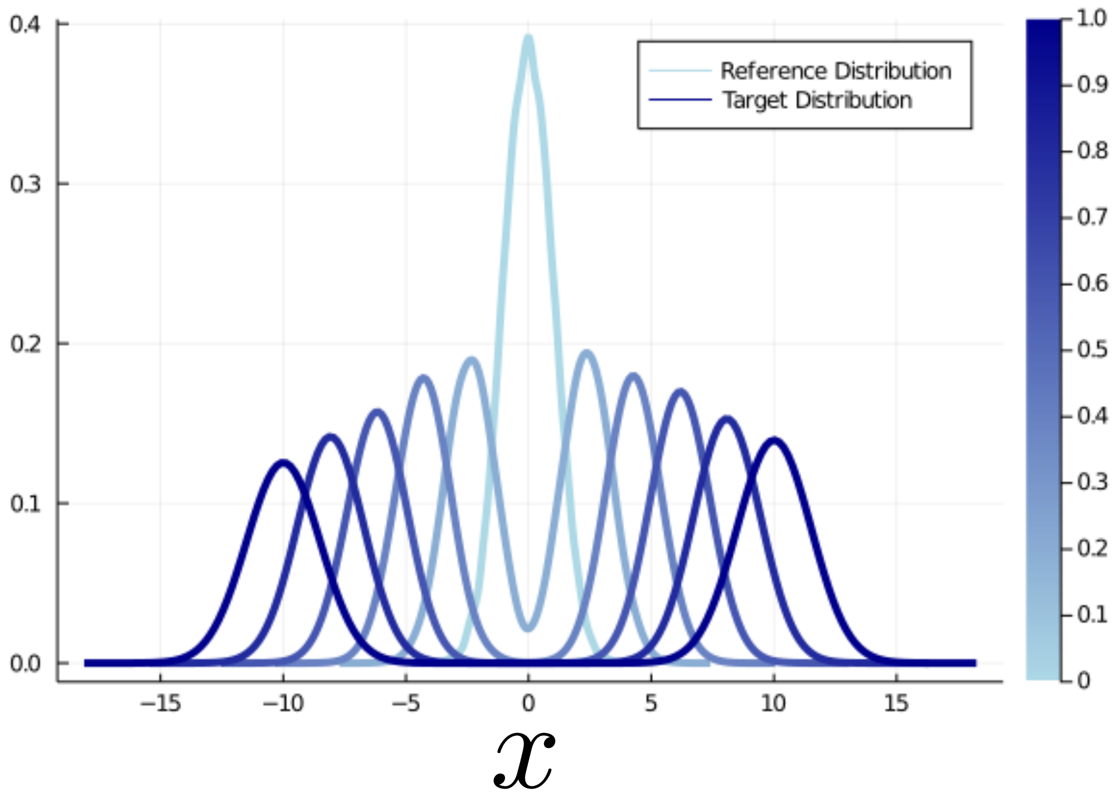

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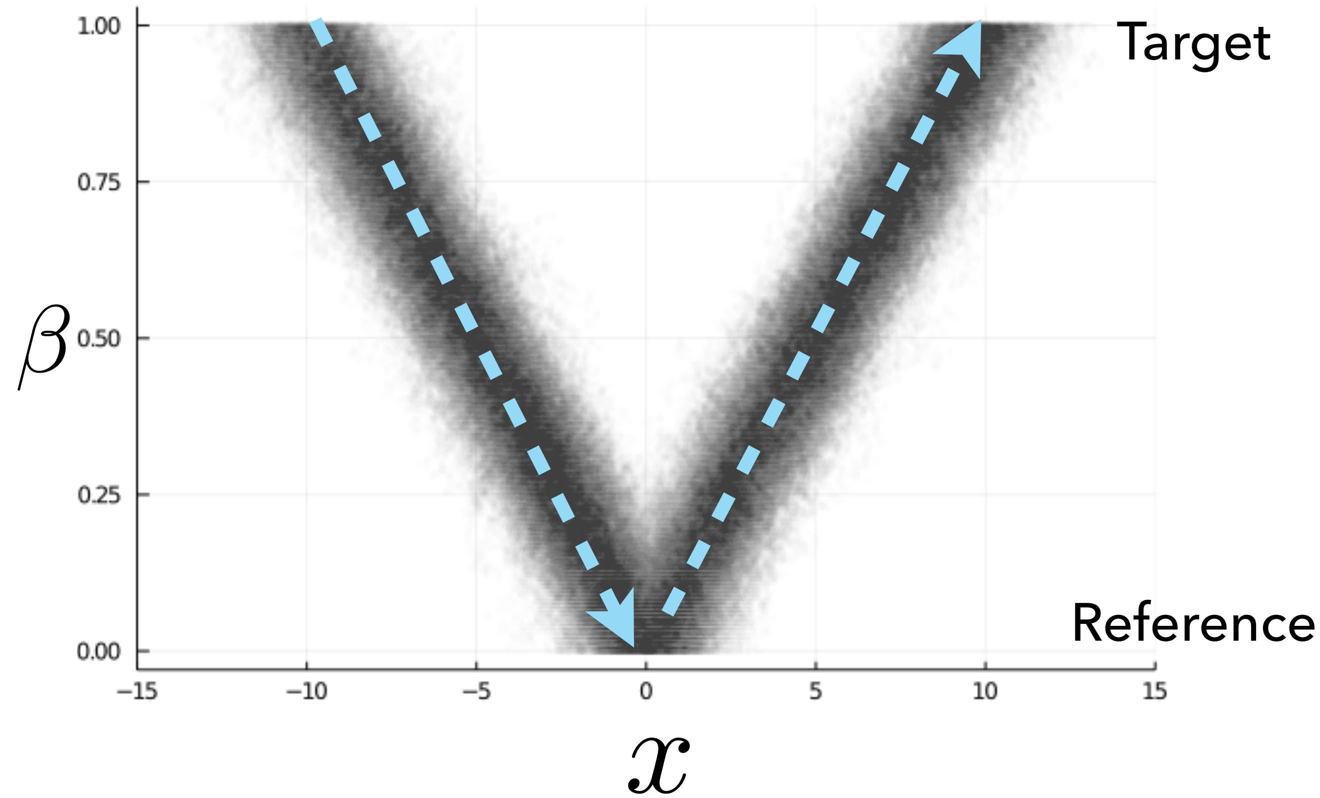

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    - Accept/reject according to Metropolis-Hastings:

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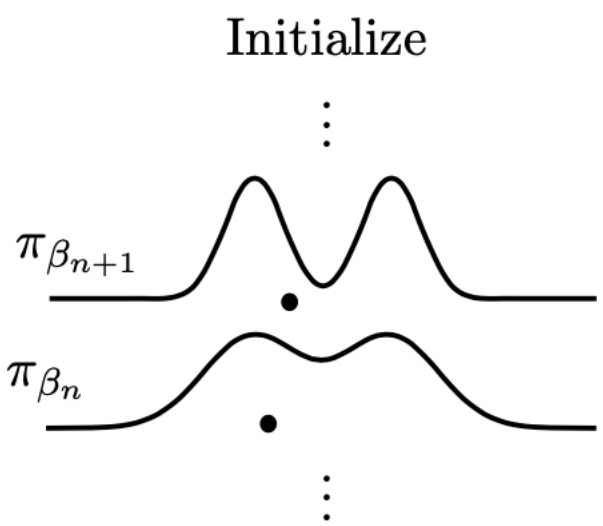

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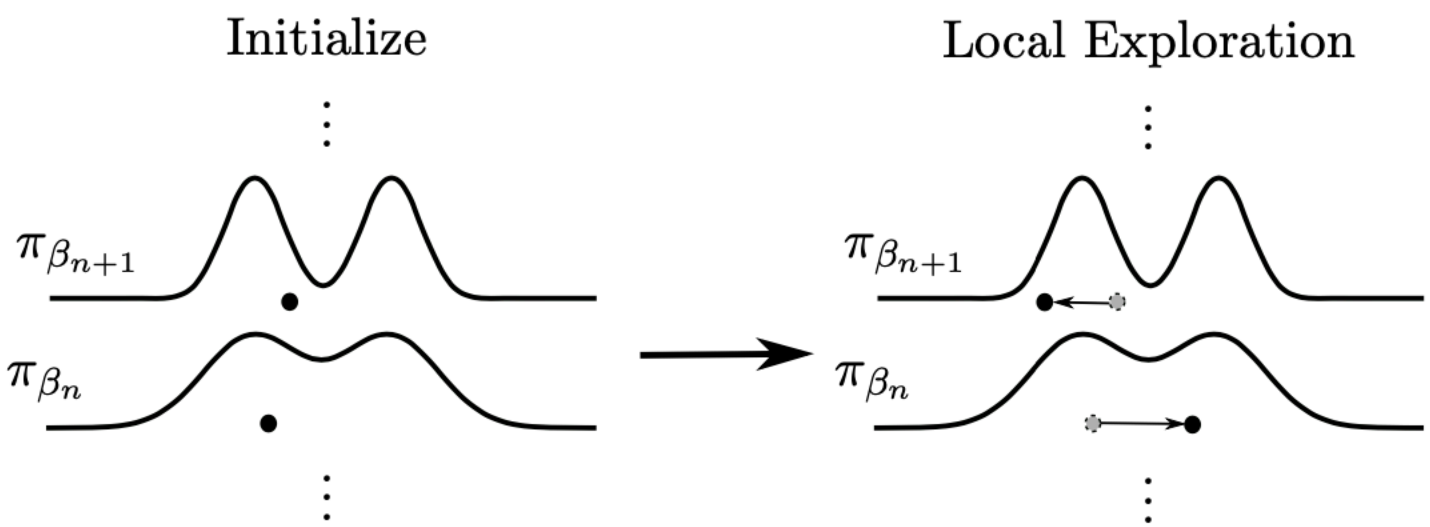

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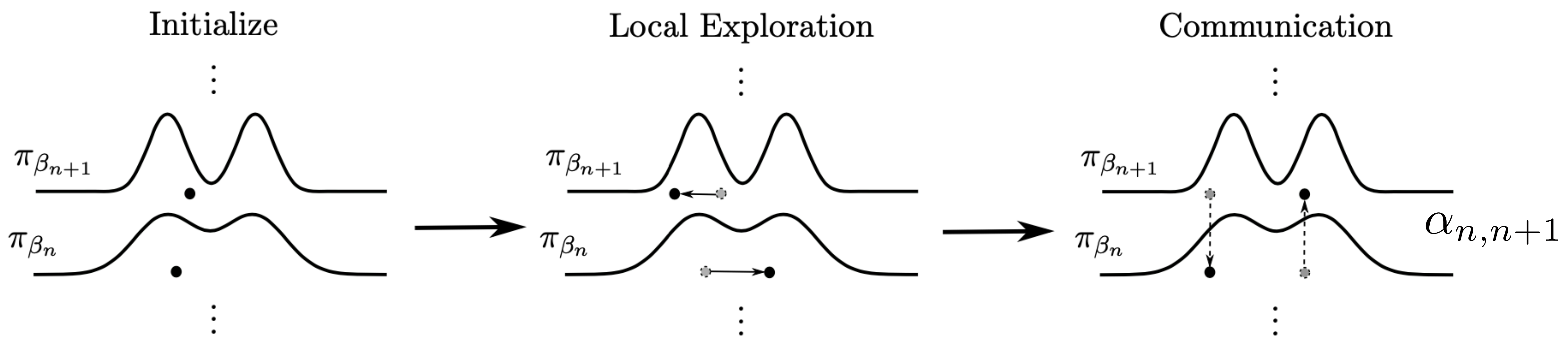

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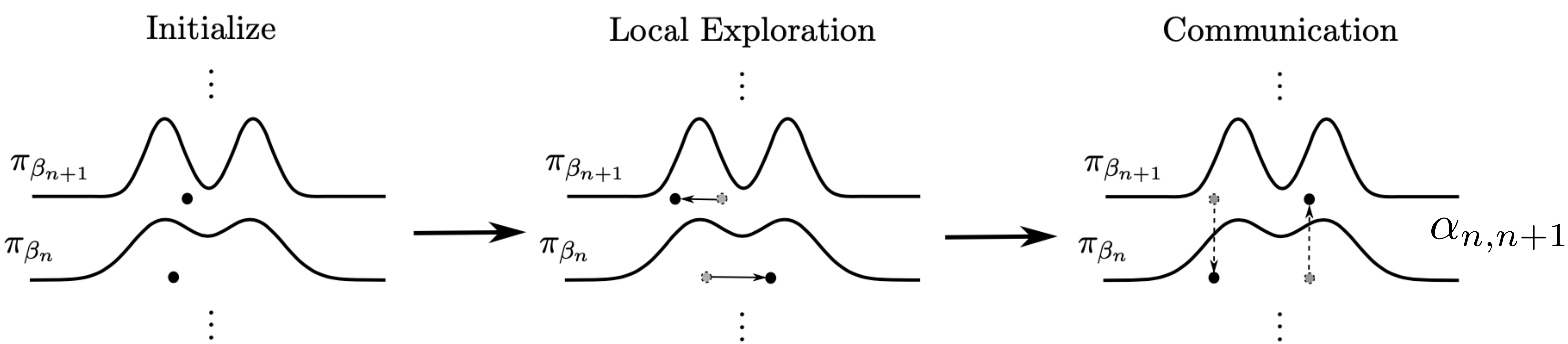

- Acceptance probability:

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

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

MCMC VS PARALLEL TEMPERING

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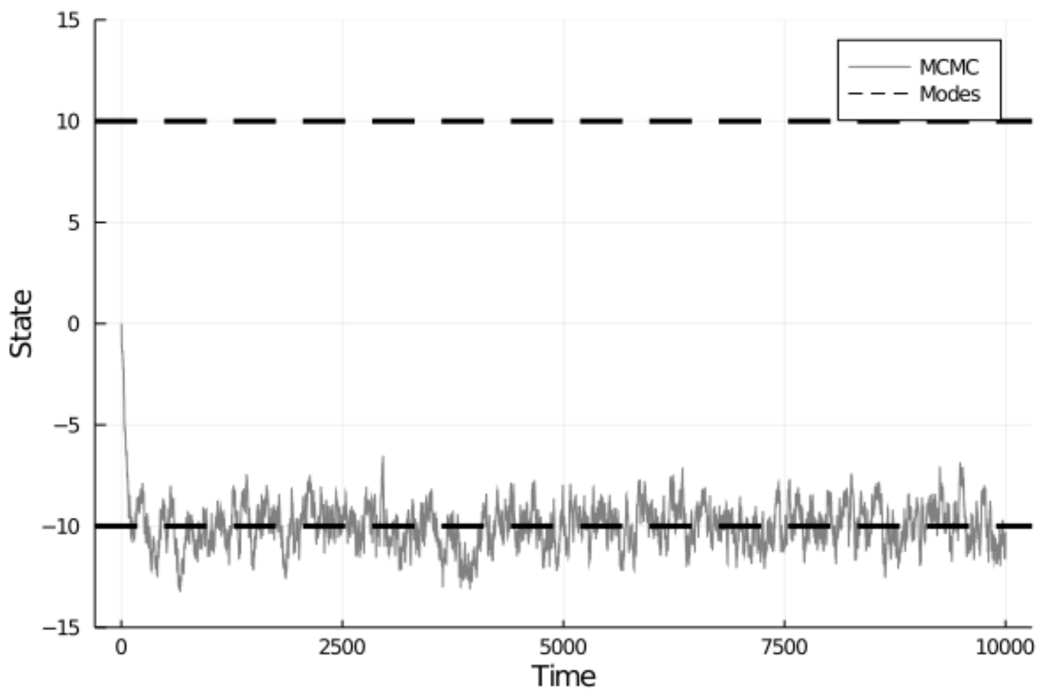
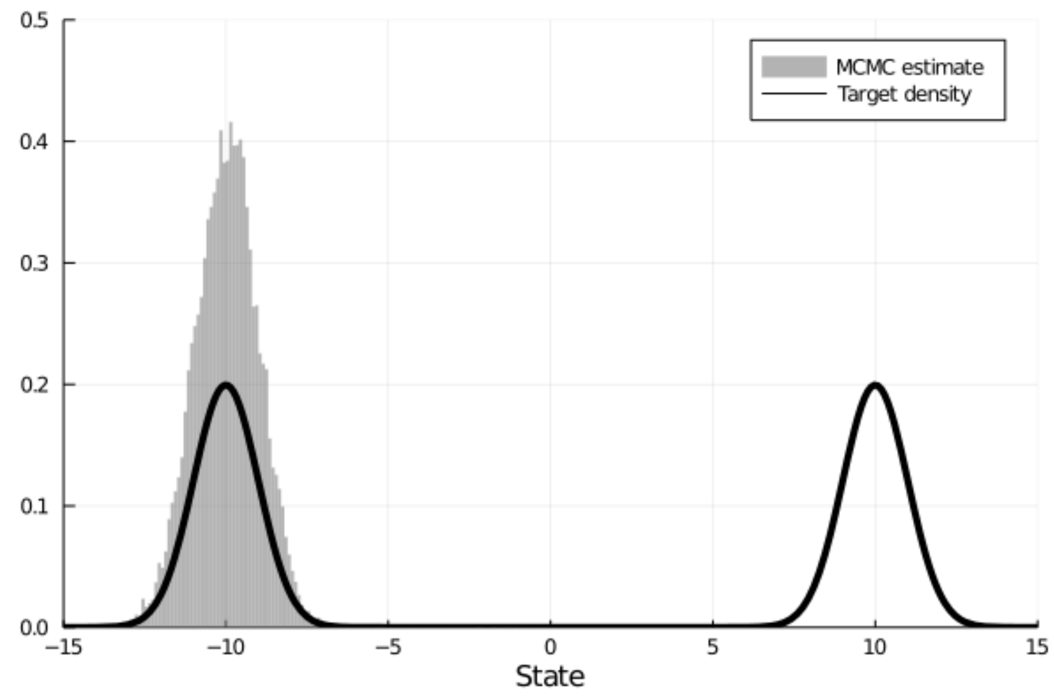
Single chain MCMC





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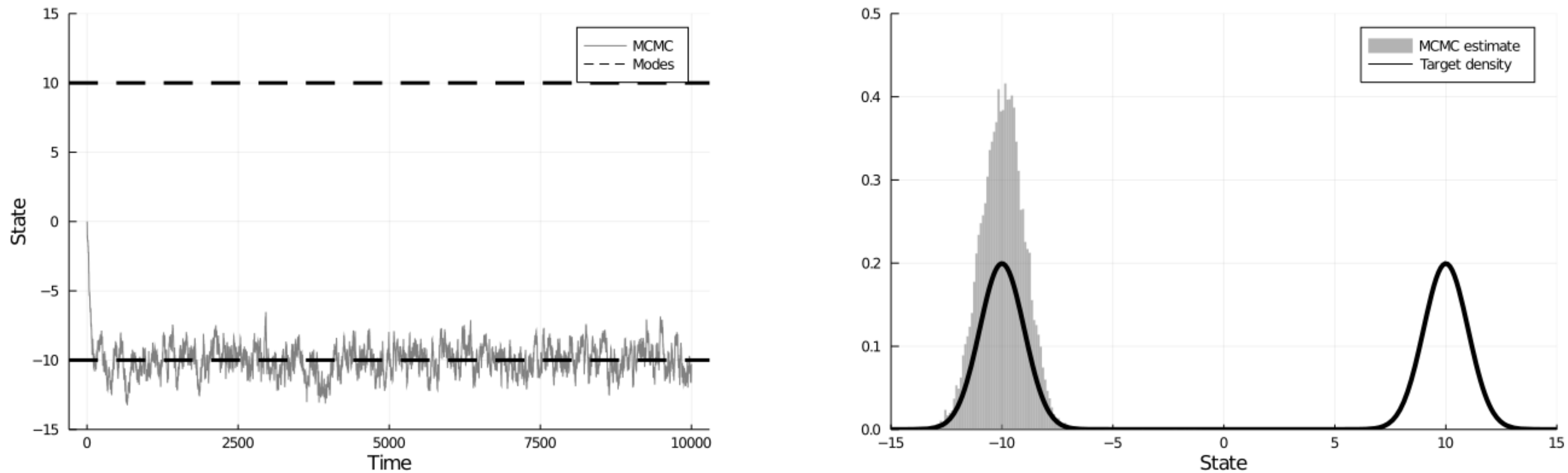
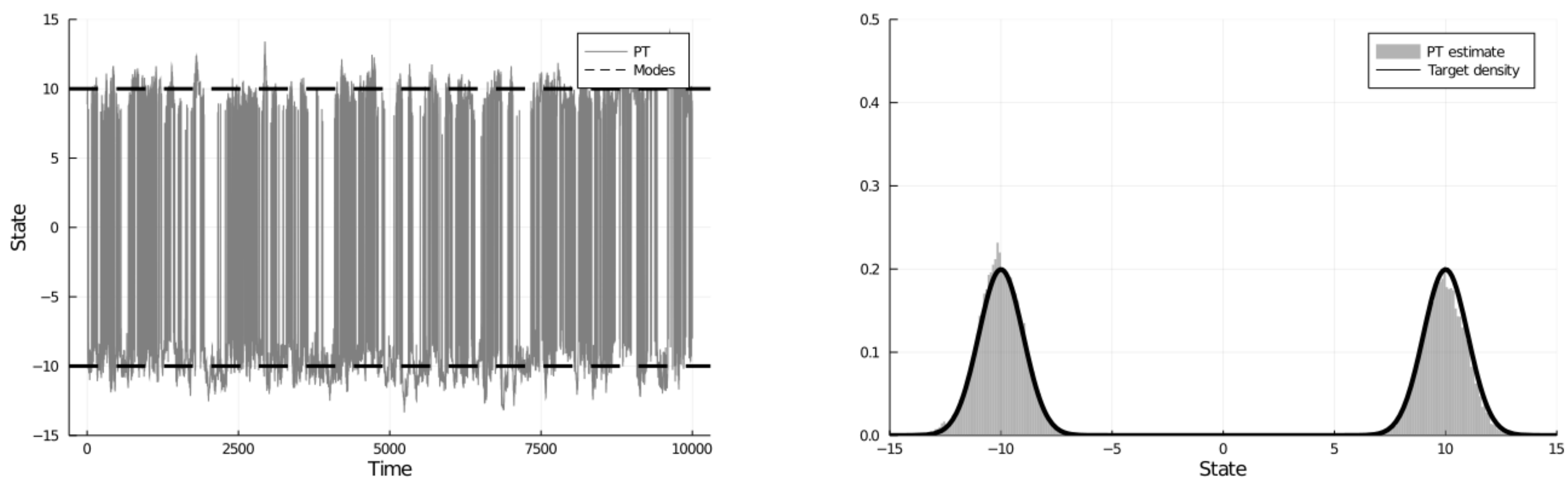


Parallel Tempering (N = 10)



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  - Introduce non-reversible PT + scaling + tuning + diagnostics

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  - Introduce non-reversible PT + scaling + tuning + diagnostics
- **Parallel tempering on optimized paths (ICML, 2021)†**
  - Introduce geometry of PT + path tuning.

Alexandre Bouchard-Côté*†

George Deligiannidis*

Arnaud Doucet*

Vittorio Romaniello†

Trevor Campbell†

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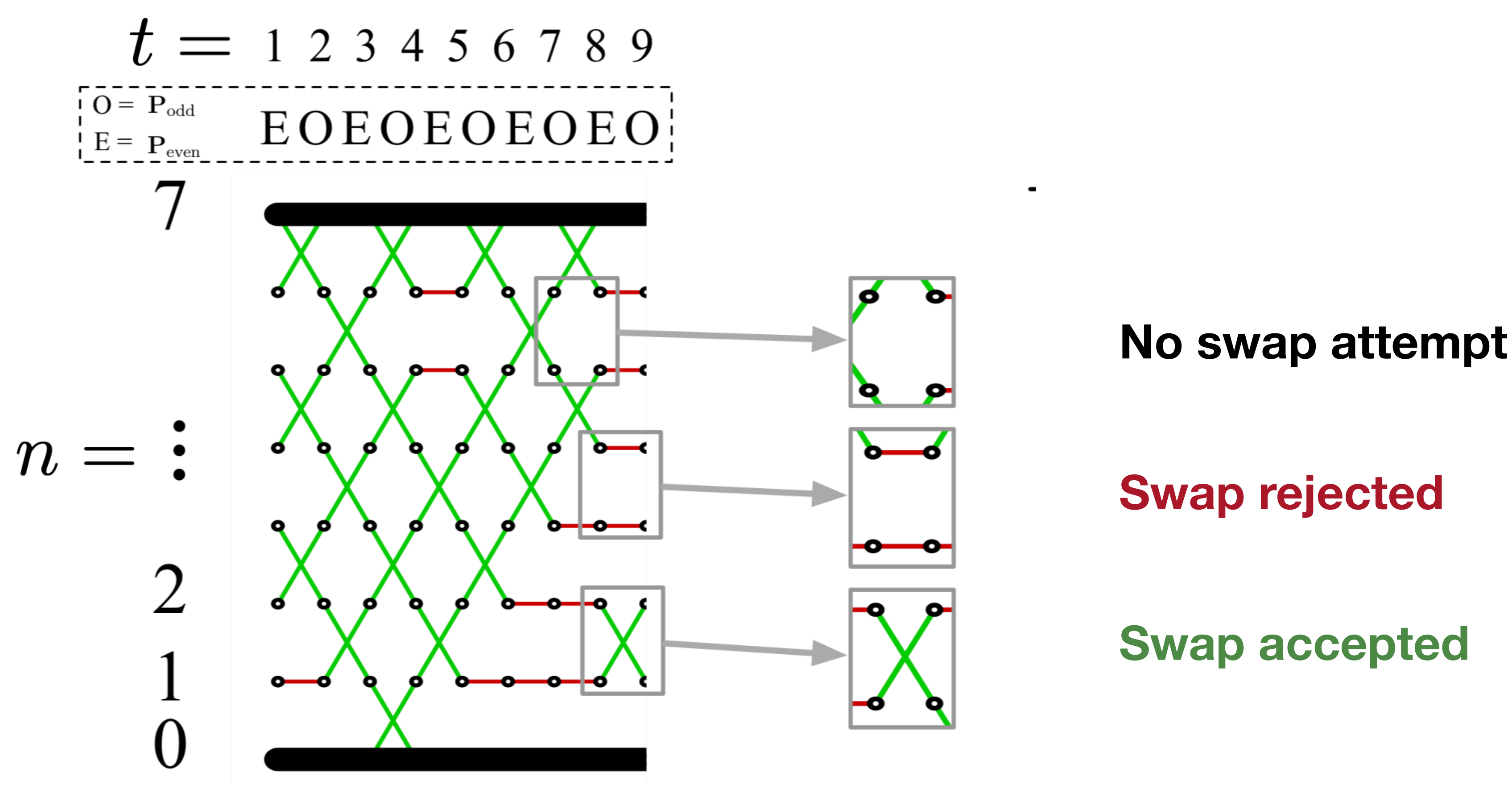
  - We can study communication through the dynamics of the permuted annealing parameters



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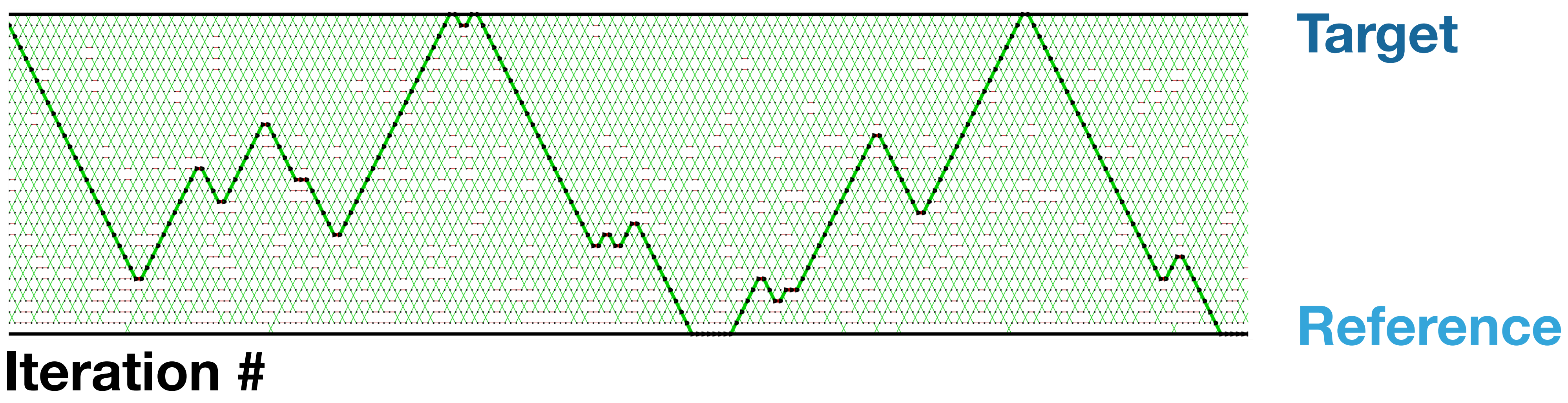

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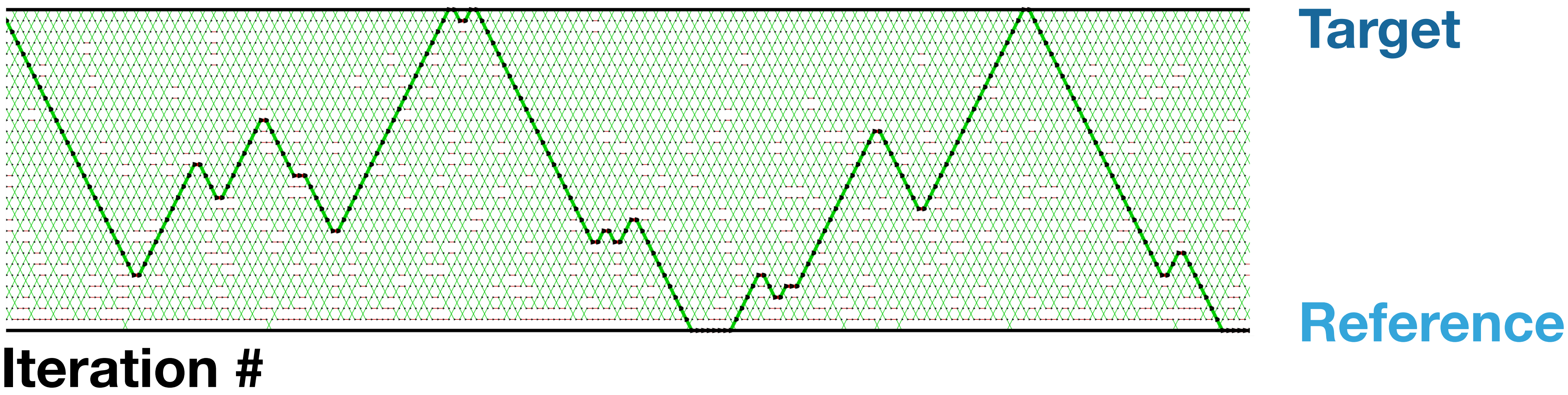

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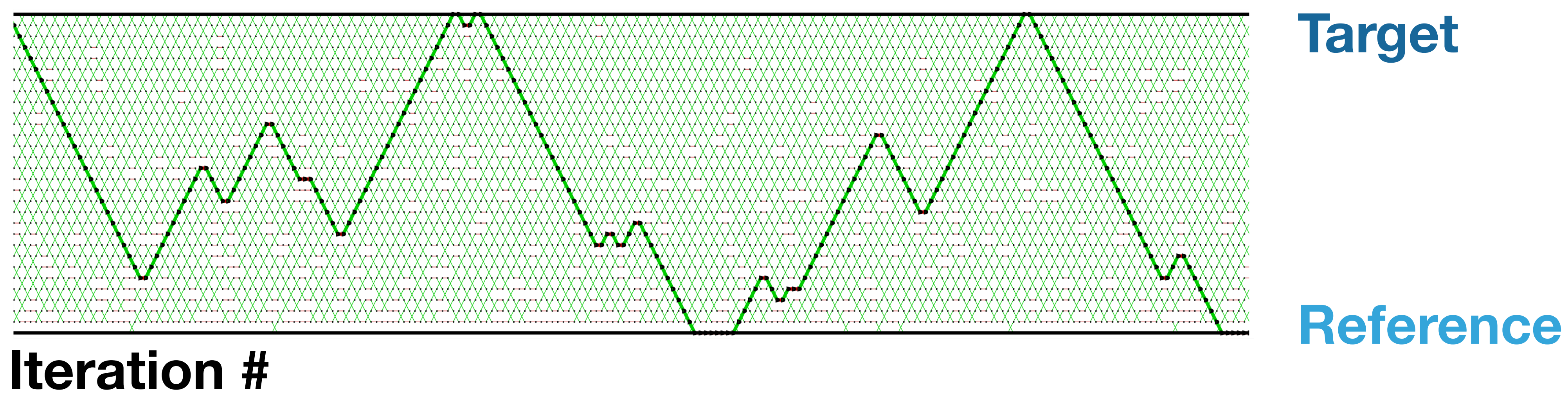

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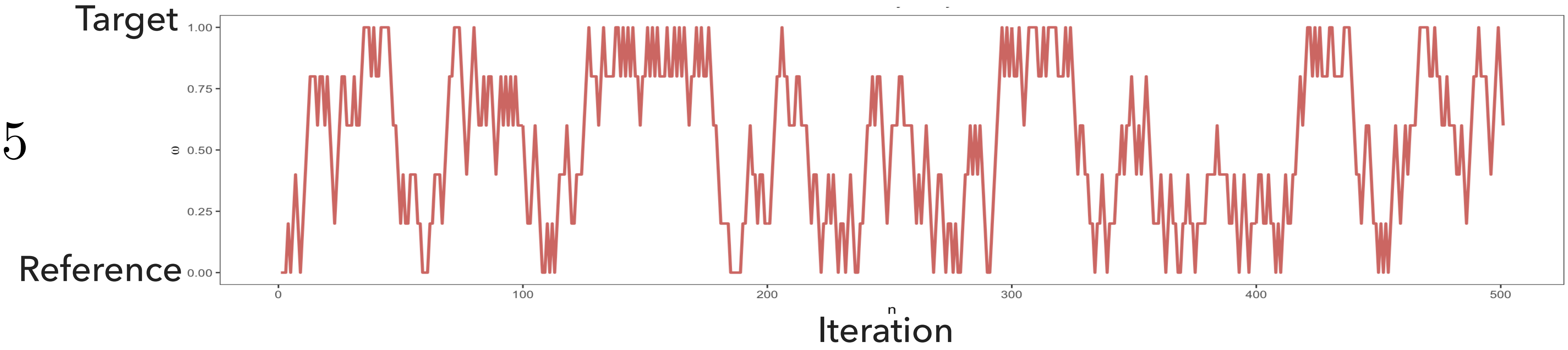

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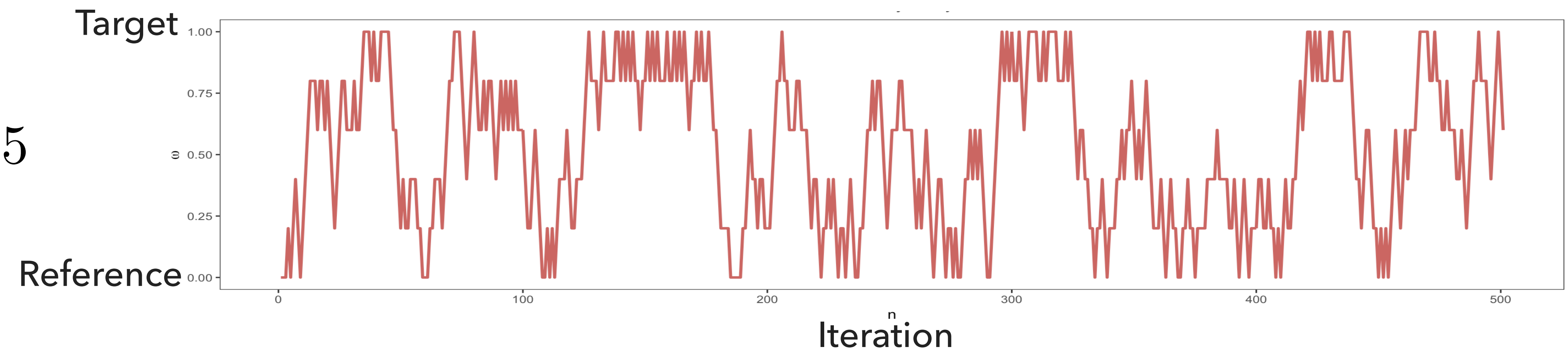

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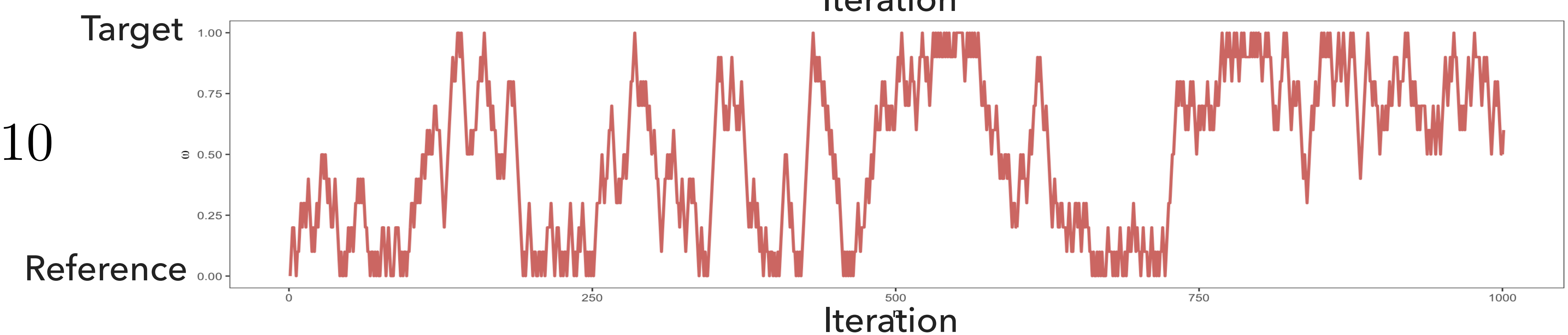

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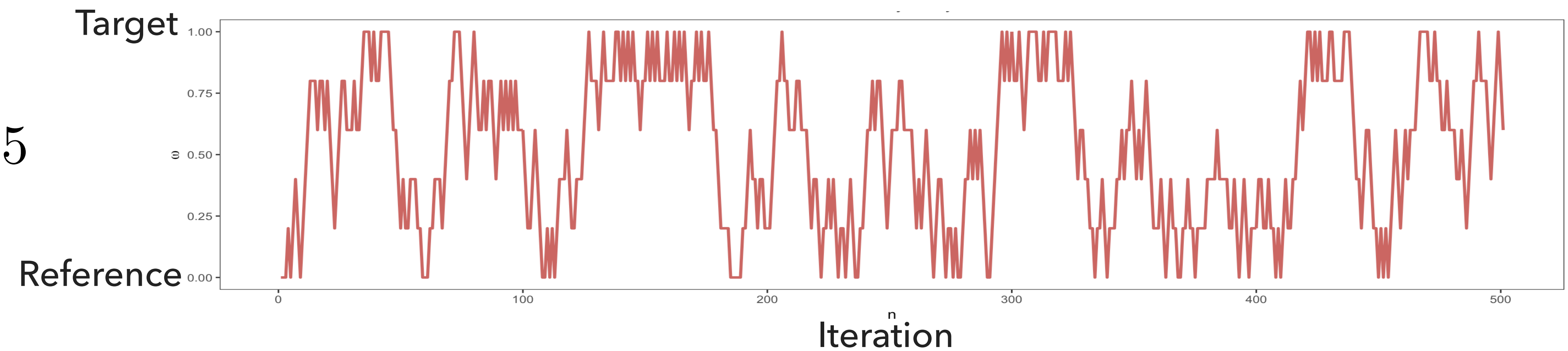

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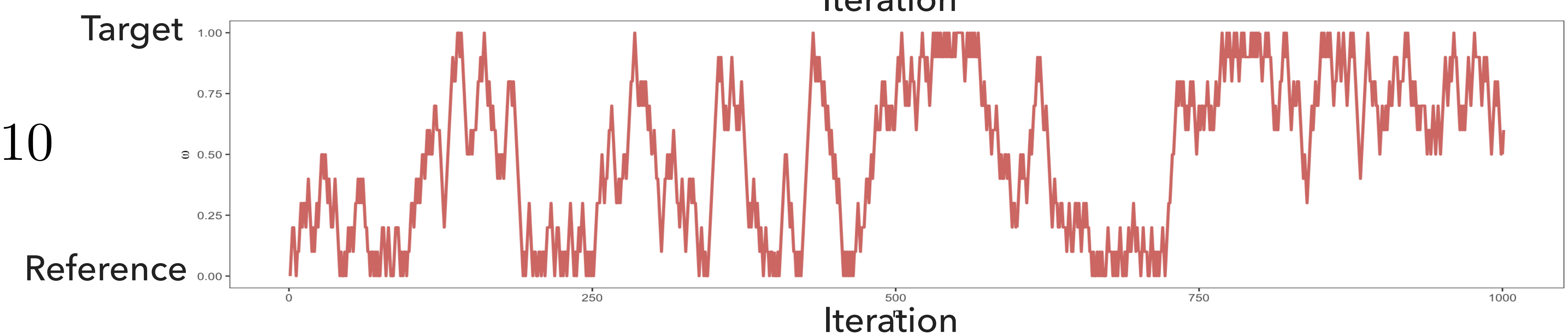

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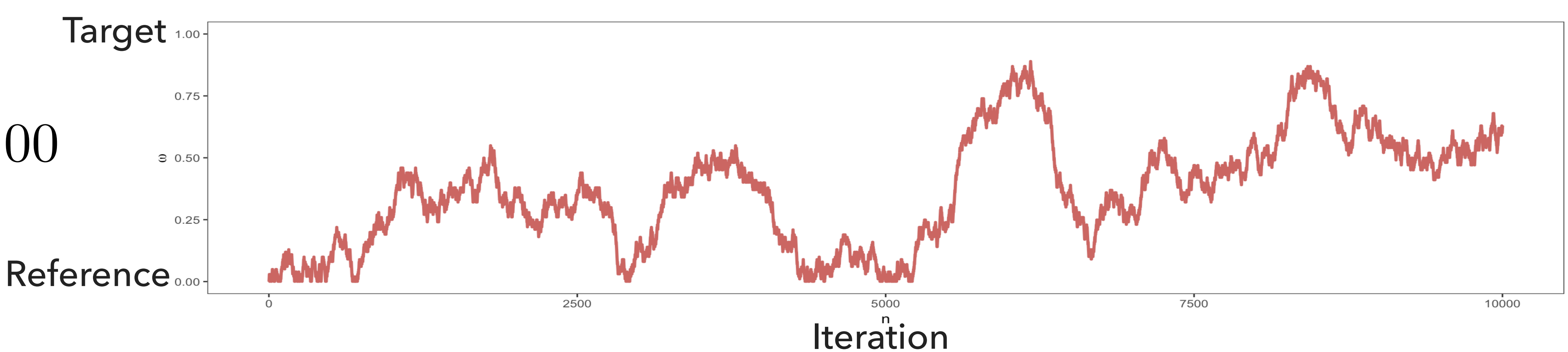

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Theorem: For any annealing schedule

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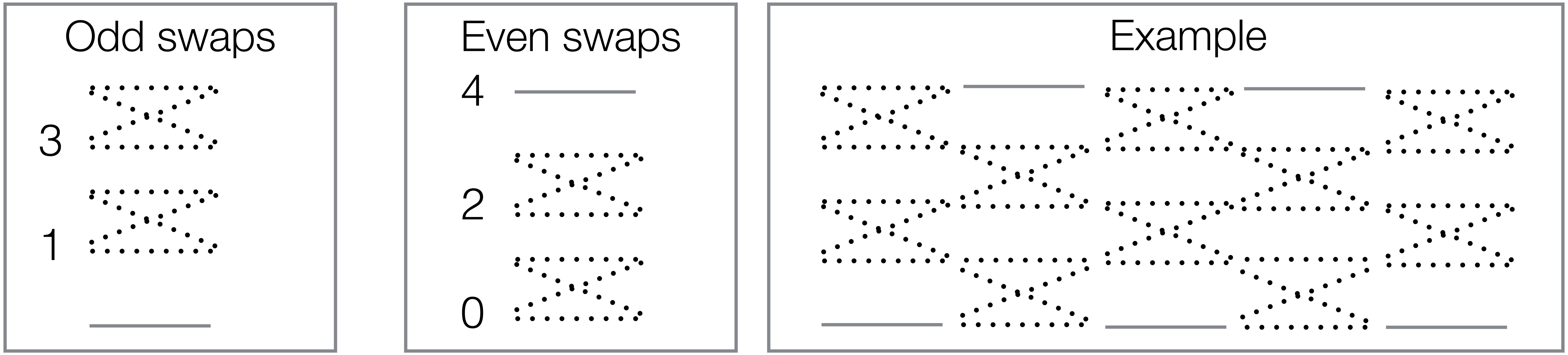
NON-REVERSIBLE PT (OKABE ET AL, 2001)

- Deterministically alternate between **Odd** and **Even** swaps



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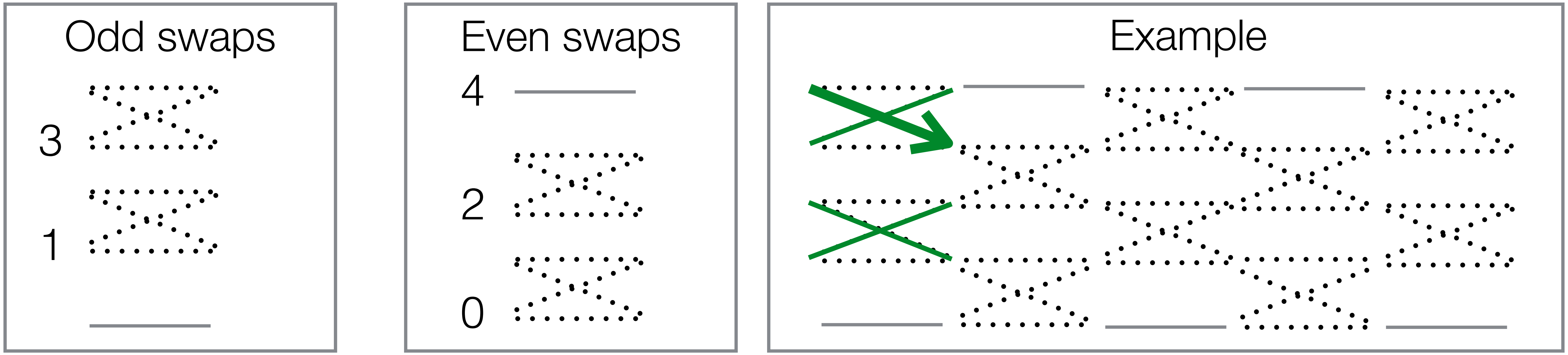

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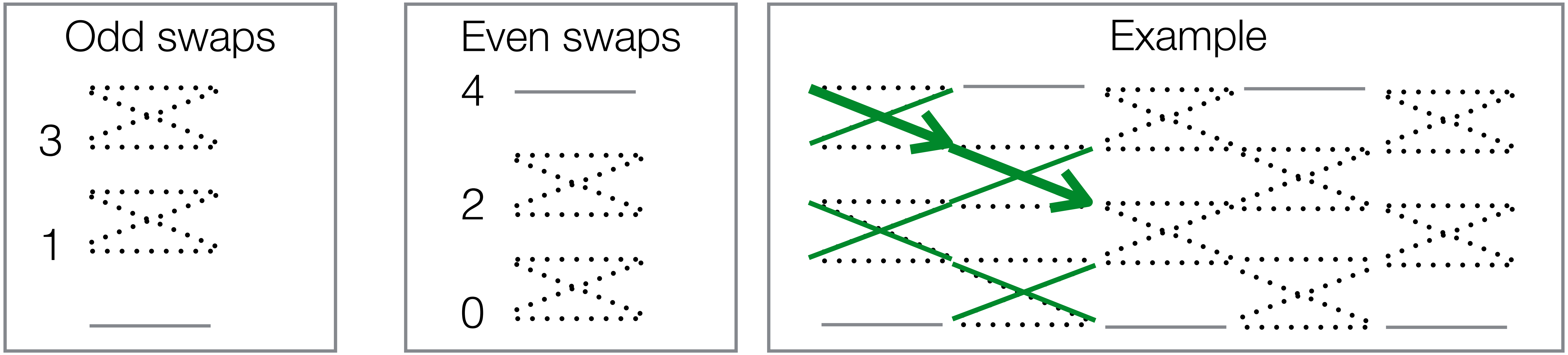

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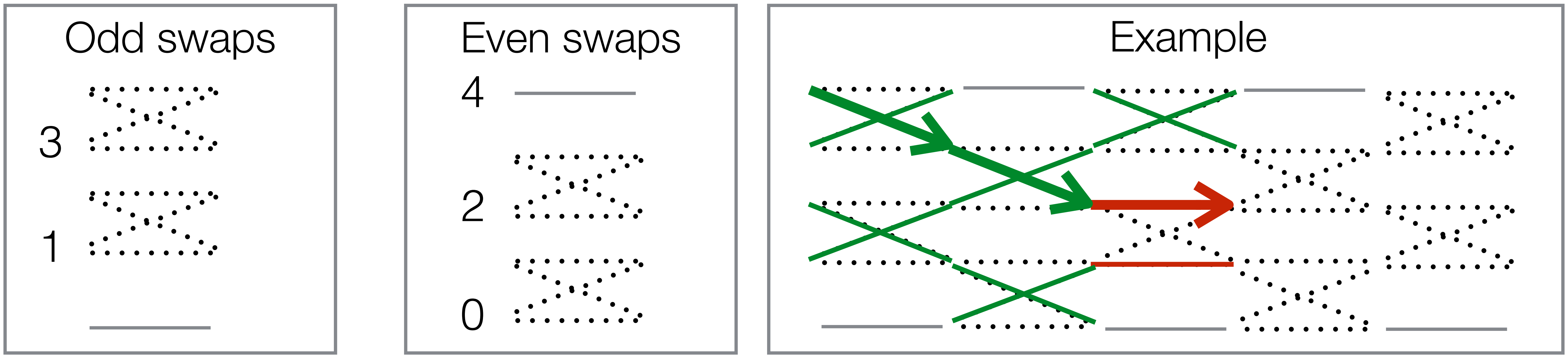

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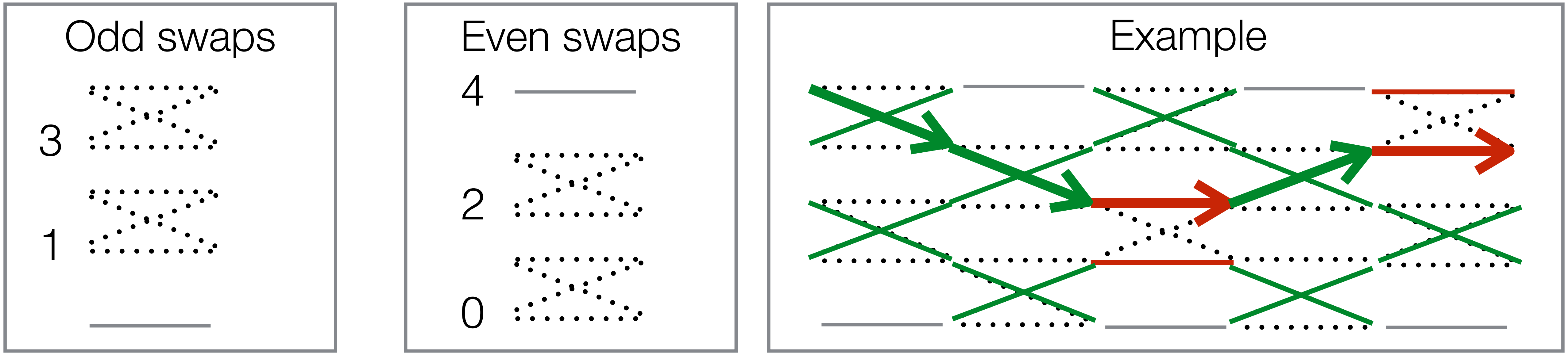

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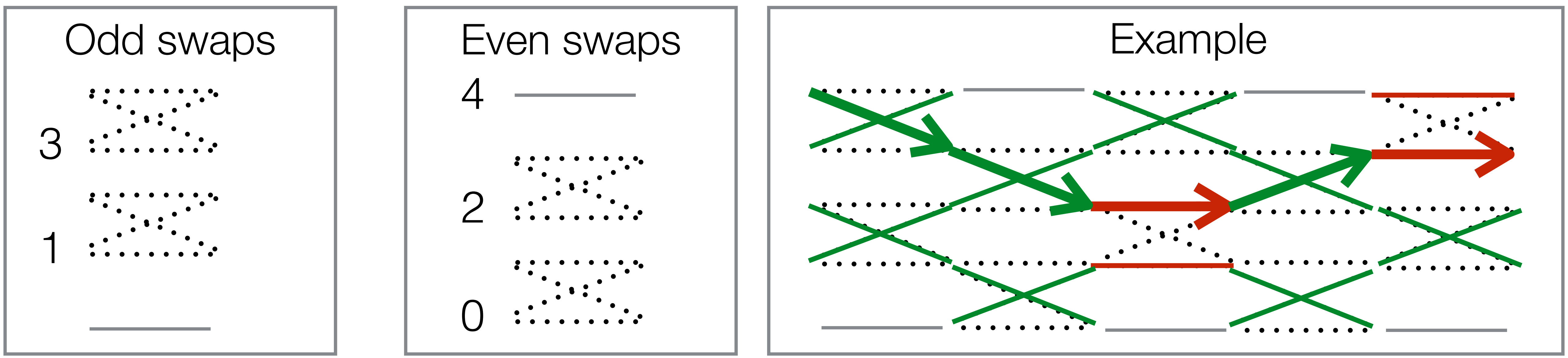

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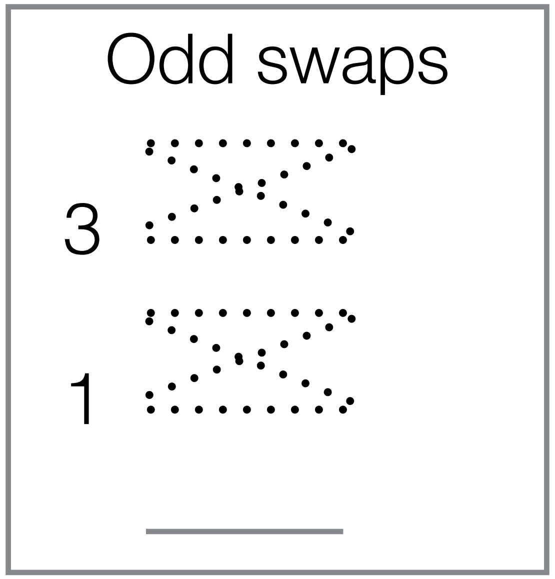

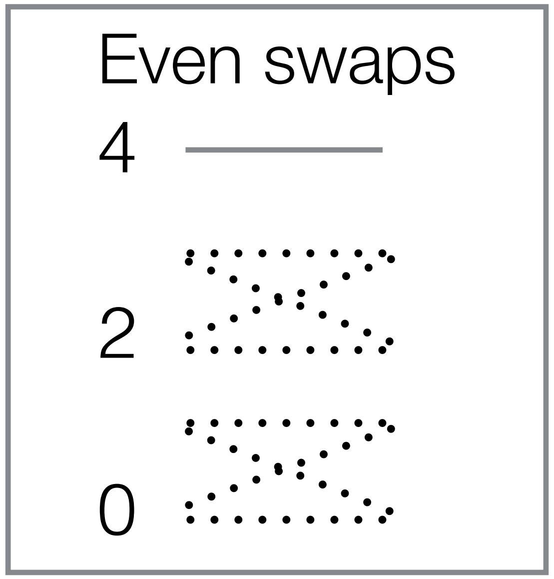

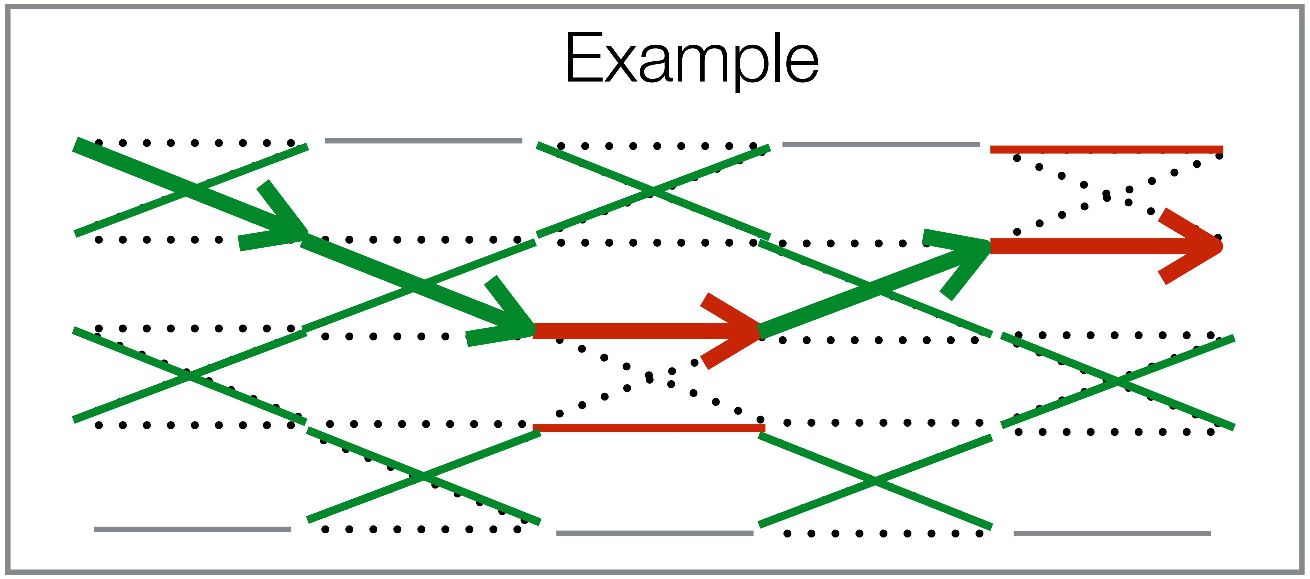

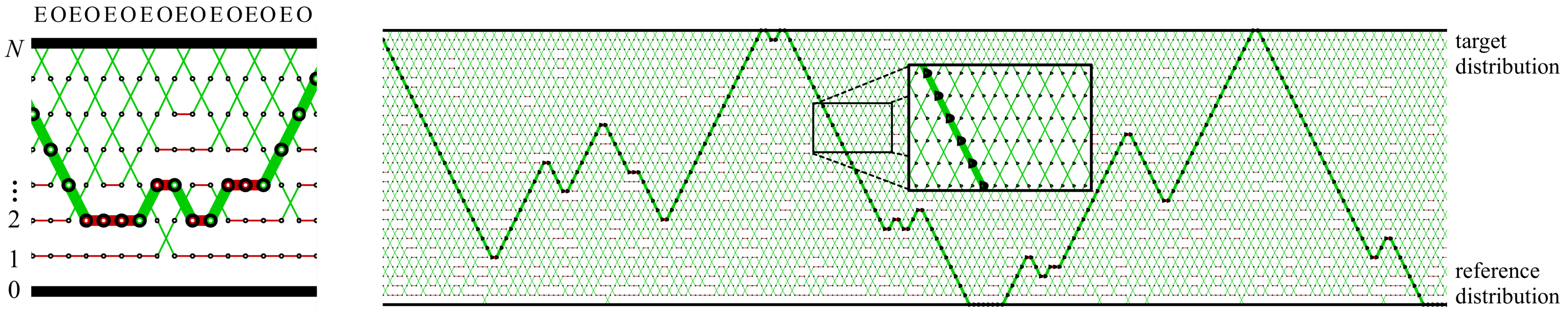

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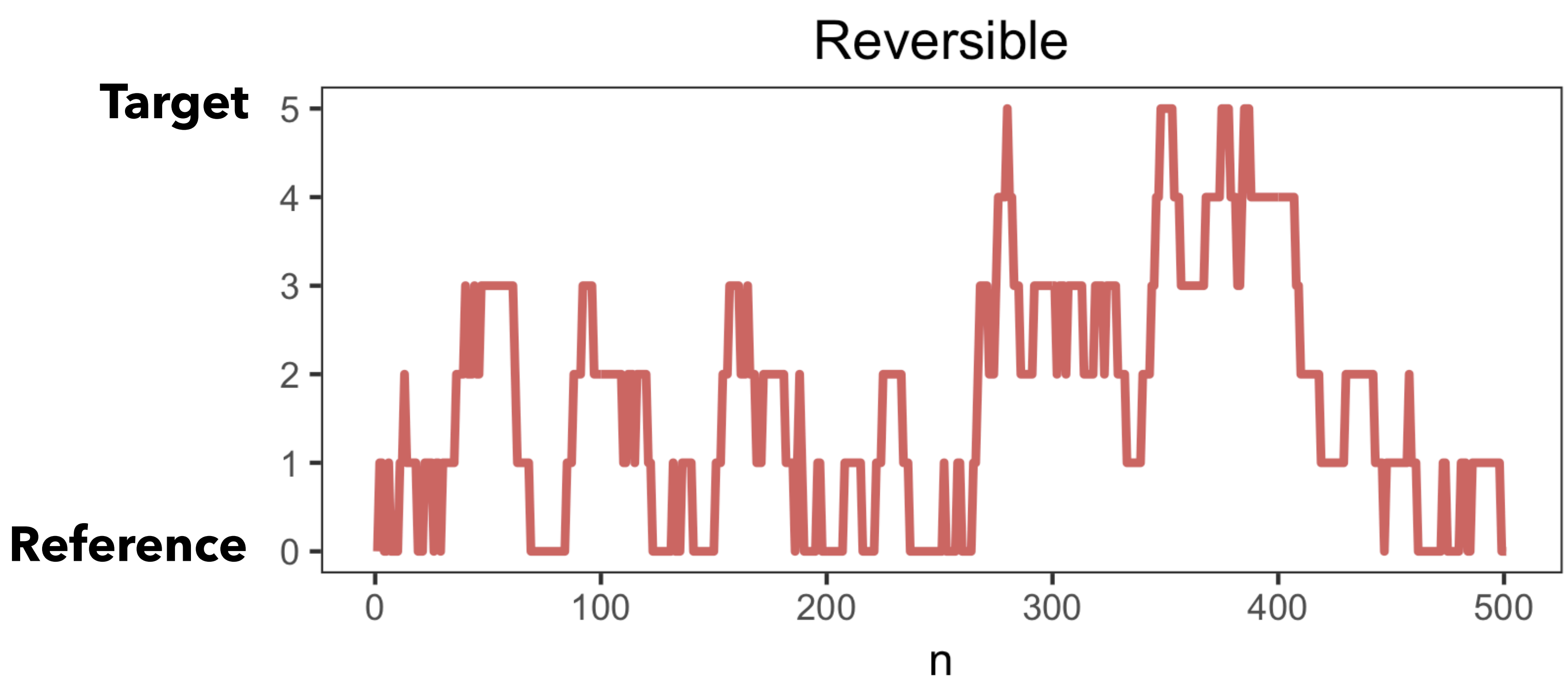
- Robust to schedule
- Scalable to GPUs

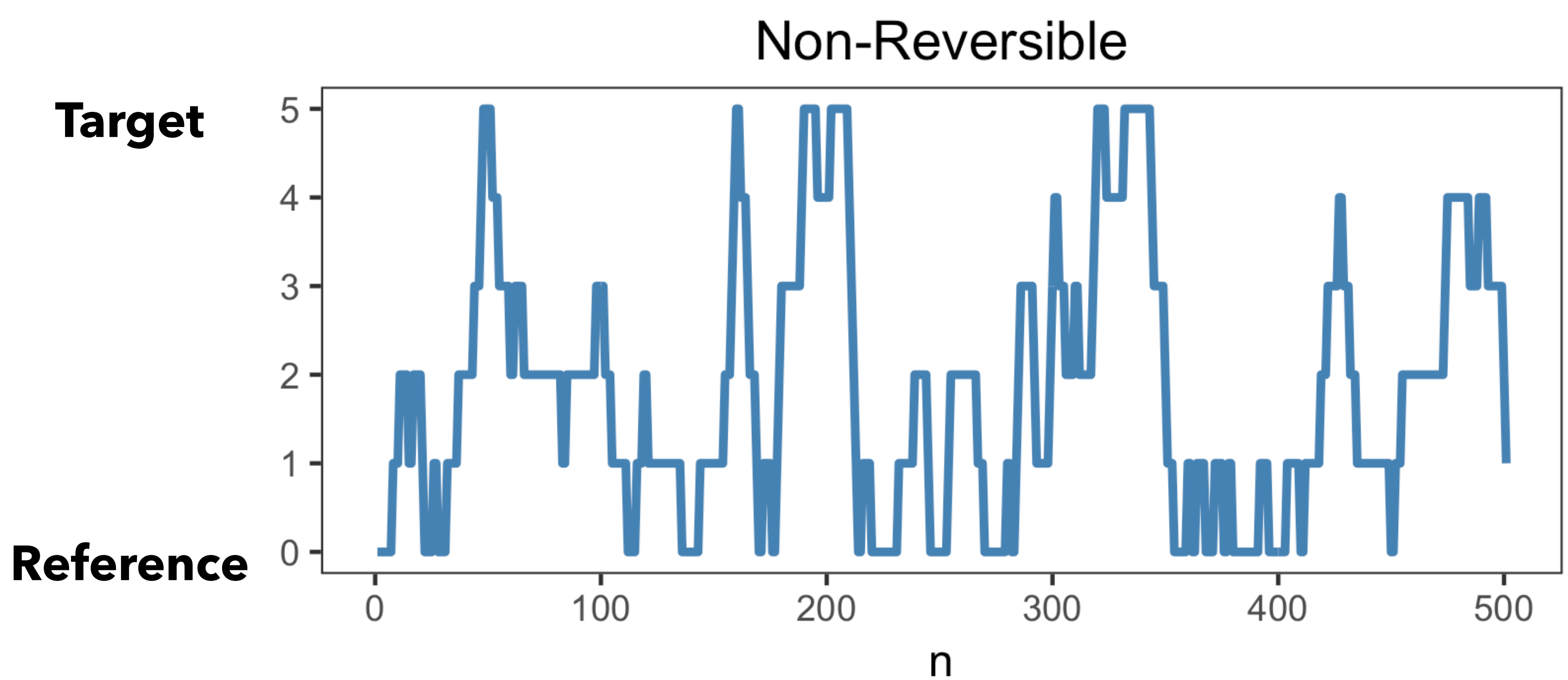
SAMPLE TRAJECTORIES

$$N = 5$$

 # Round Trips



$$1$$

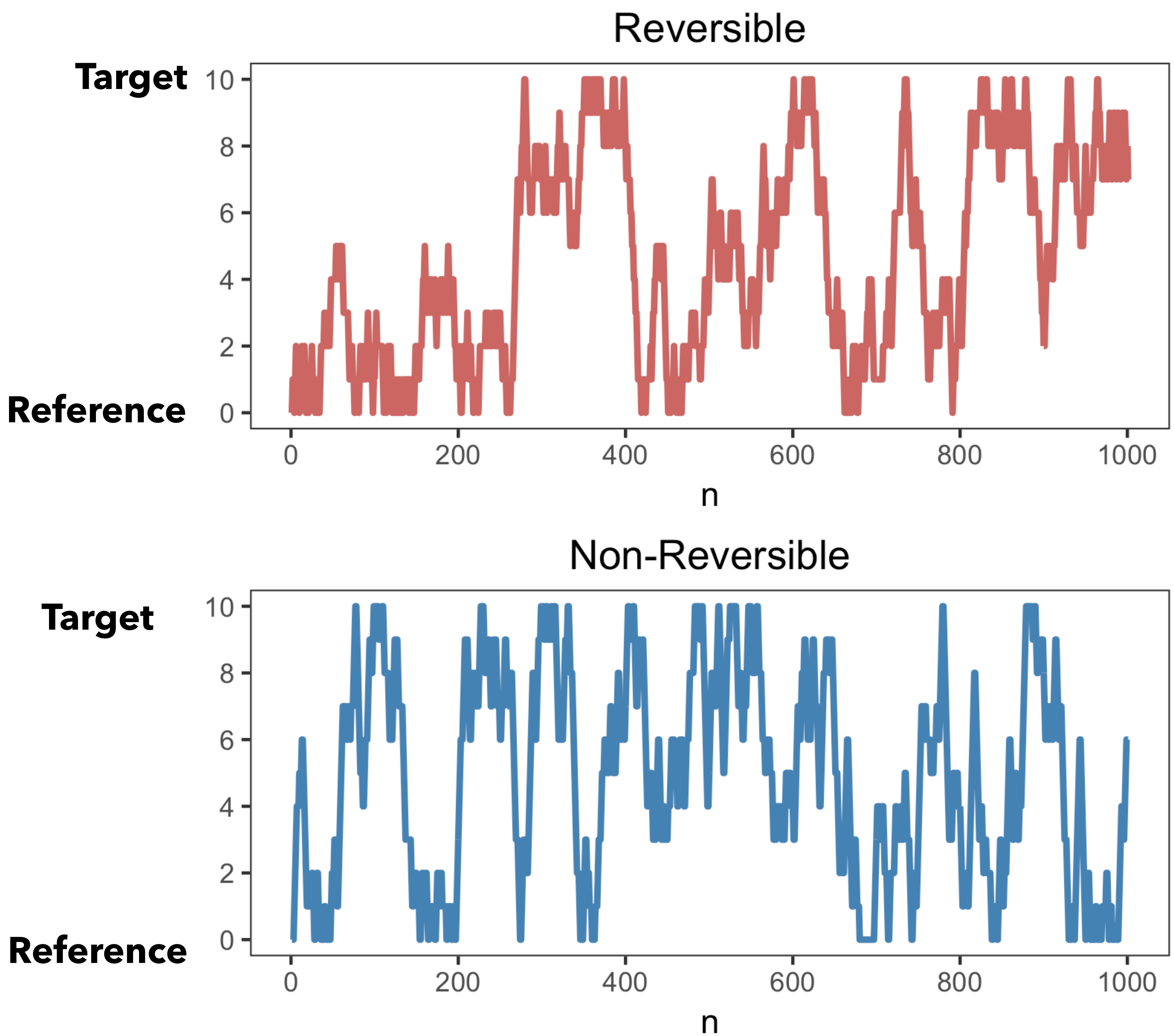


$$4$$

SAMPLE TRAJECTORIES

$$N = 10$$

 # Round Trips



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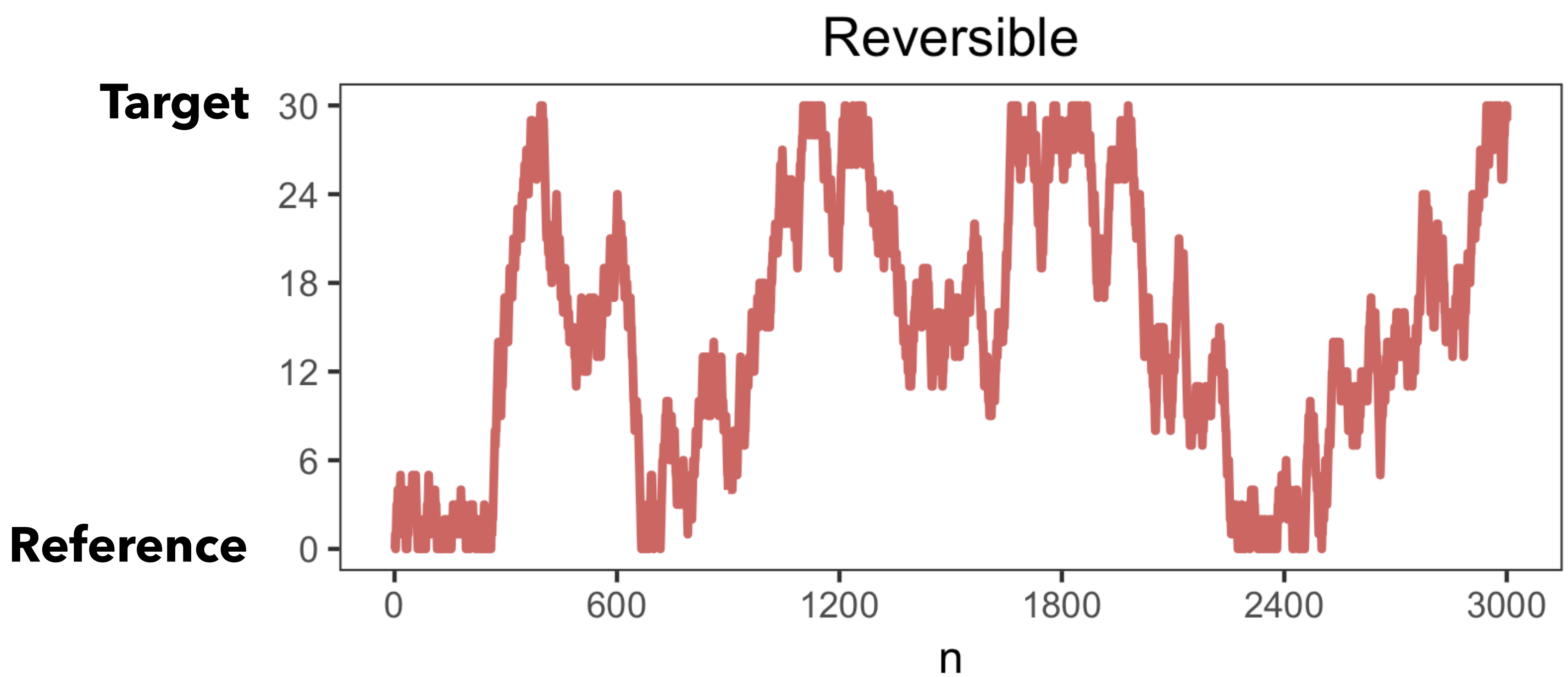
6

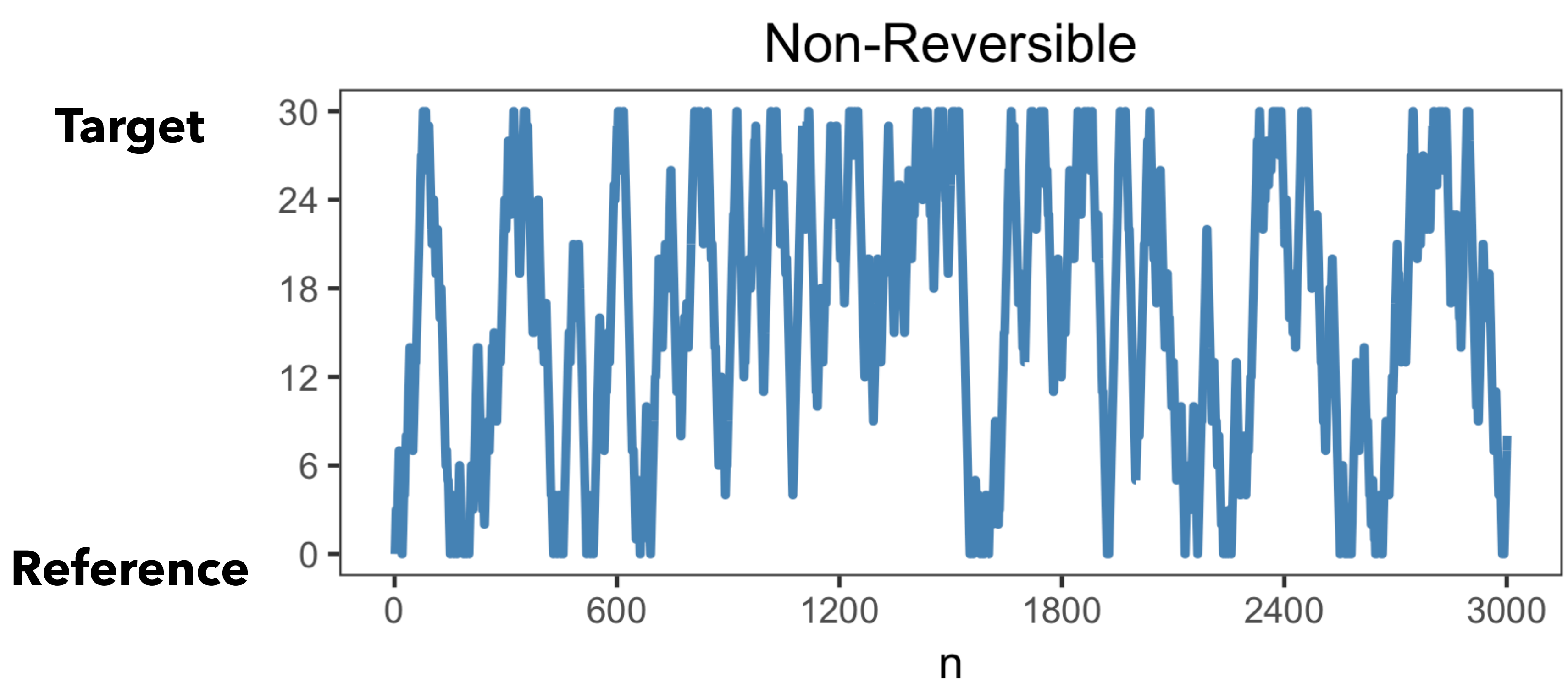
SAMPLE TRAJECTORIES

$$N = 30$$

Round Trips



2

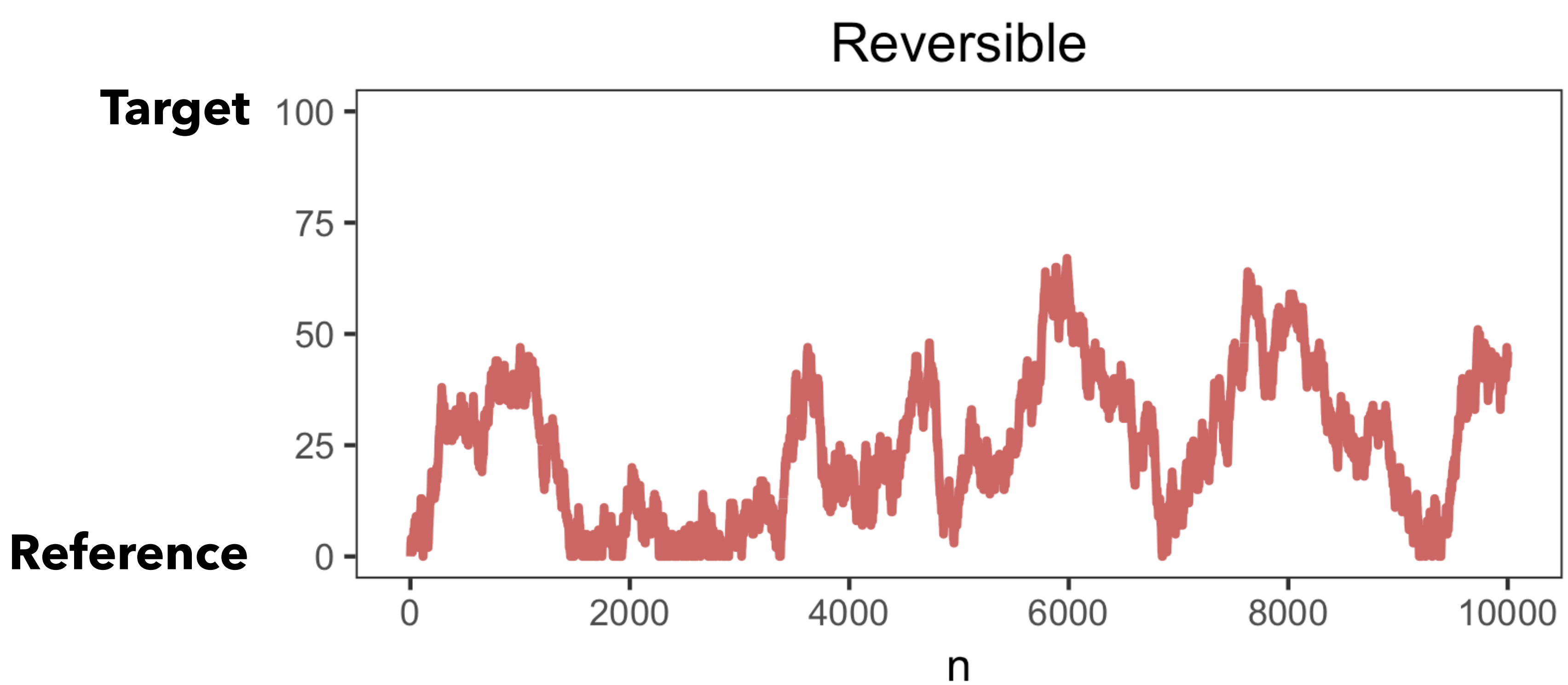


8

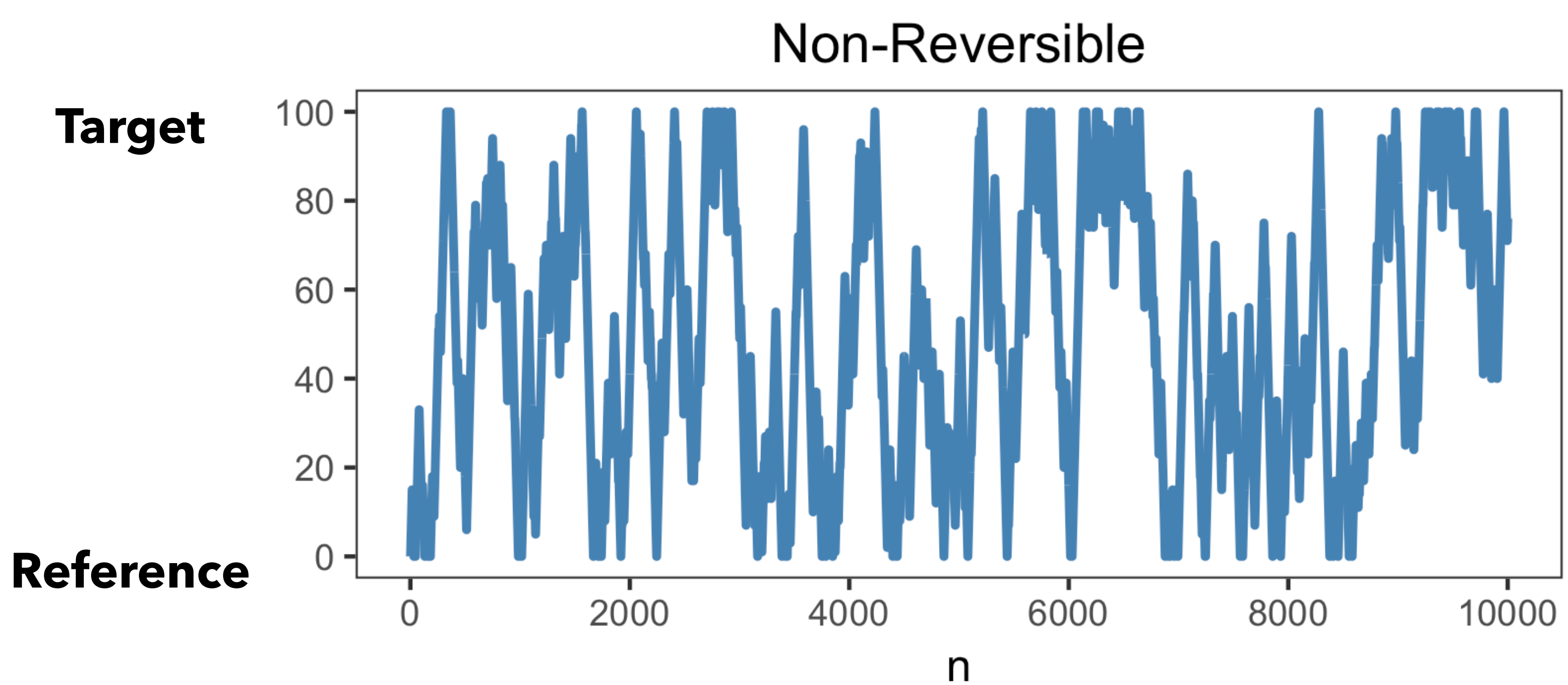
SAMPLE TRAJECTORIES

$$N = 100$$

 # Round Trips



0



9

SCALING LIMIT (REVERSIBLE)

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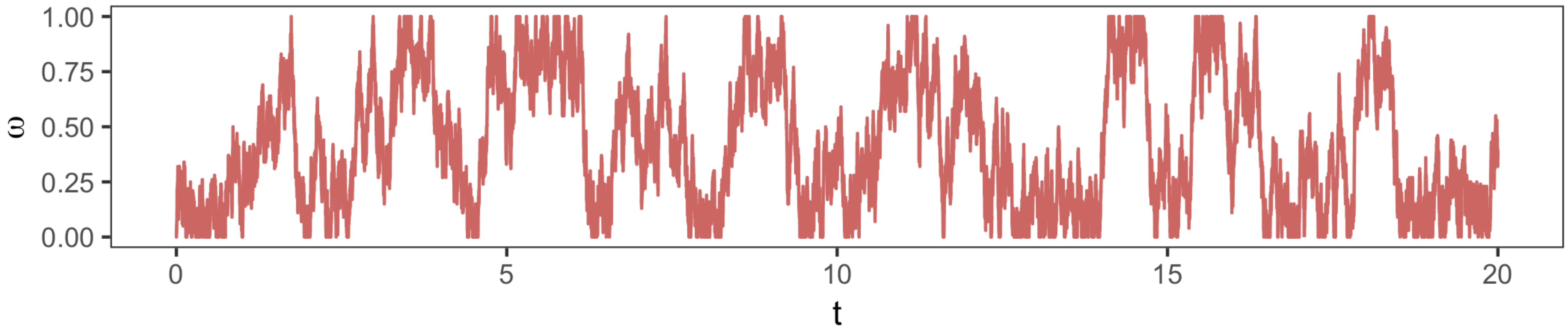

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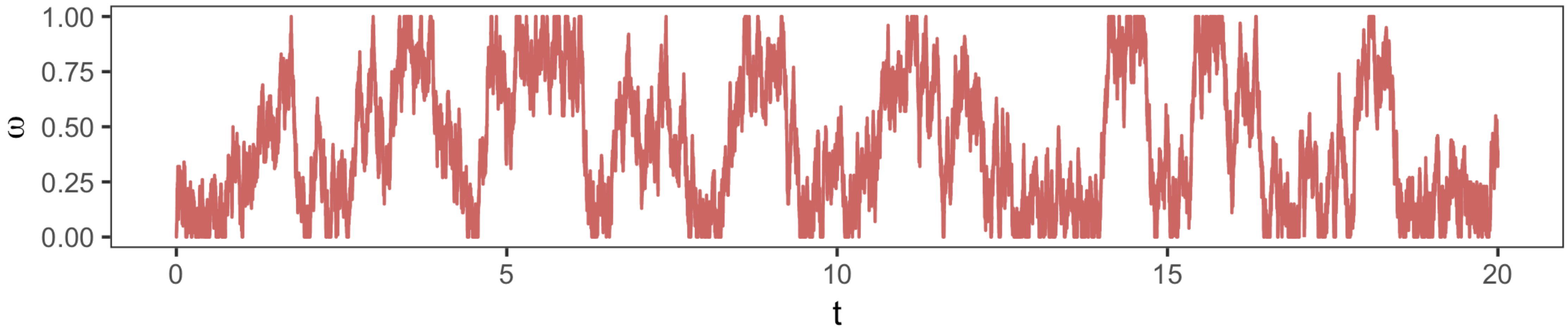

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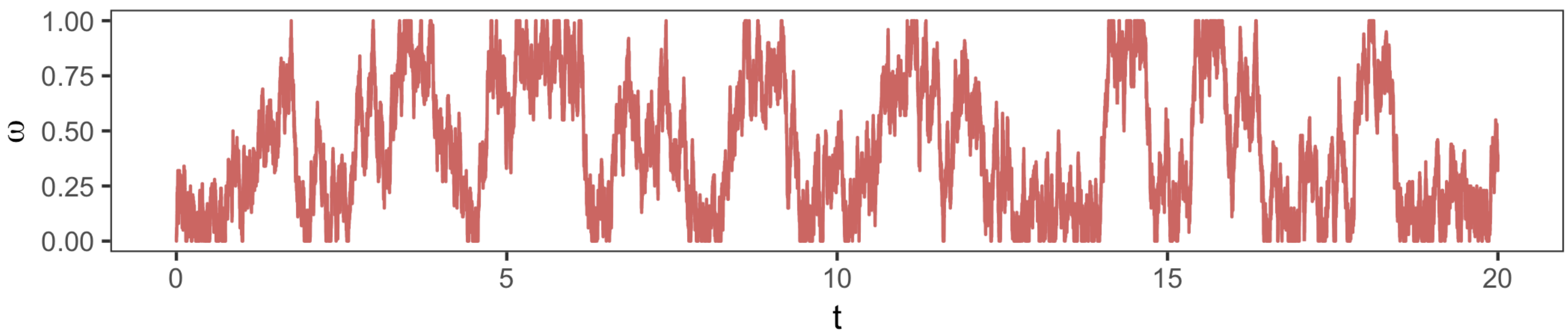

- As N grows large, noise from diffusivity dominates
- Modifying reference, target, or path leads to marginal gains

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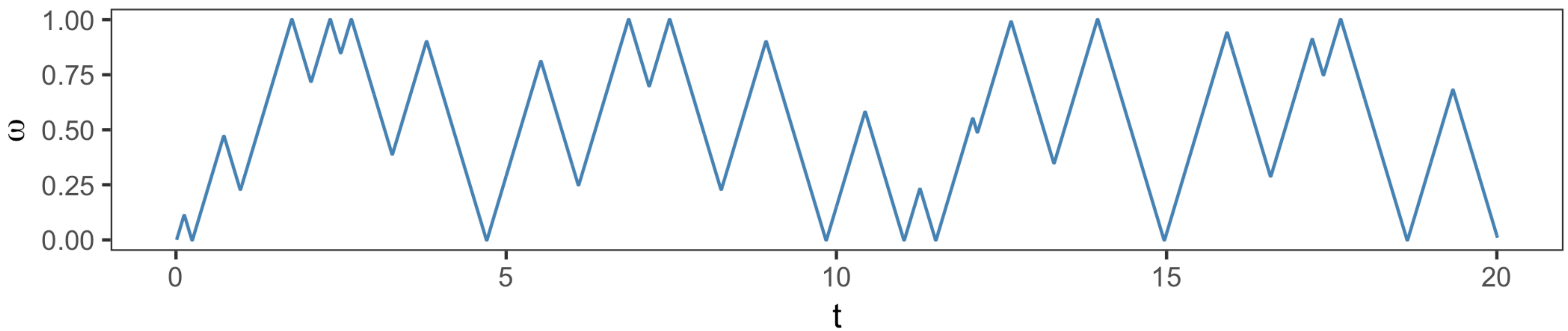

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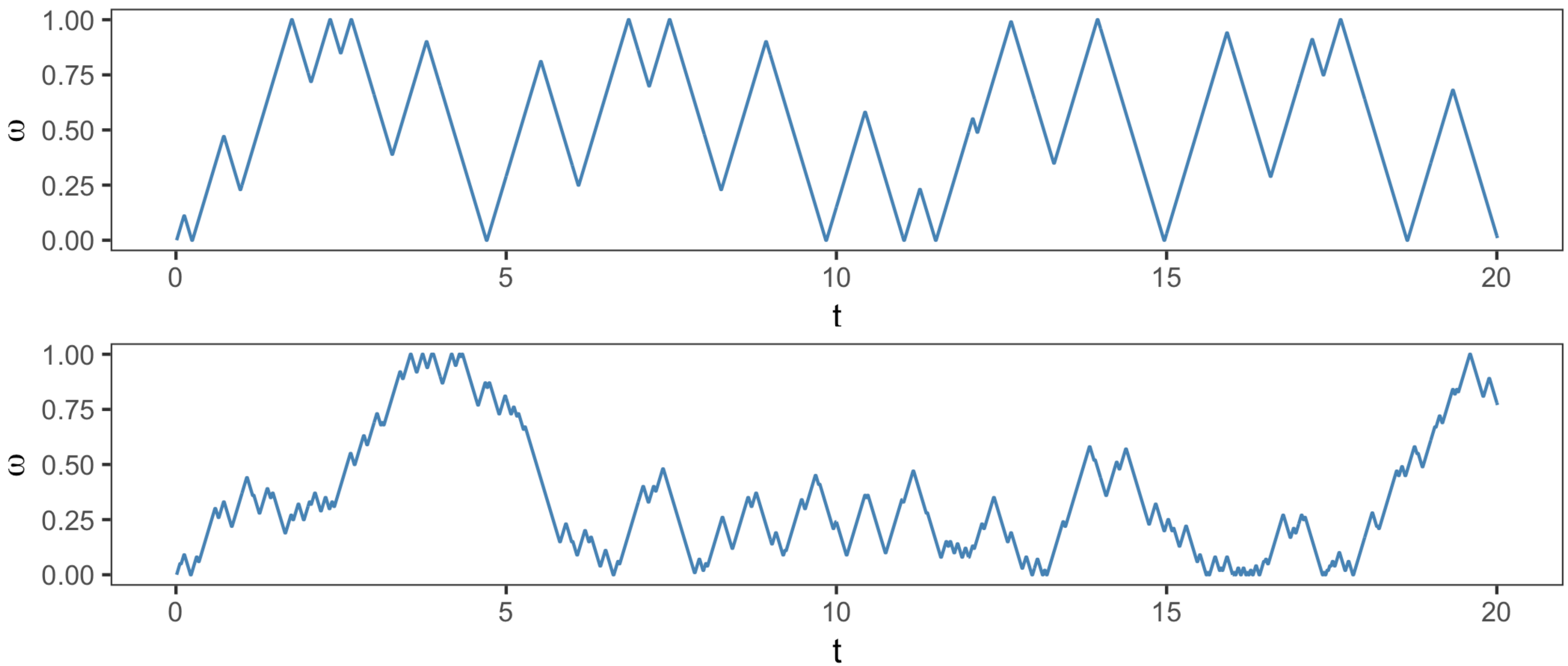

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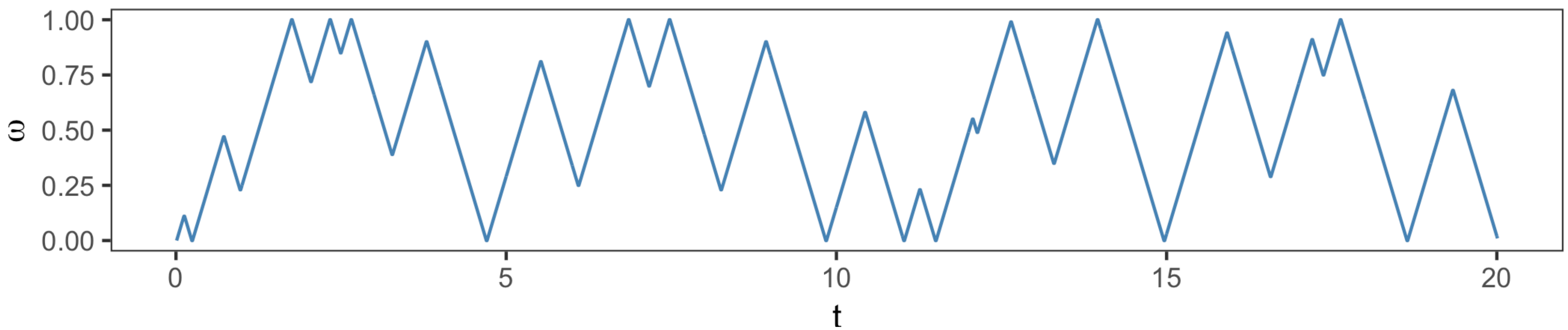

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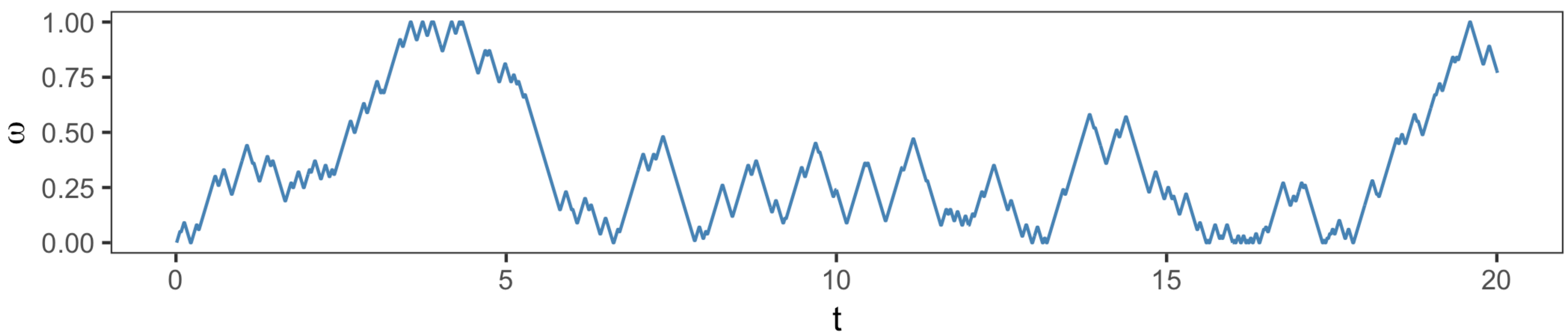

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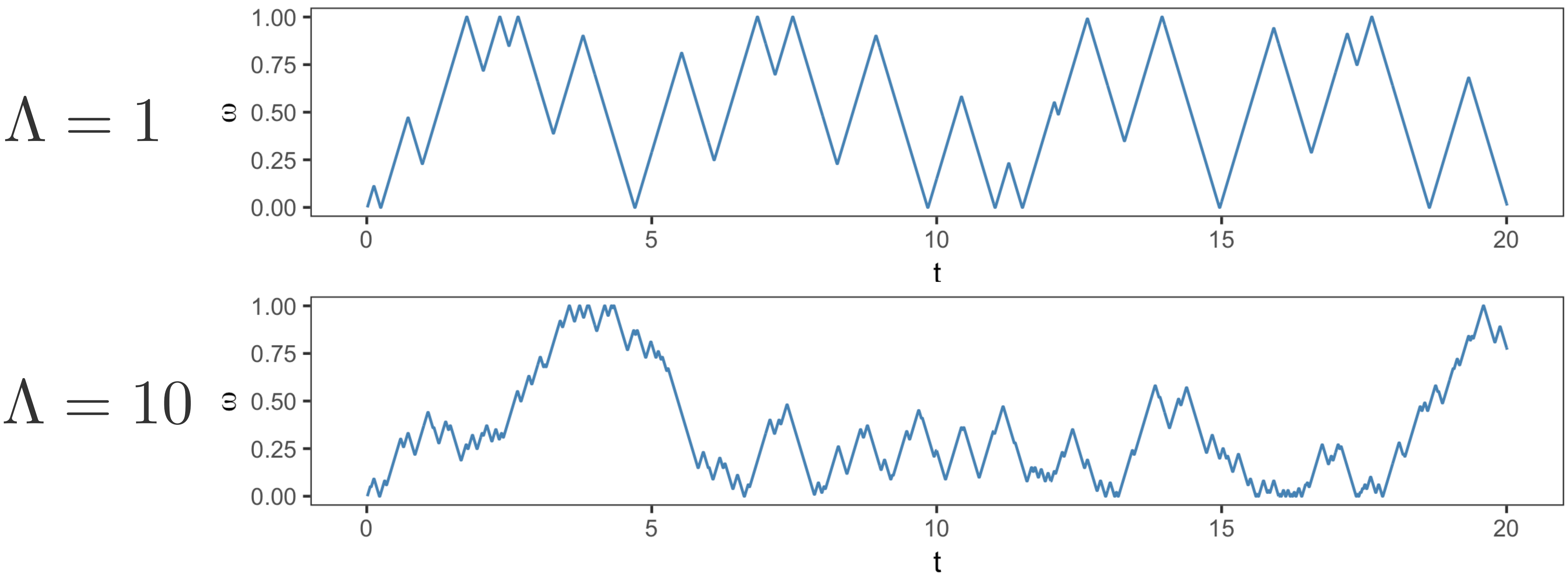

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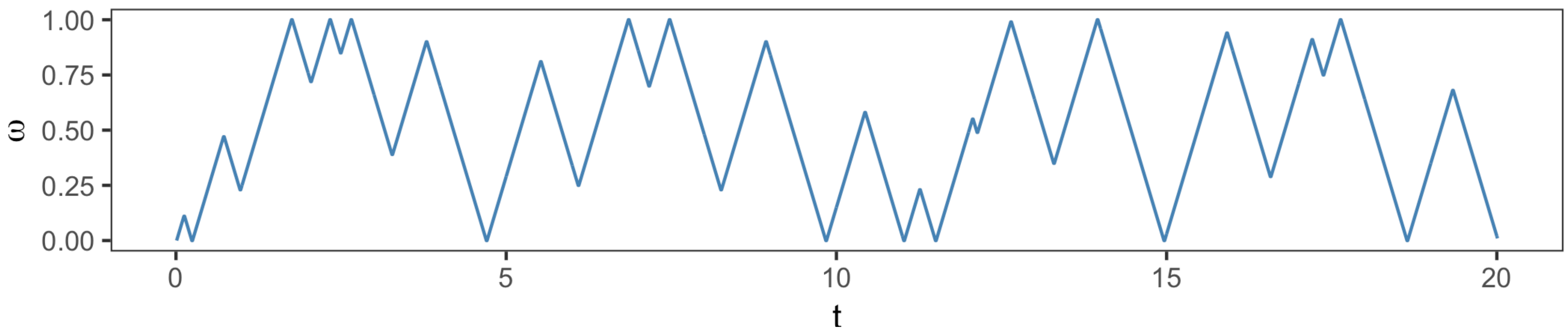

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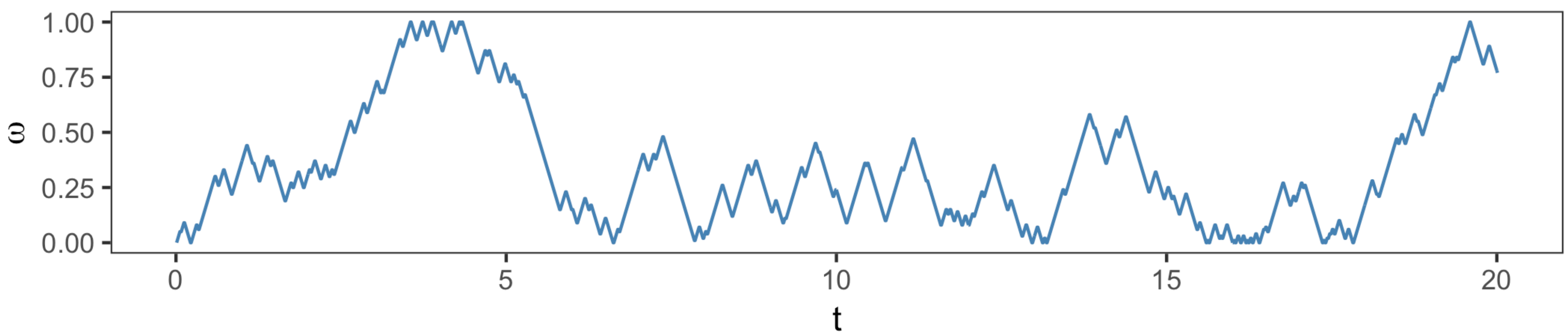

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- As N increases, NRPT stabilizes.
- Asymptotic behaviour of NRPT depends on the annealing path through communication barrier.

COMMUNICATION BARRIER

- **Rejection rate:** $r(\beta, \beta')$ the probability a swap rejected between π_β and $\pi_{\beta'}$

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

Cumulative rejection rate along path

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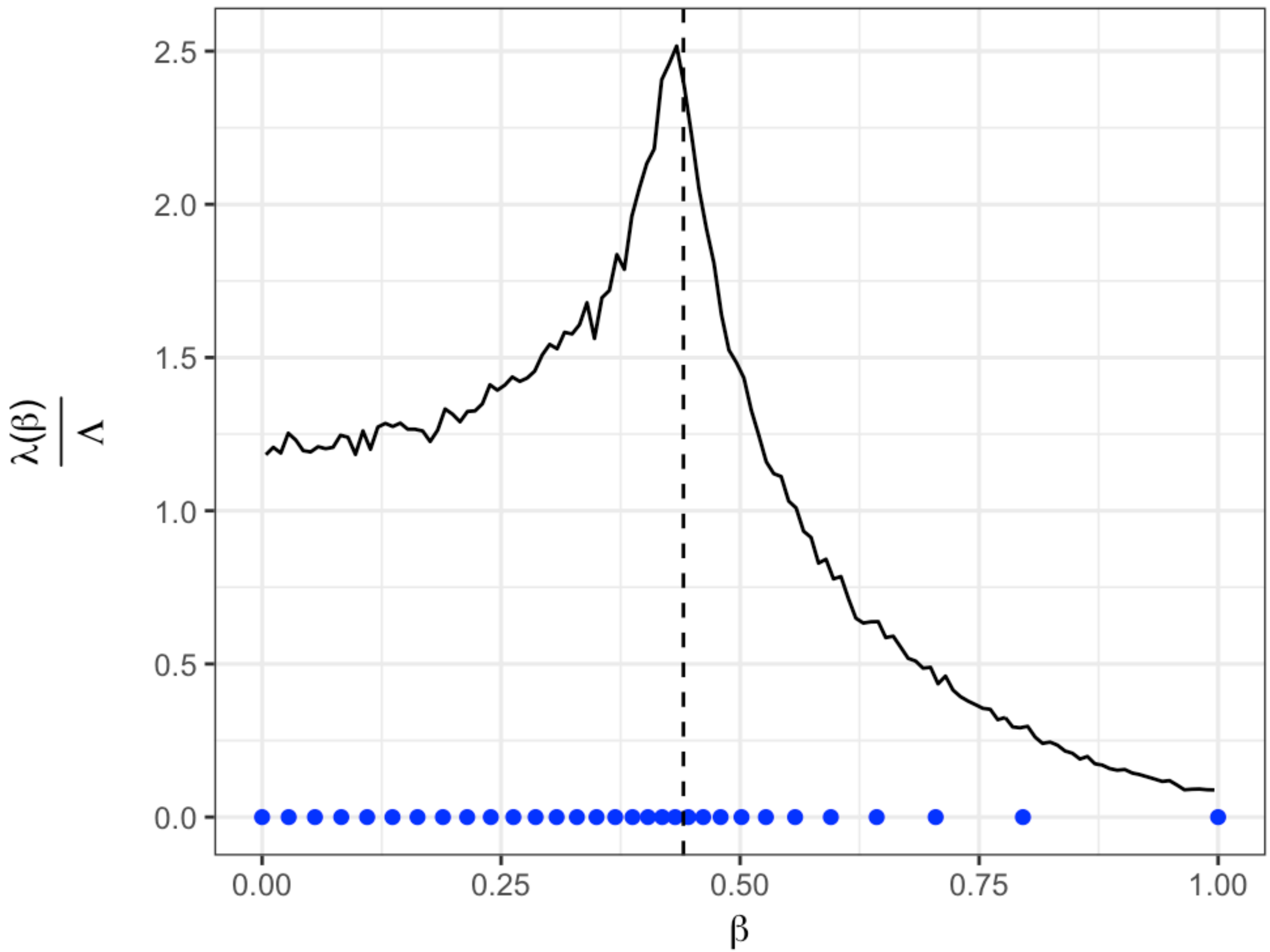
- Theorem implies:

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

EXAMPLE ISING MODEL



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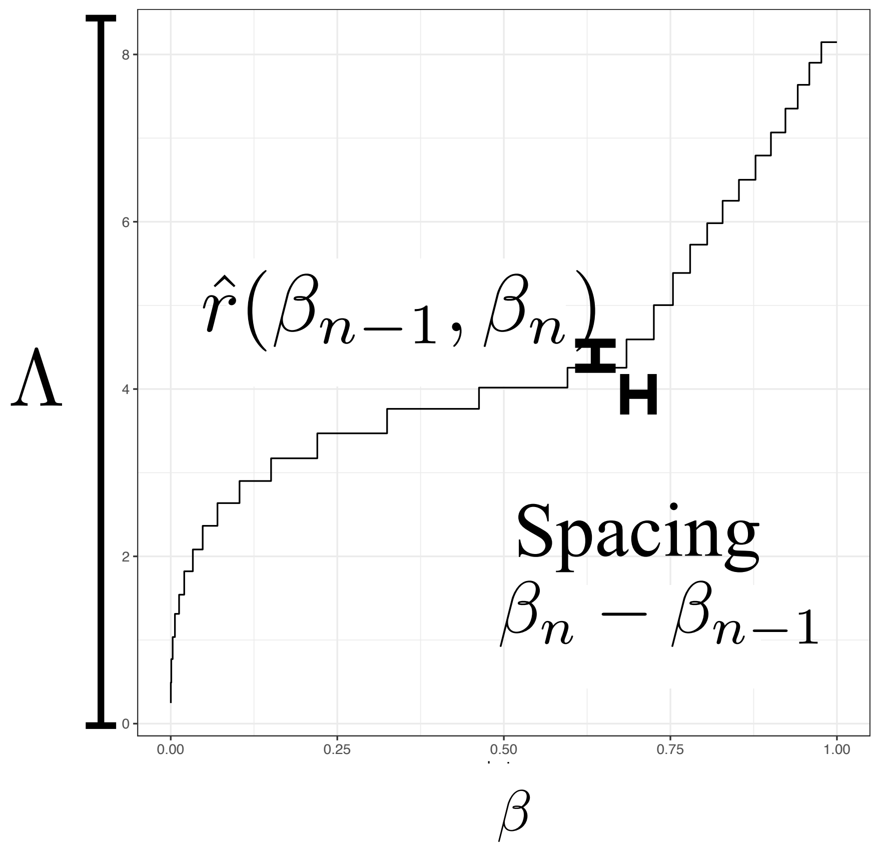

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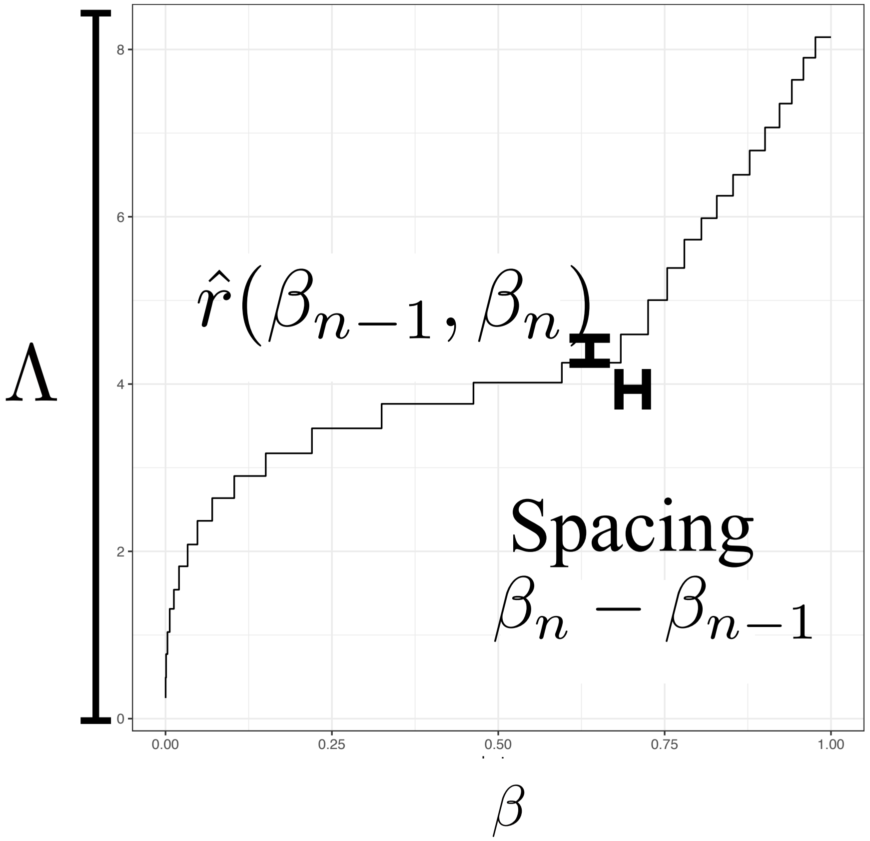

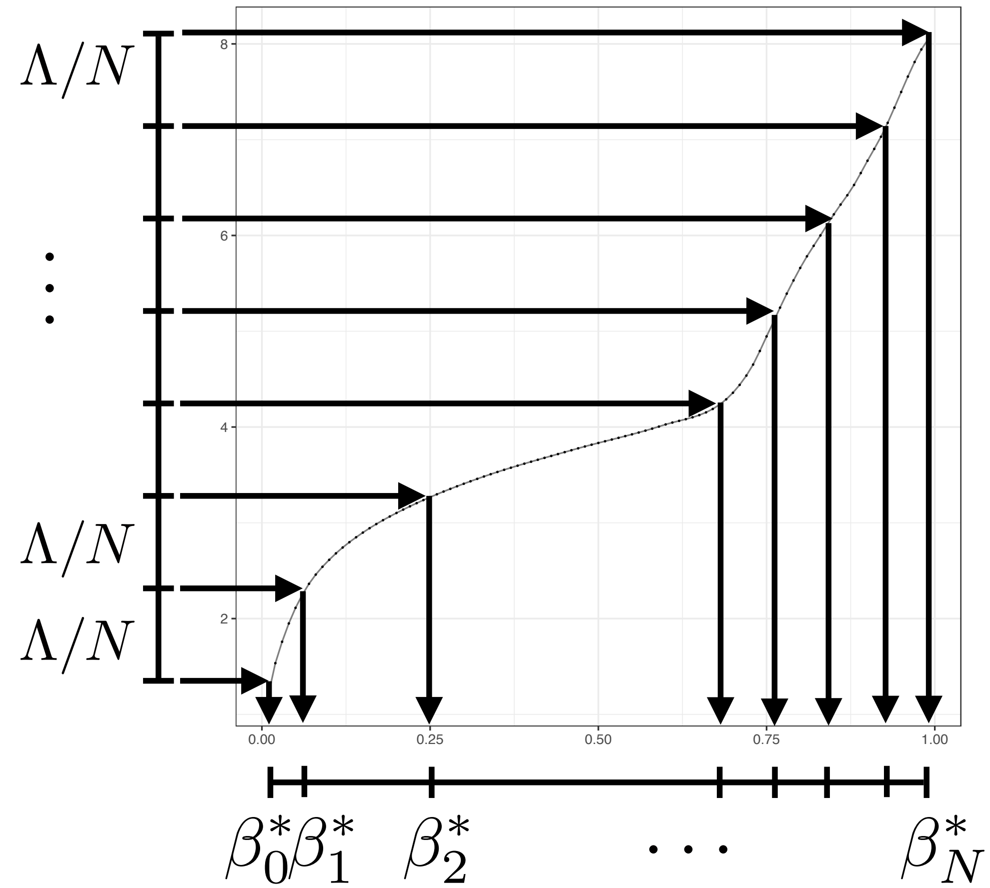

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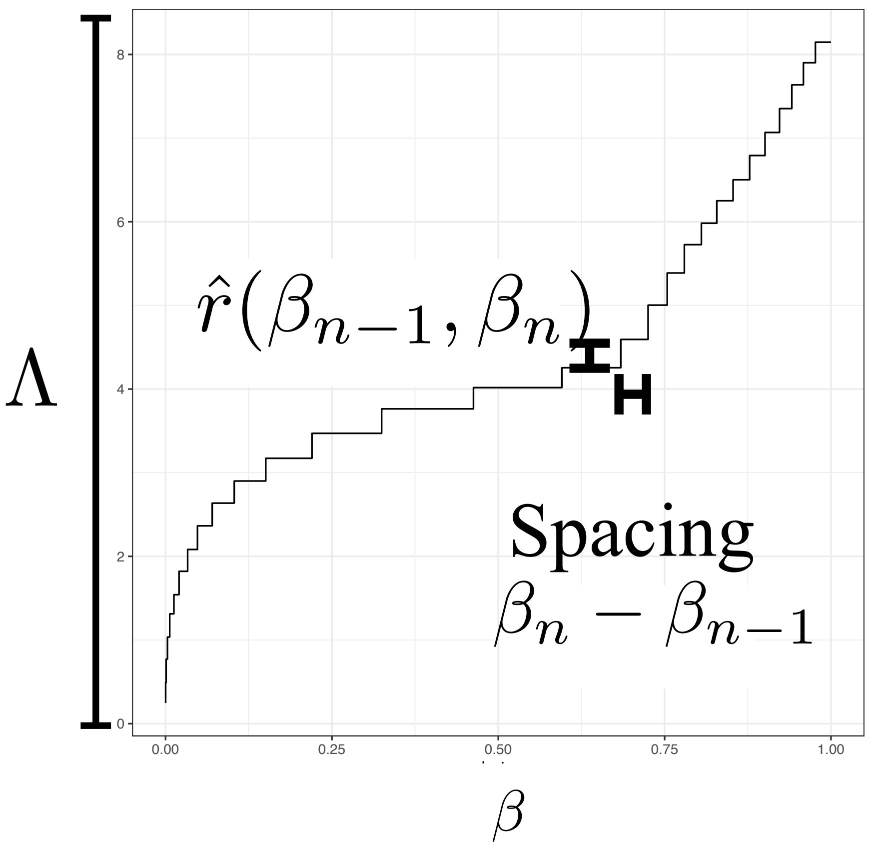

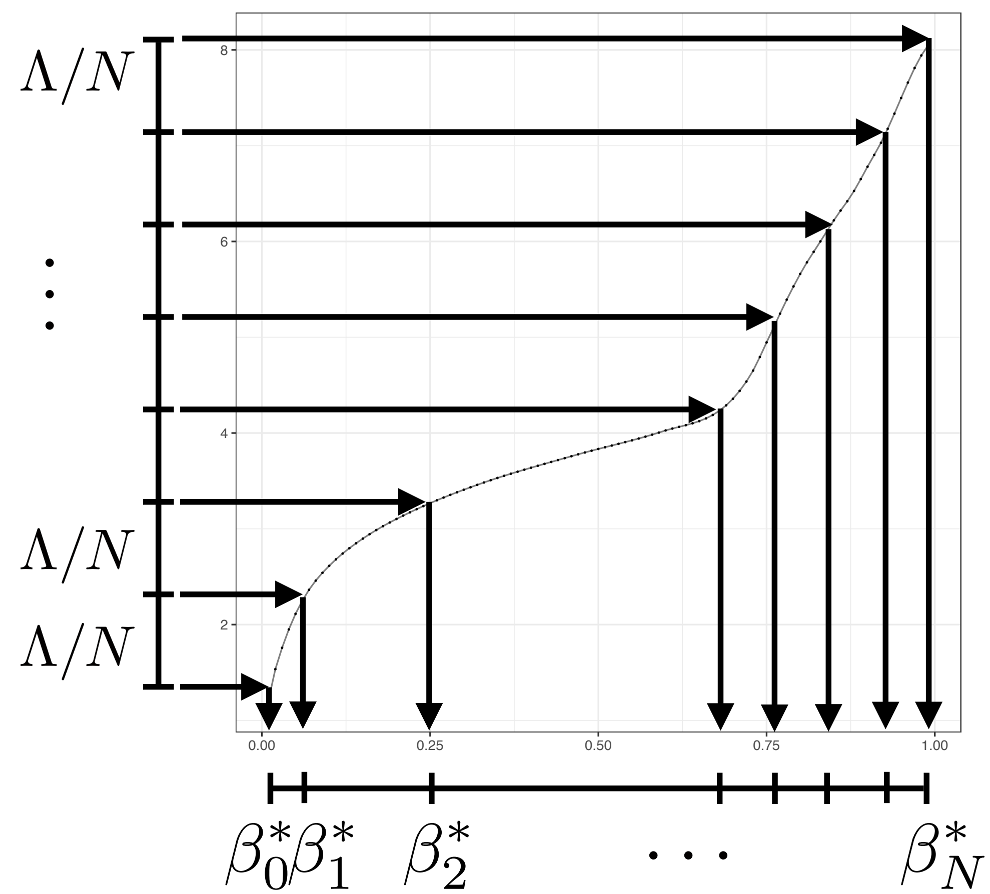

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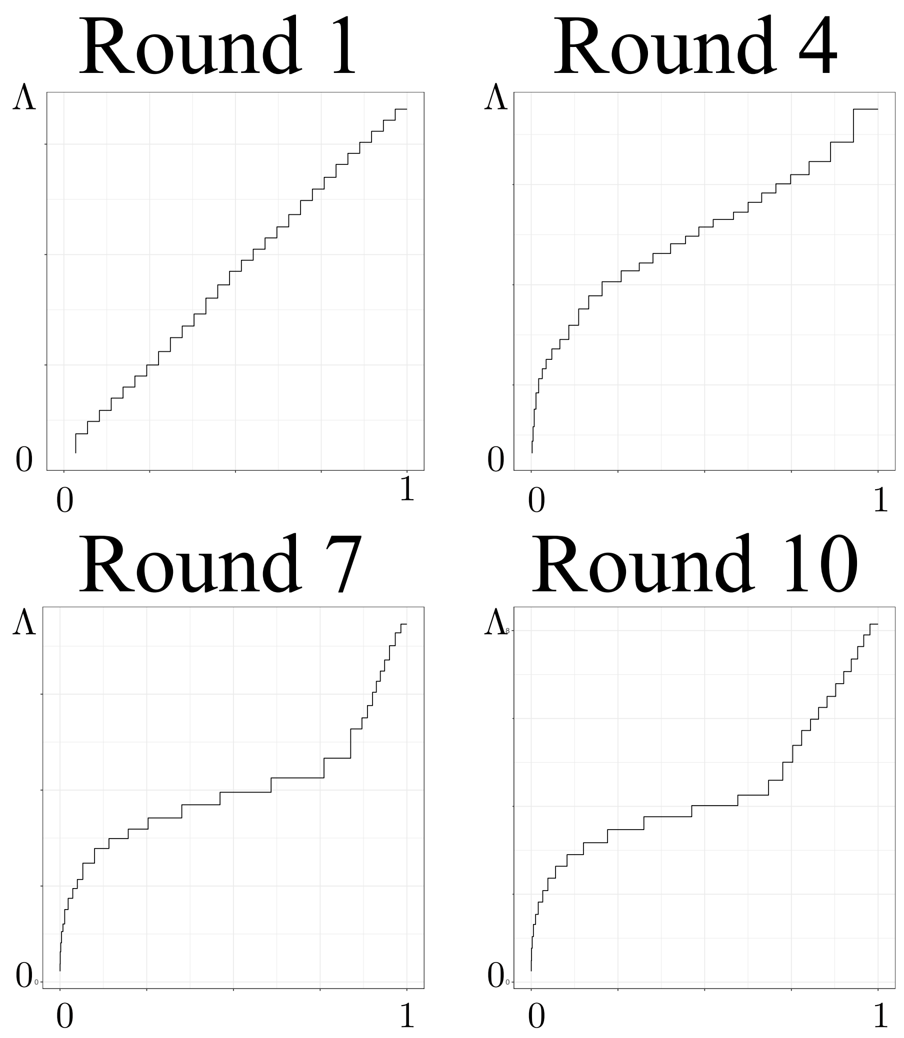
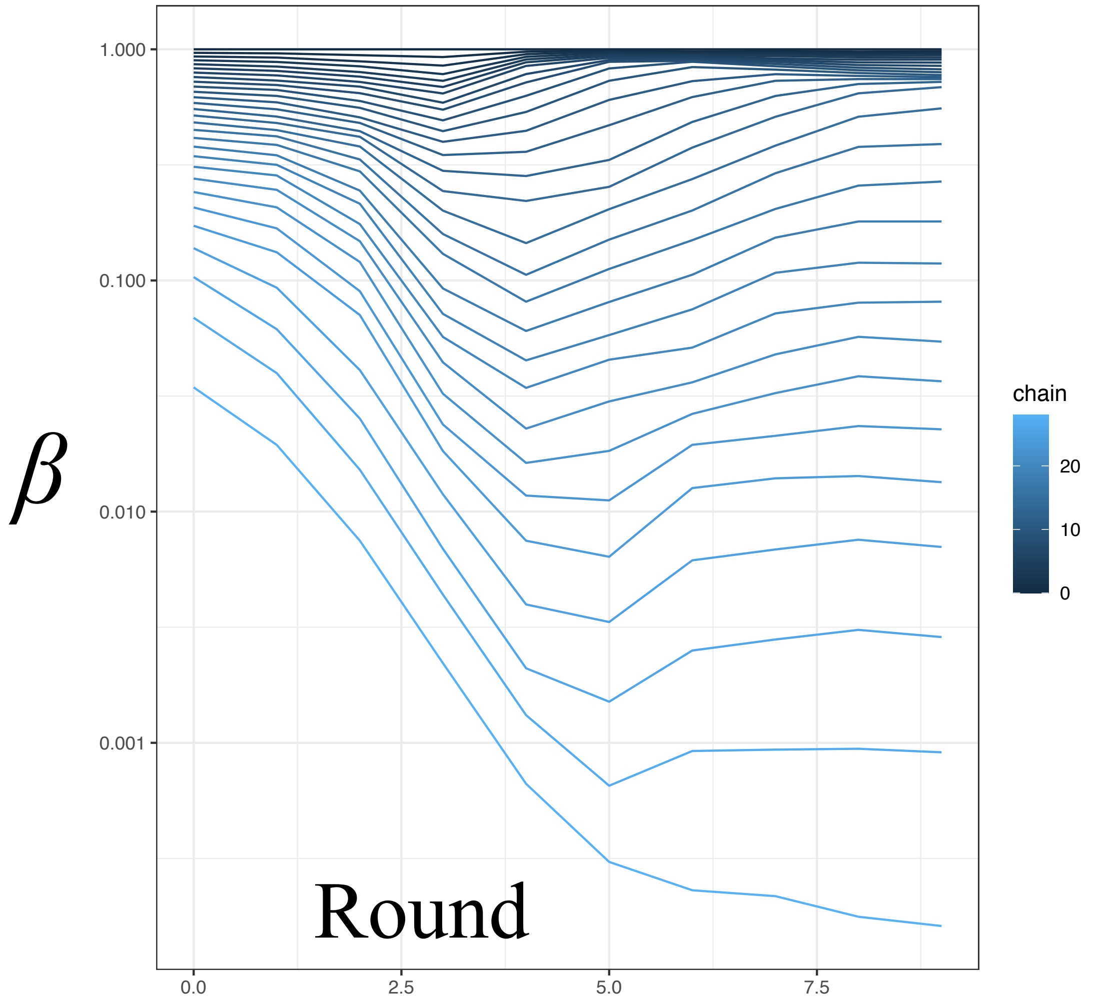
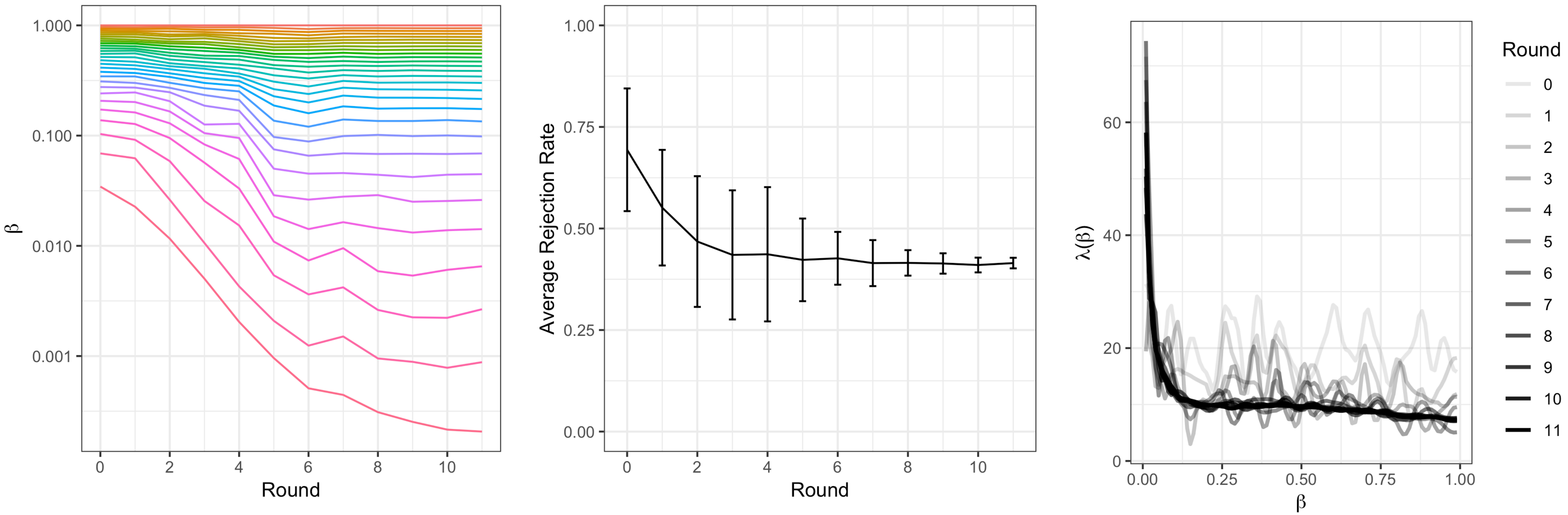


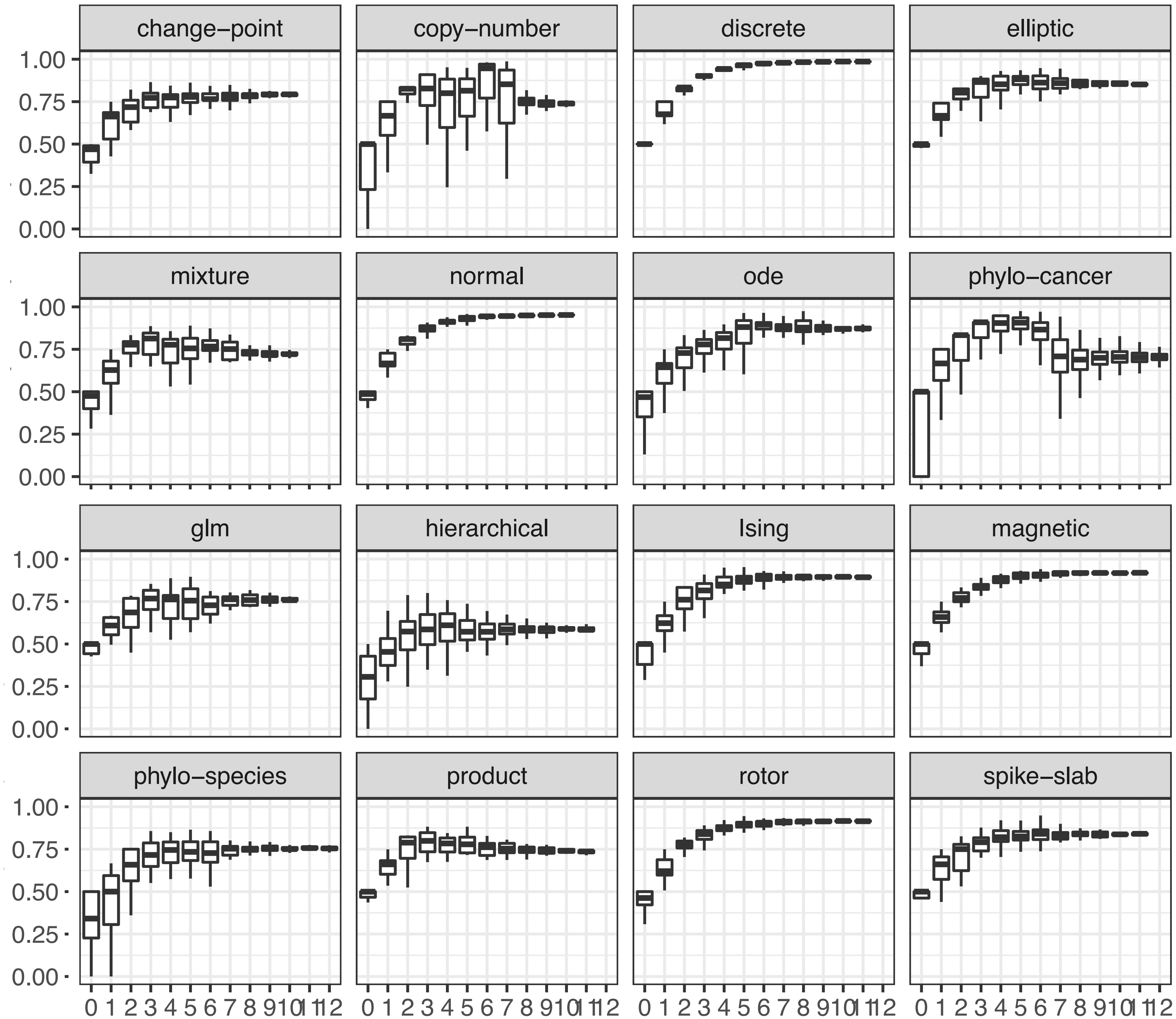


HIERARCHICAL BAYESIAN MODEL (D = 369)



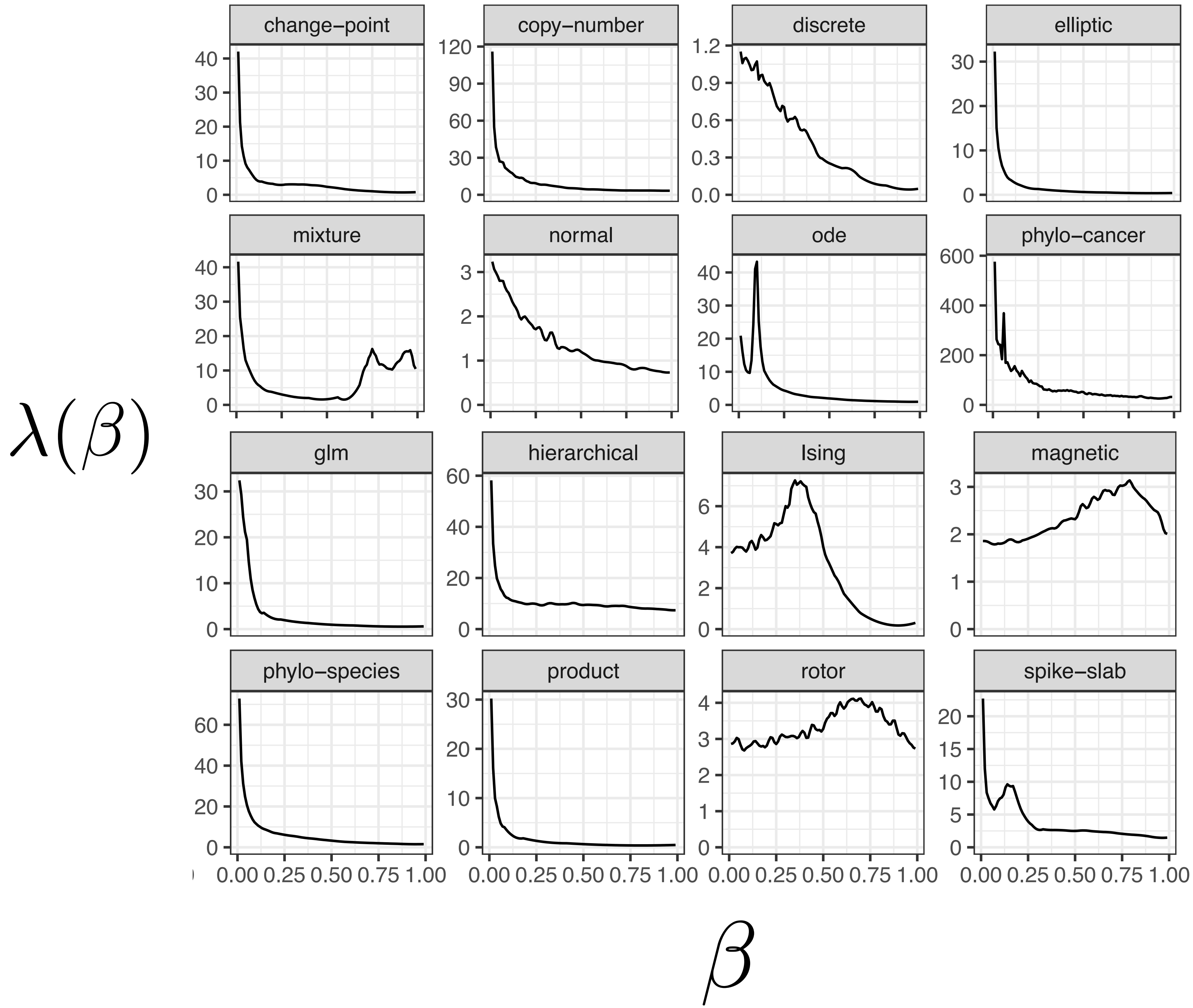
NRPT IN PRACTICE

Acceptance rates



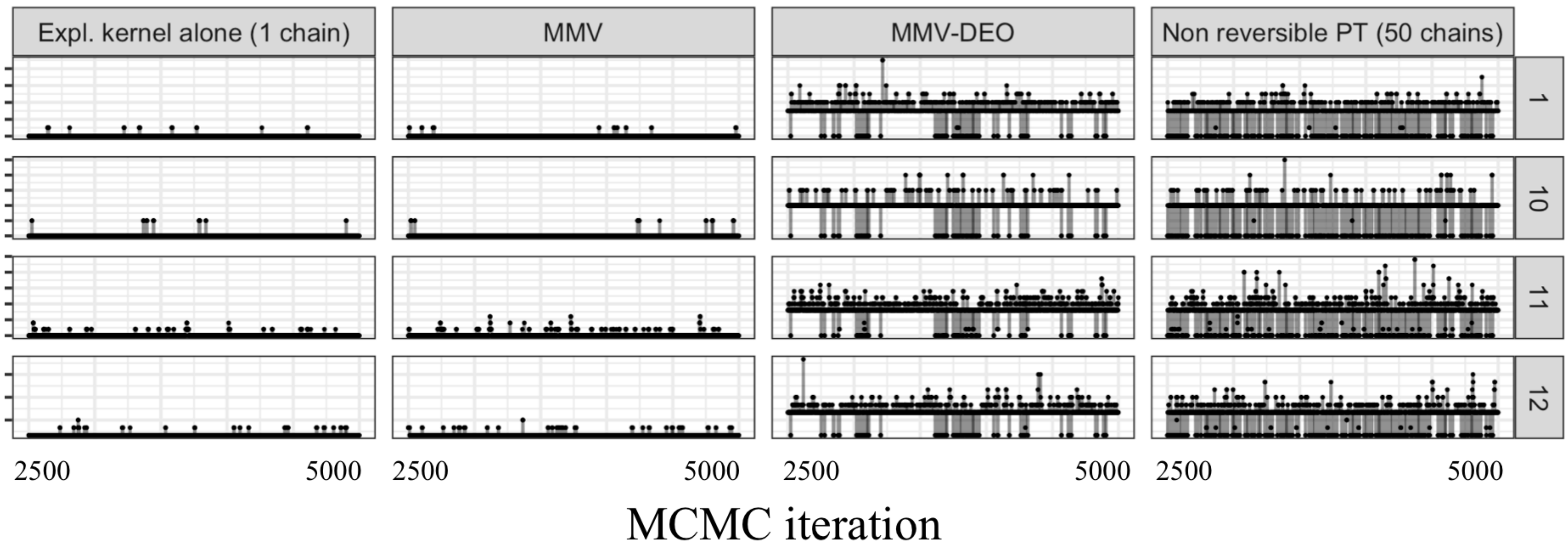
Round

LOCAL COMMUNICATION BARRIER



EXAMPLE: COPY NUMBER INFERENCE (D = 30)

1 Chain | Reversible PT | Reversible PT + Schedule Tuning | Non-Reversible PT + Schedule Tuning



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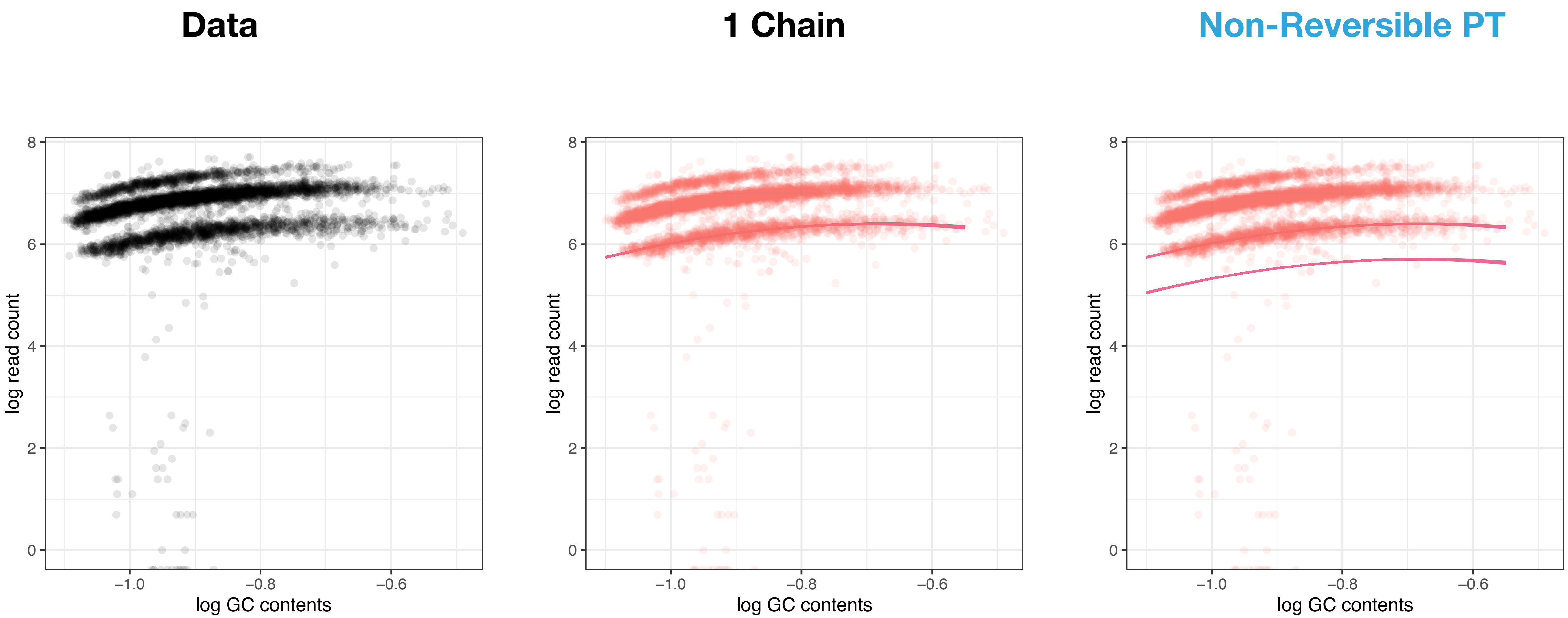
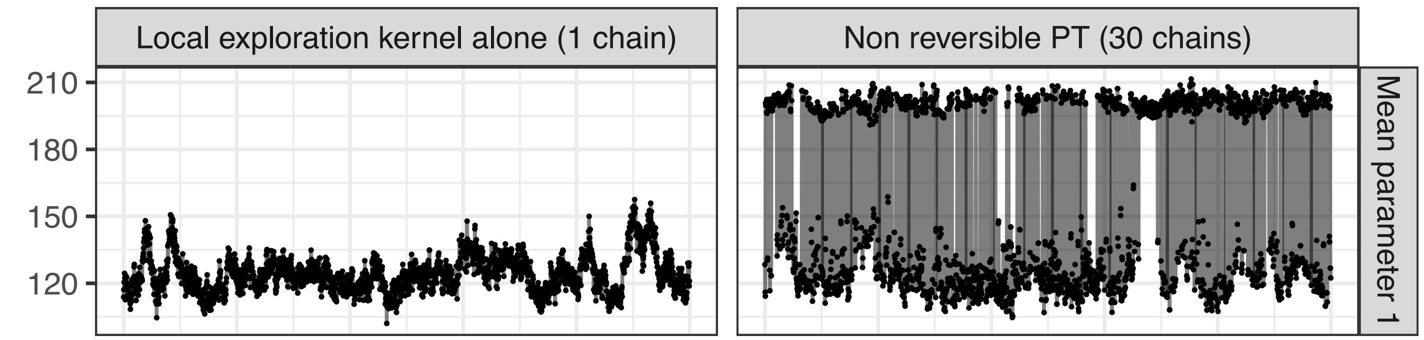
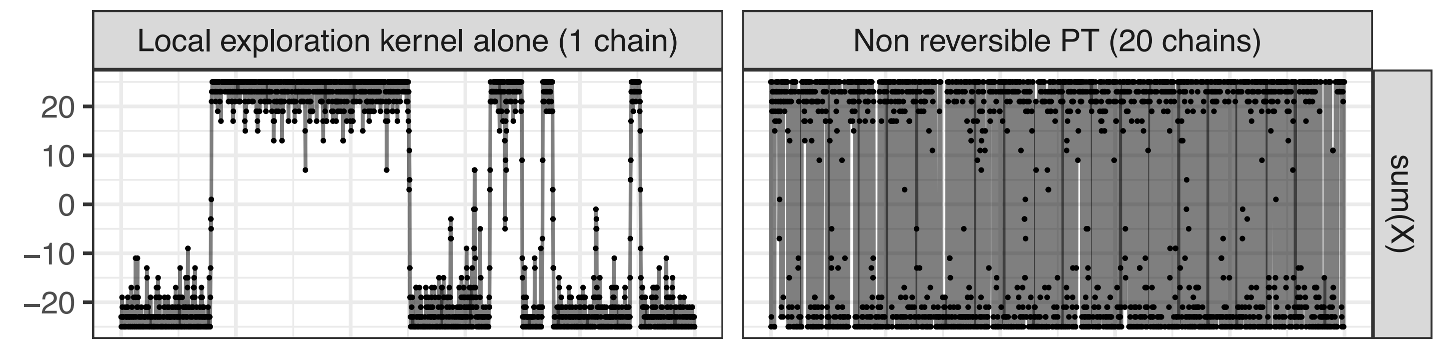


EXAMPLE: MULTIMODAL TARGETS

Bayesian Mixture Model
(d = 155)



Ising Model
(d = 25)



Copy number inference
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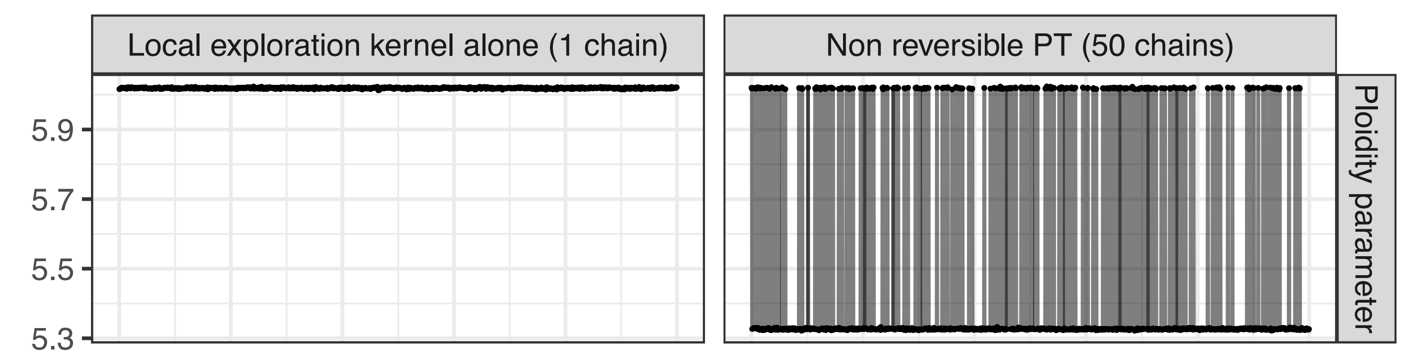
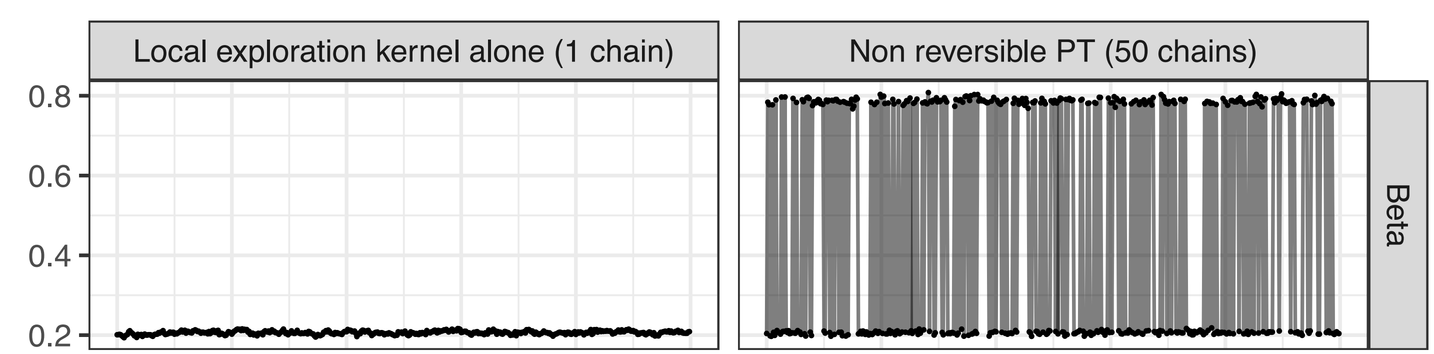


ODE parameter inference
(d = 9)



COMPARISON TO STATE OF THE ART

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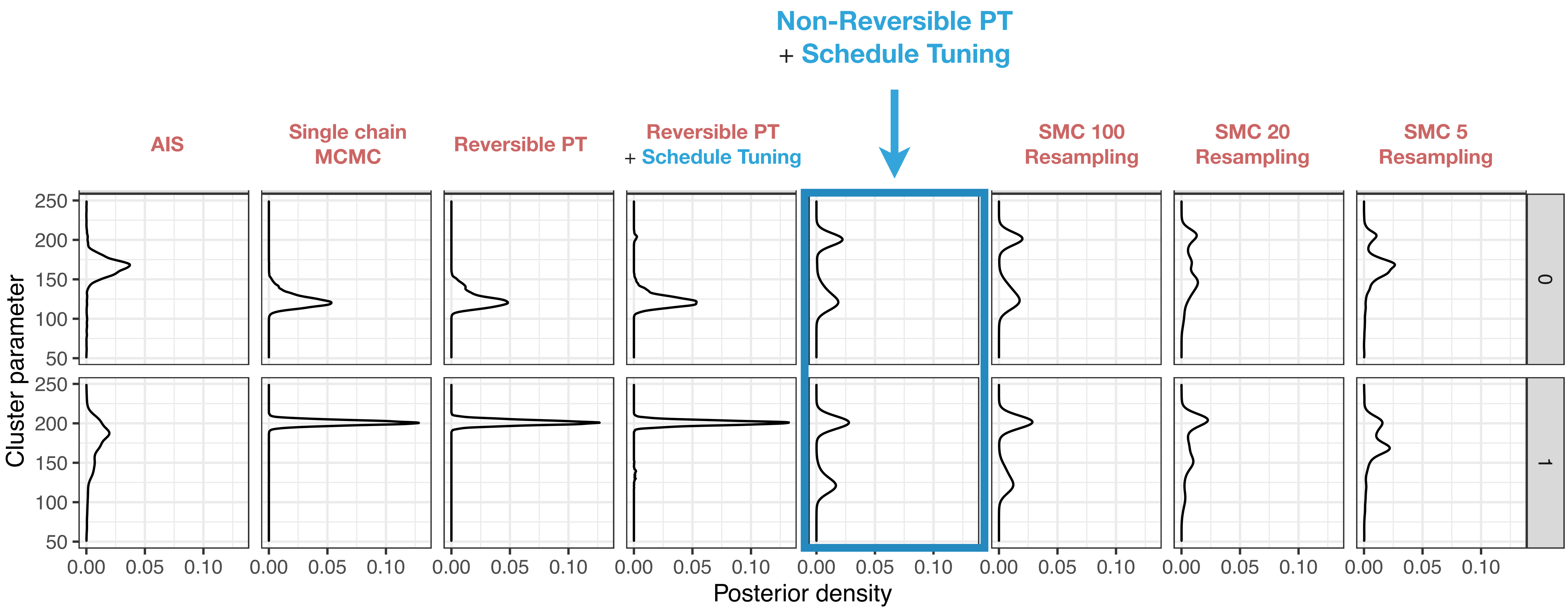
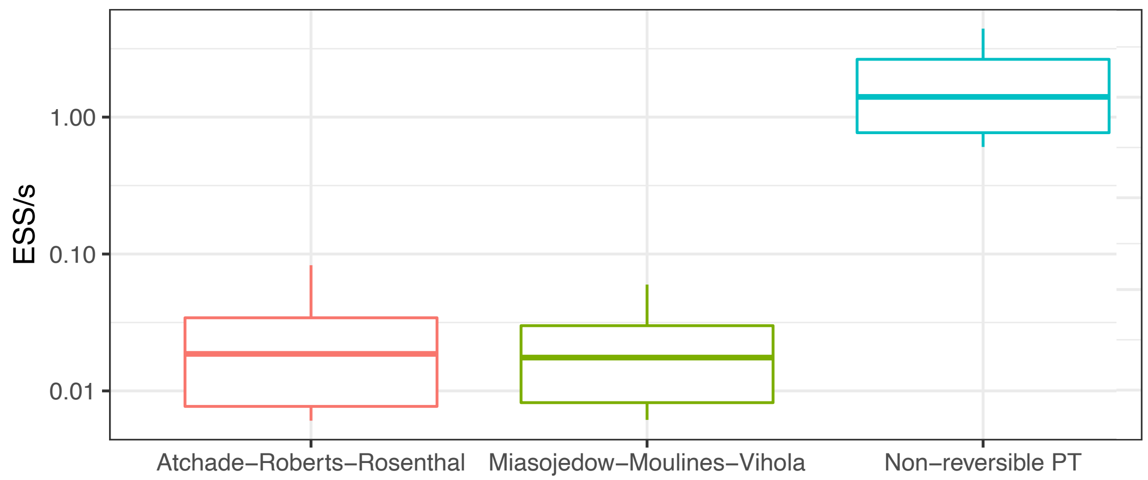


ESS COMPARED TO REVERSIBLE PT

Spike–and–Slab (RMS Titanic passengers dataset)



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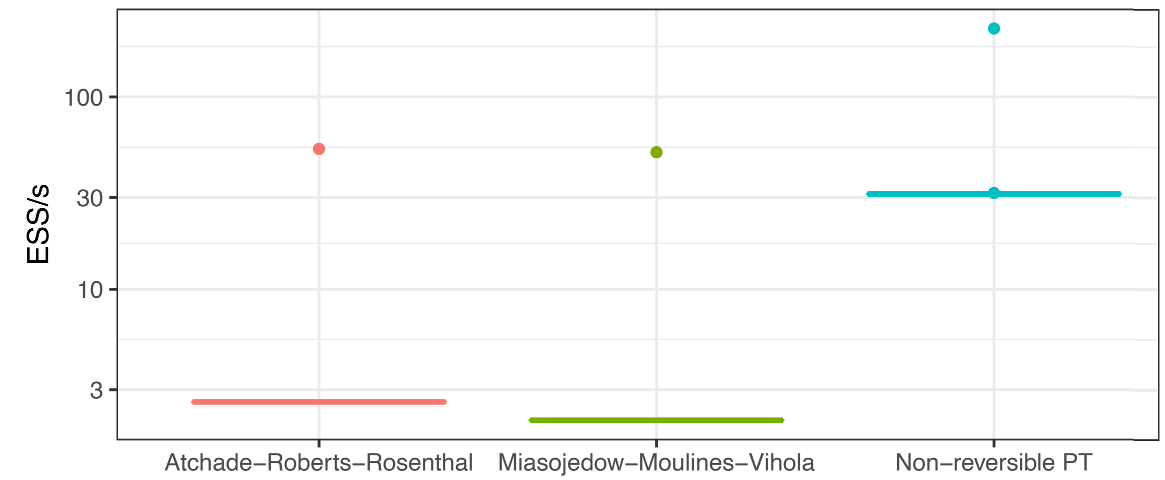
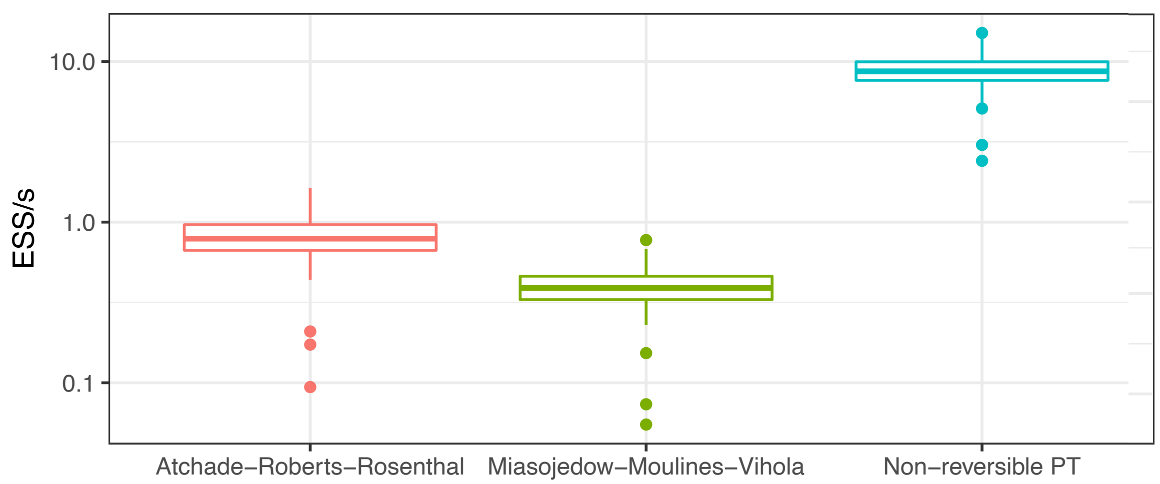


Hierarchical model (rocket launches dataset 1957–2017)



Wright–Fisher SDE

State of the art for Reversible PT

Non-Reversible PT

APPLICATIONS

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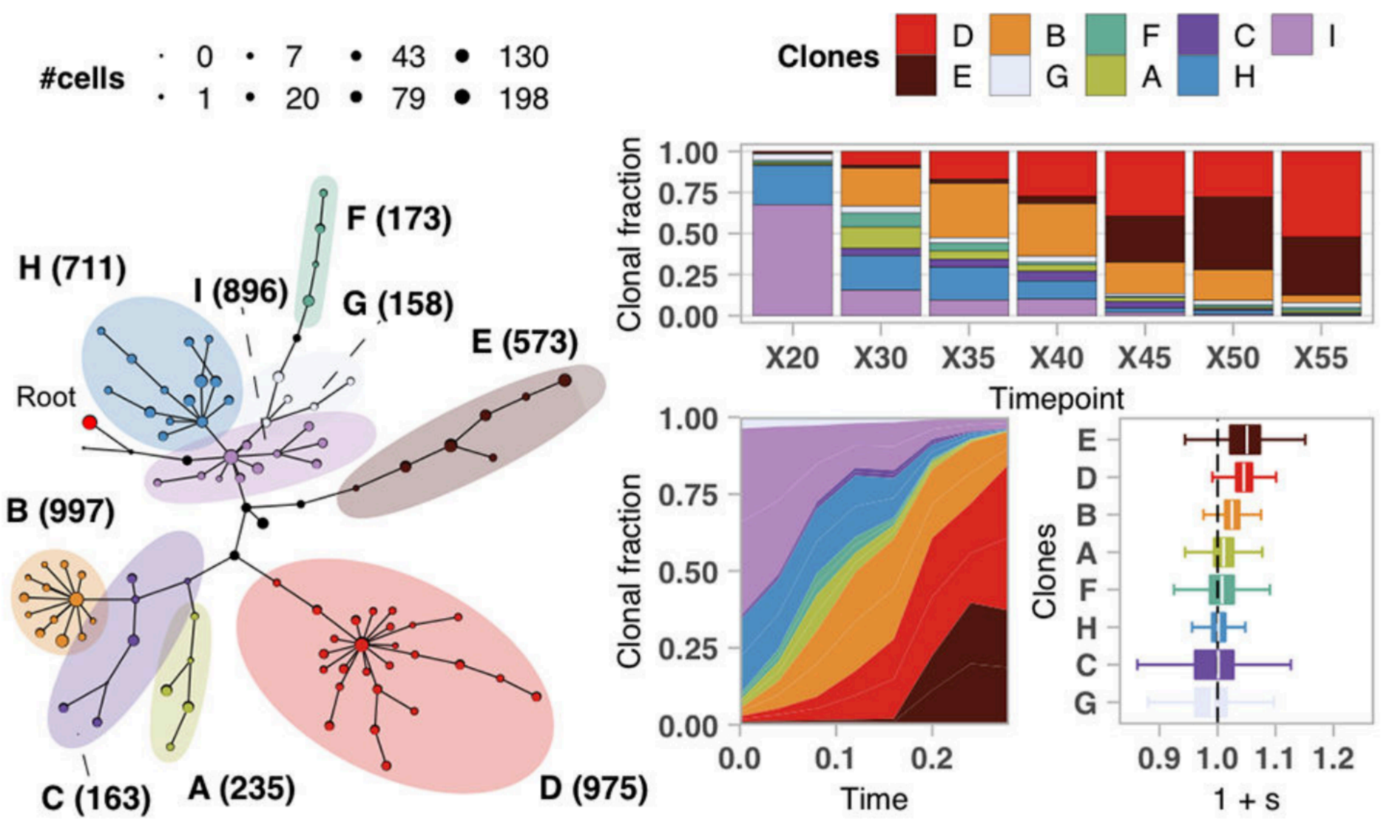
- BC Cancer Research Center and MSK used NRPT to model time-series of single-cell cancer genomes
  (Dorri et al 2020, Salehi et al, 2021) in Nature



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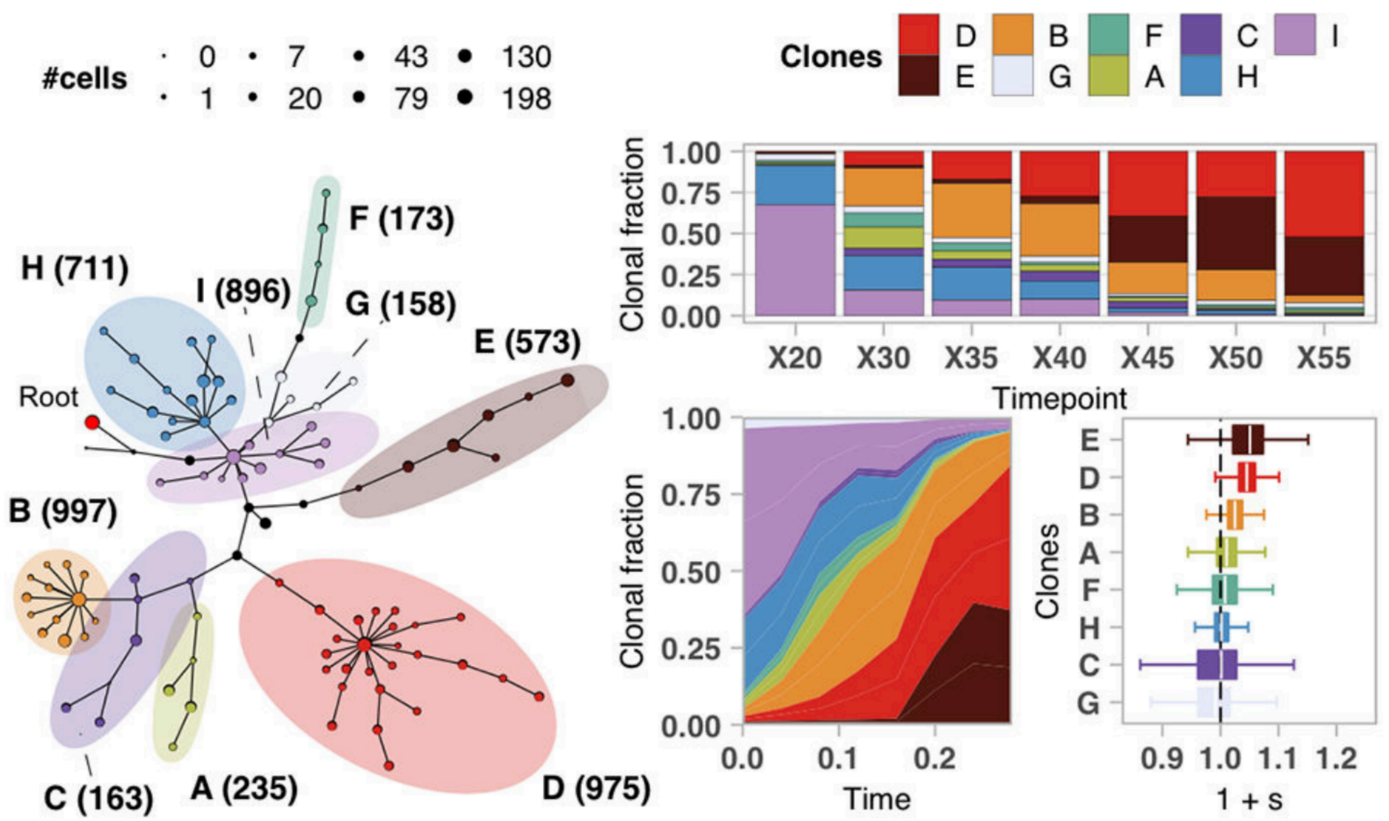

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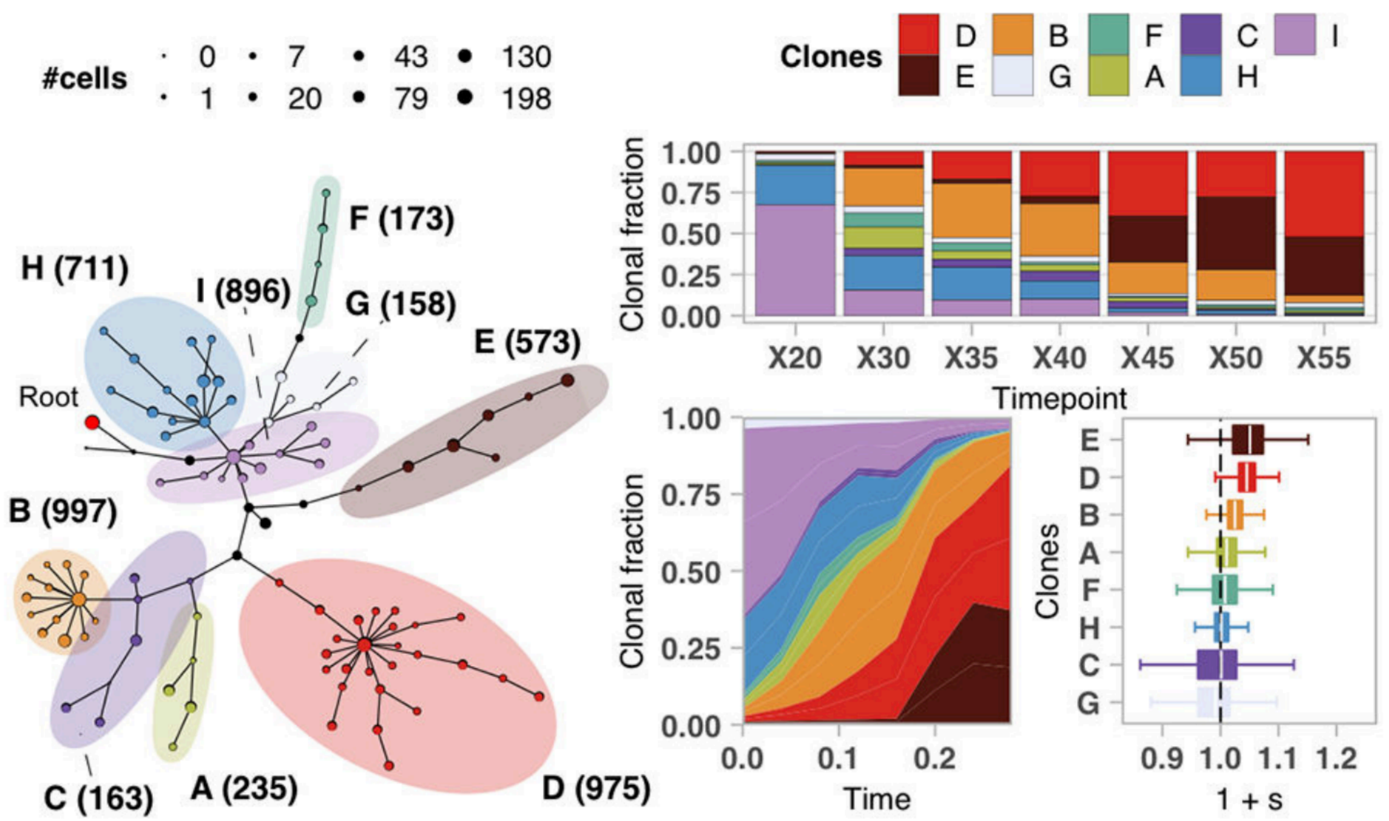

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- Google research used NRPT for tackle ill-conditioned Bayesian inverse problems applied to nuclear fusion *(Langmore, et al 2021)*

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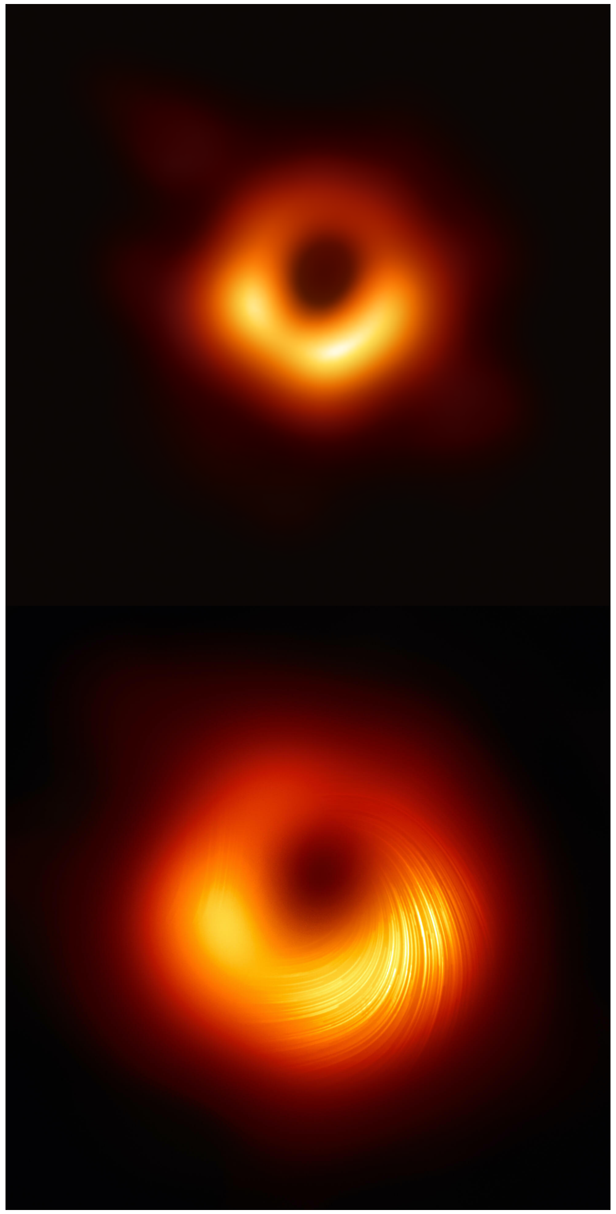

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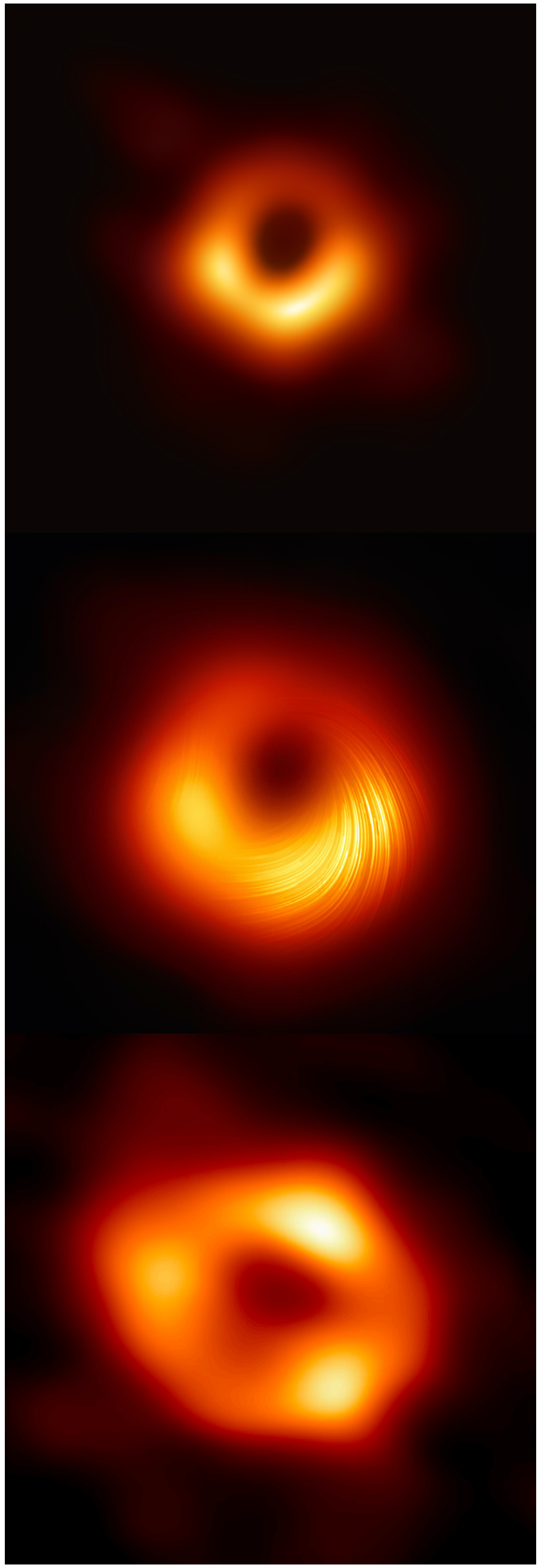
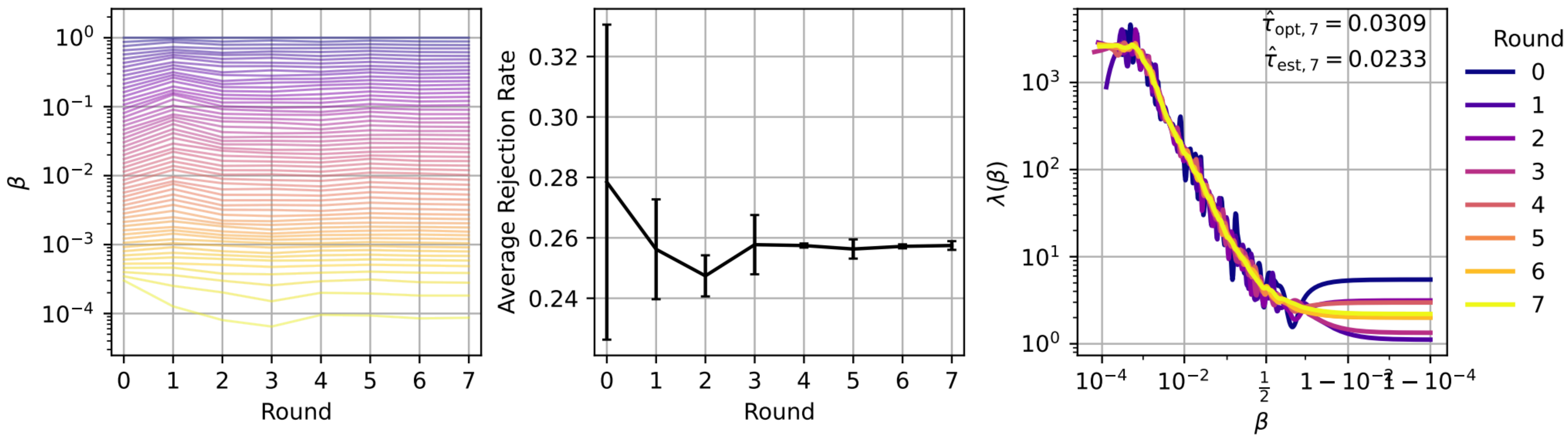
- NRPT used to capture photo of Sagittarius A*, the suppermassive blackhole in center of Milky Way
  (EHT, 2022)



NRPT FOR BLACK HOLE PHOTO



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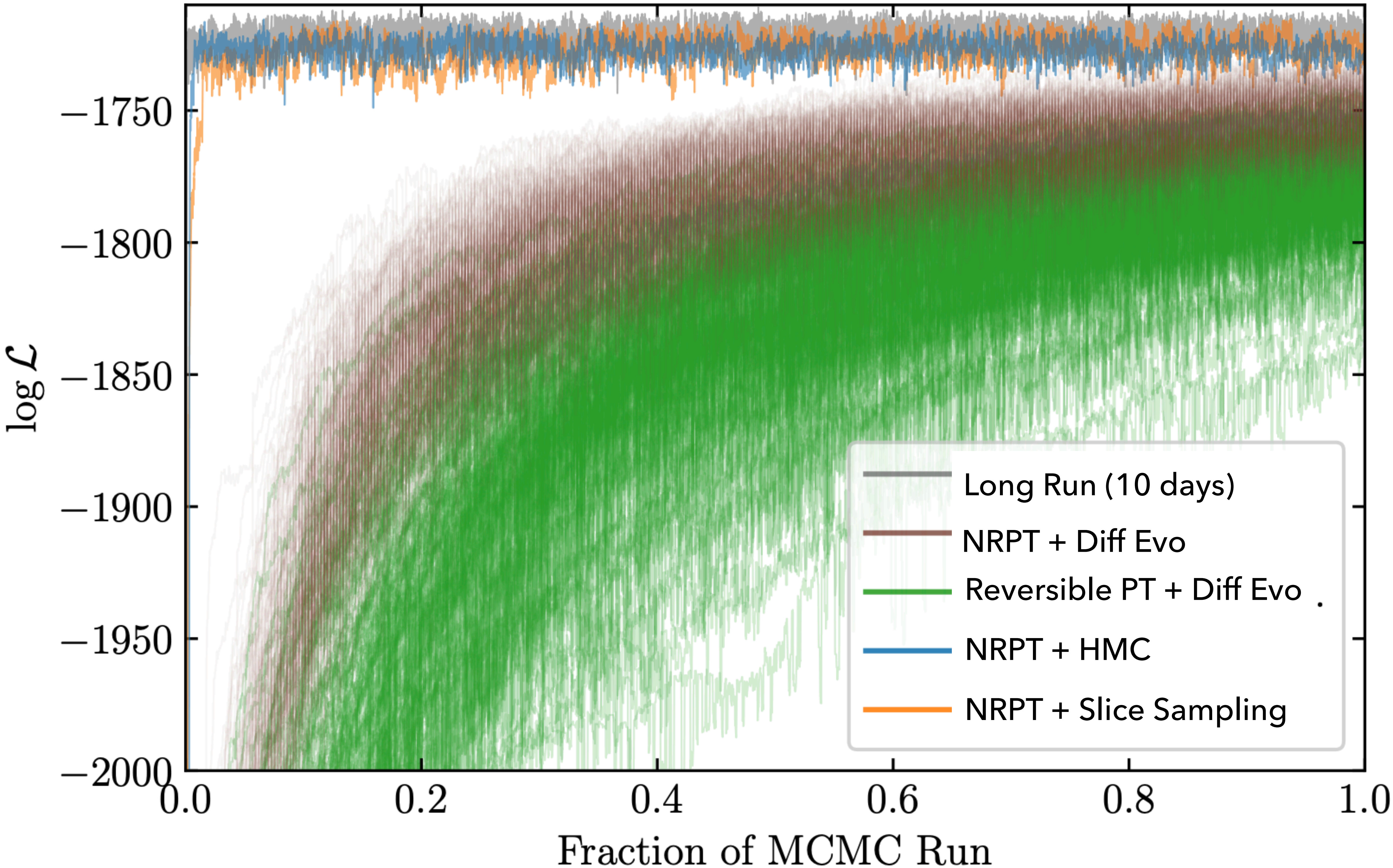

REJECTION RATE AS A DIVERGENCE

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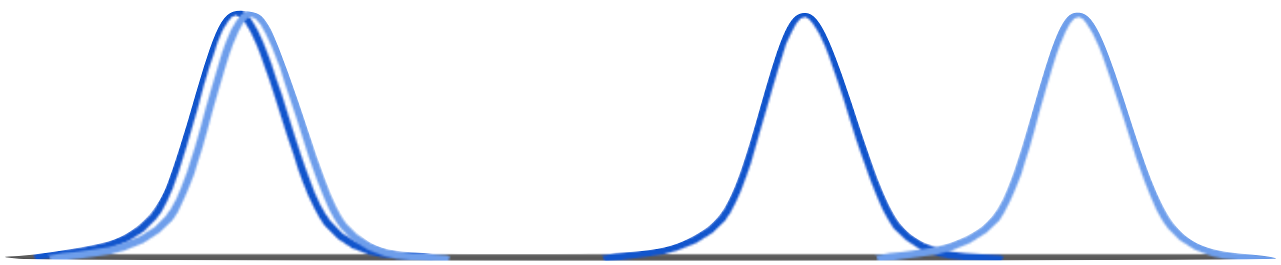

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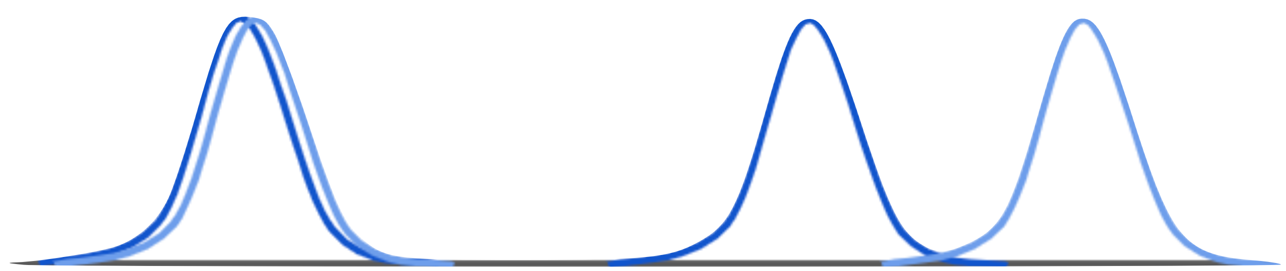

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$$r_n = r\left(\pi_{\beta_{n-1}}, \pi_{\beta_n}\right)$$

$$r(p,q) = \|p \times q - q \times p\|_{\mathrm{TV}}$$

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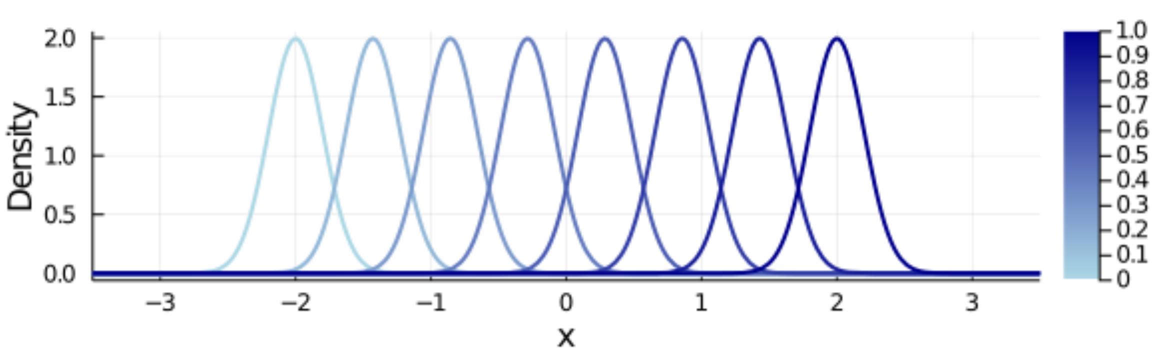

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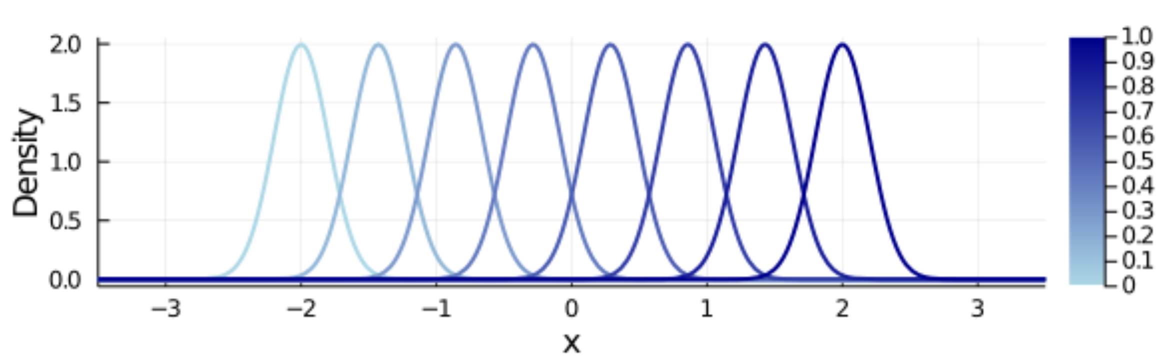
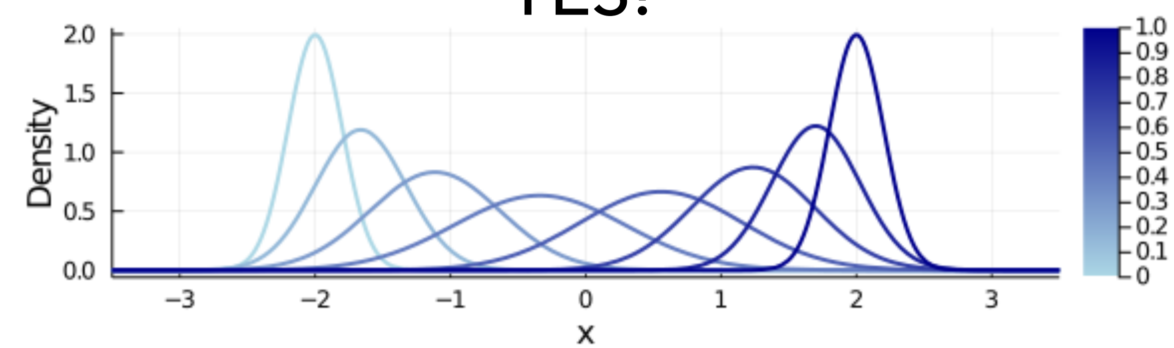


YES!



ANNEALING PATHS ON PARAMETRIC FAMILIES

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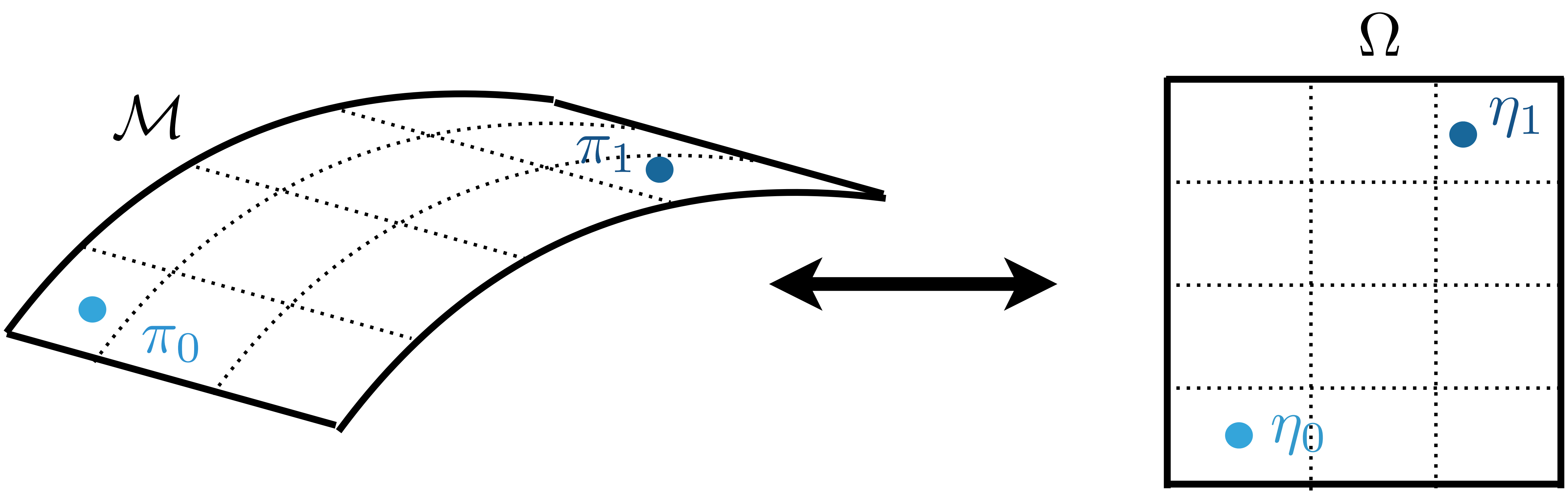

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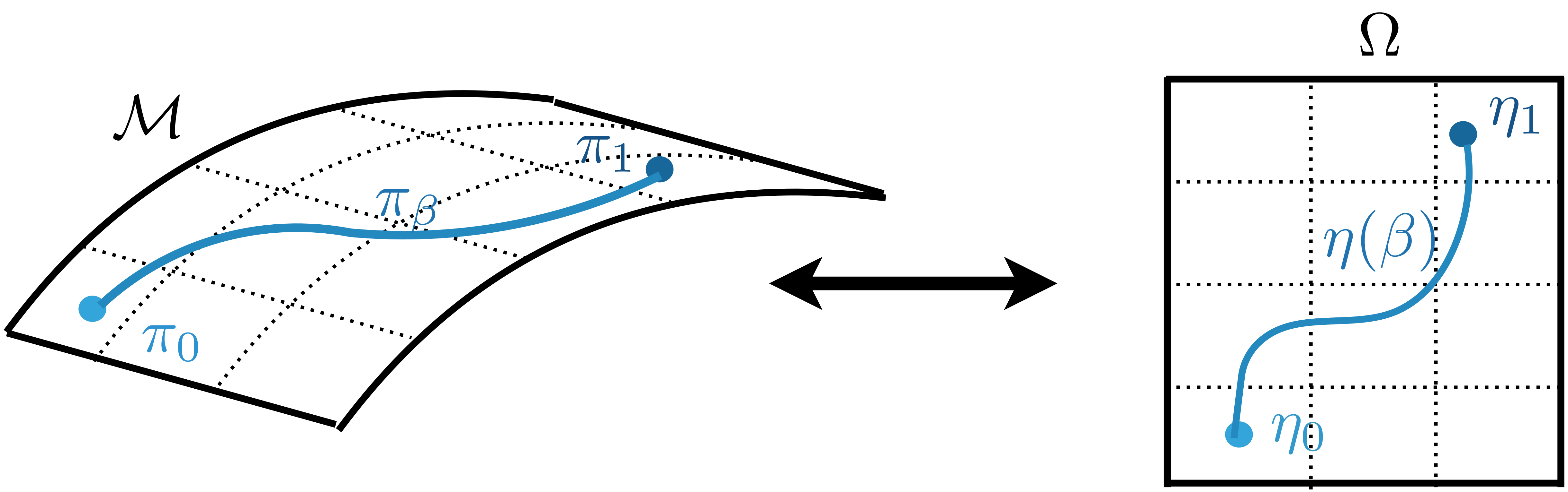
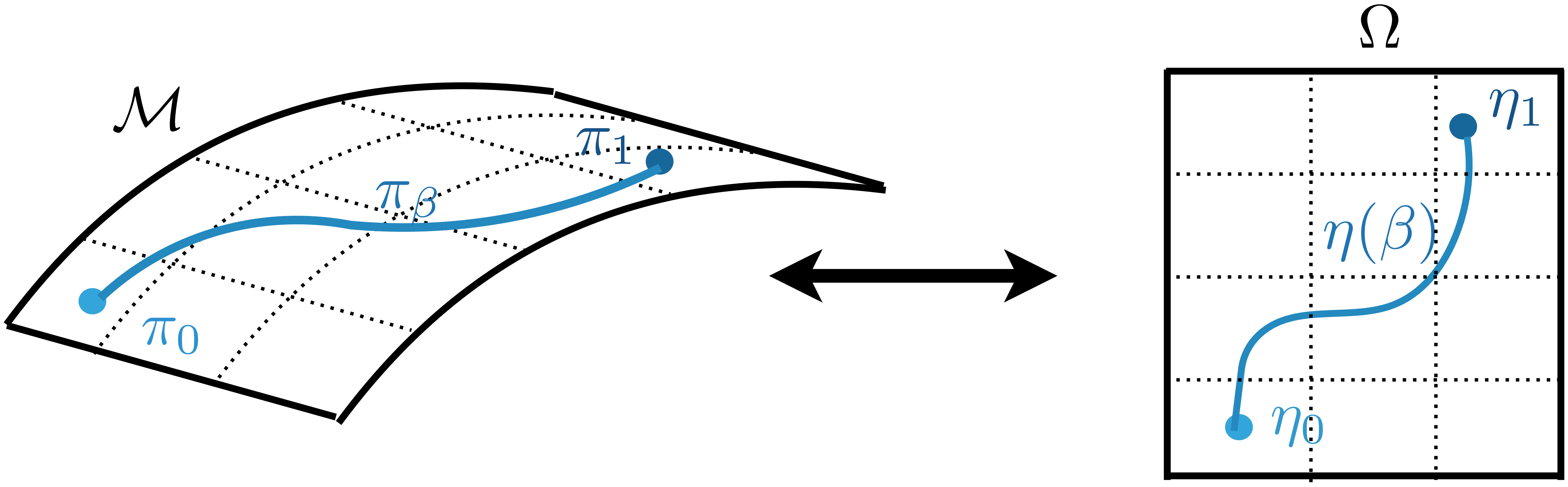


DIFFERENTIABLE ANNEALING PATHS



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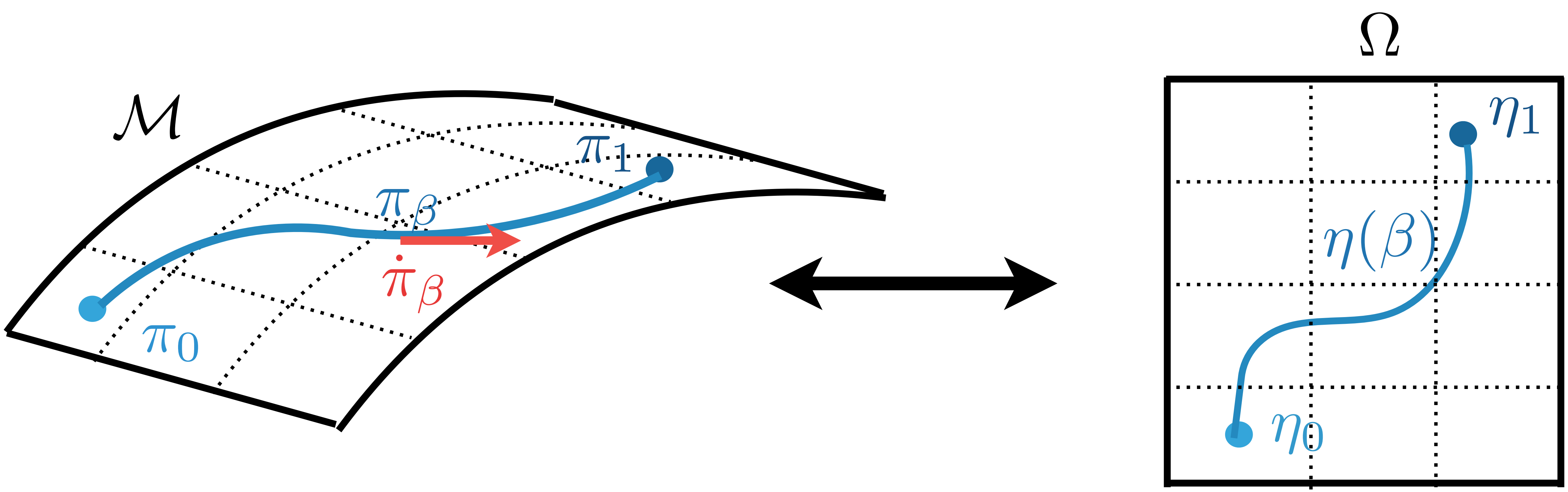

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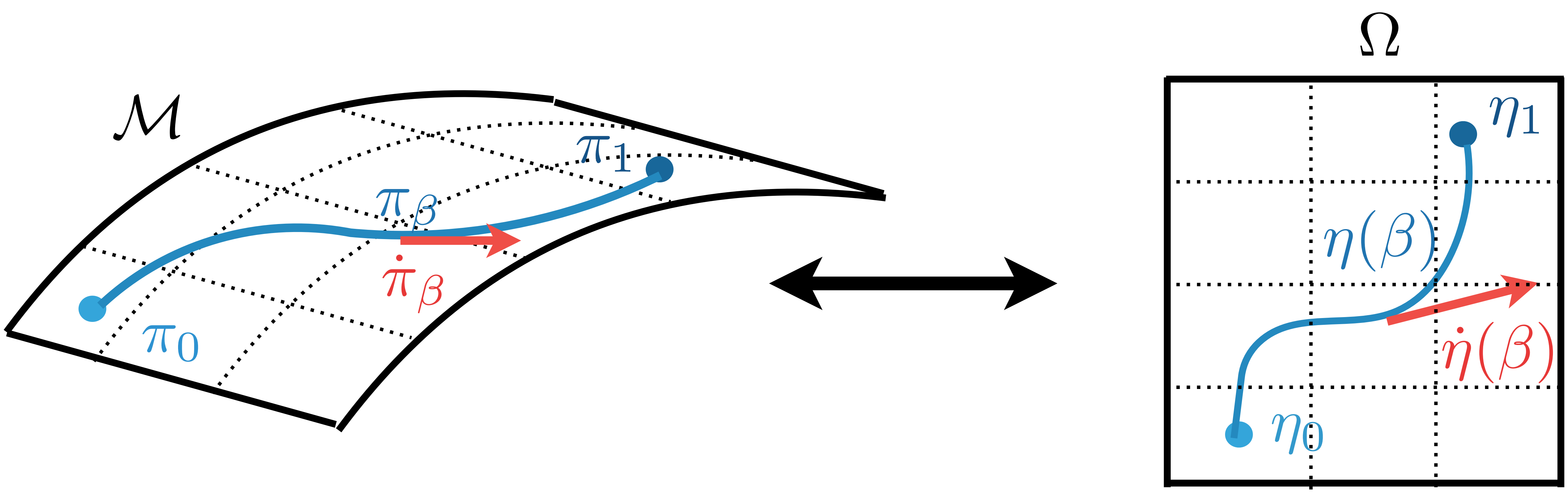
- Differentiable annealing paths in $\mathcal{M}$ are in bijective correspondence to differentiable parametric paths in Ω via chain rule.

$$\dot{\pi}_\beta = \dot{\eta}(\beta)^T S_{\eta(\beta)} \qquad S_\eta(x) = \nabla_\eta \log p_\eta(x)$$



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Theorem: Local and global communication barriers are "speed" and "length" of the path

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- We can find geodesics in Riemannian manifold $(\mathcal{M}, g)$, where g is the Fisher information metric

$$\lambda(\beta)^2 \leq \dot{\pi}_\beta^T g_{\pi_\beta} \pi_\beta \qquad\qquad g_p(\dot{p}) = \mathrm{Var}_p(\dot{p})$$

EXAMPLE GAUSSIAN

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- For example univariate Gaussians:

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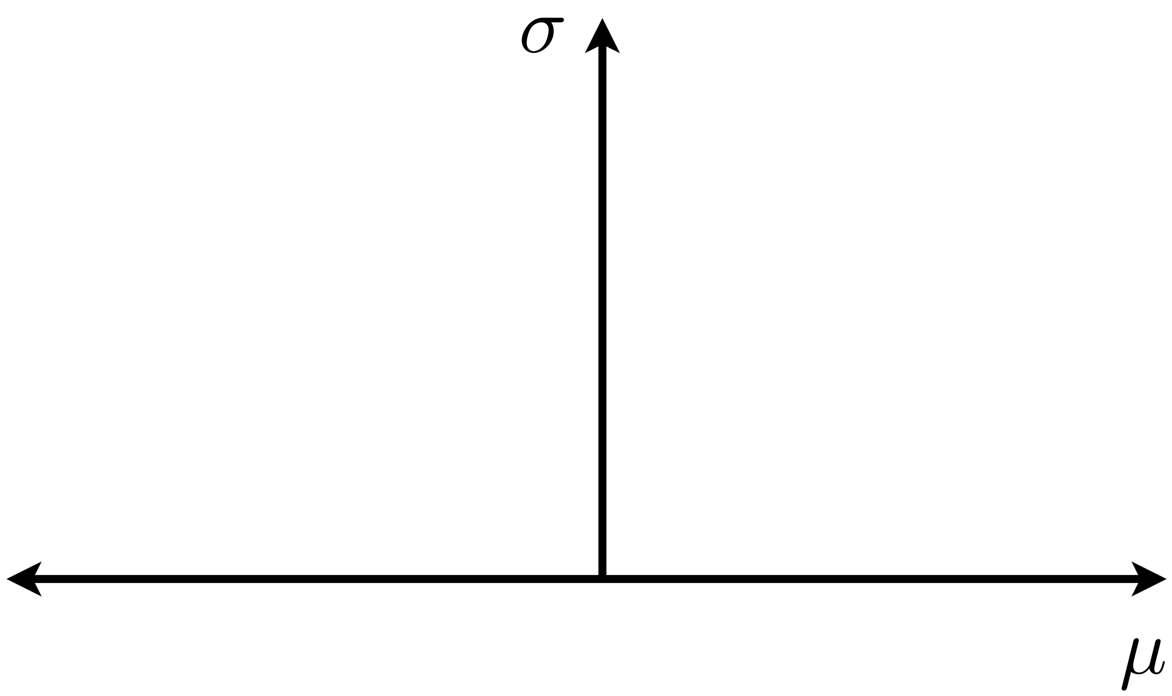

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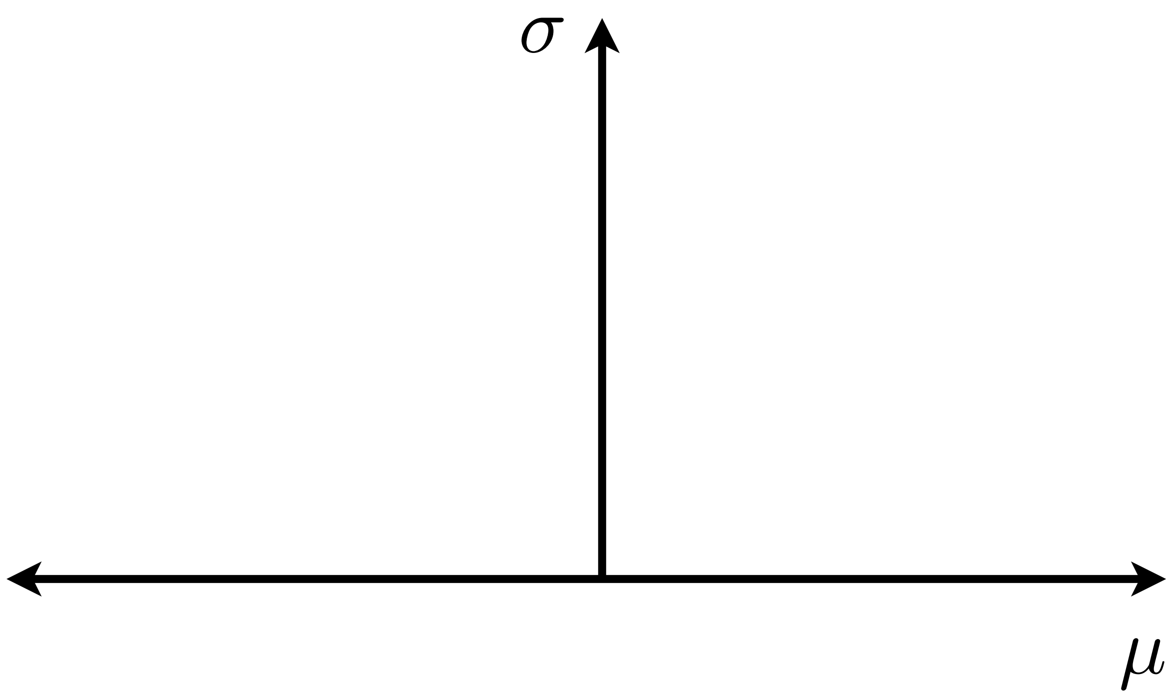

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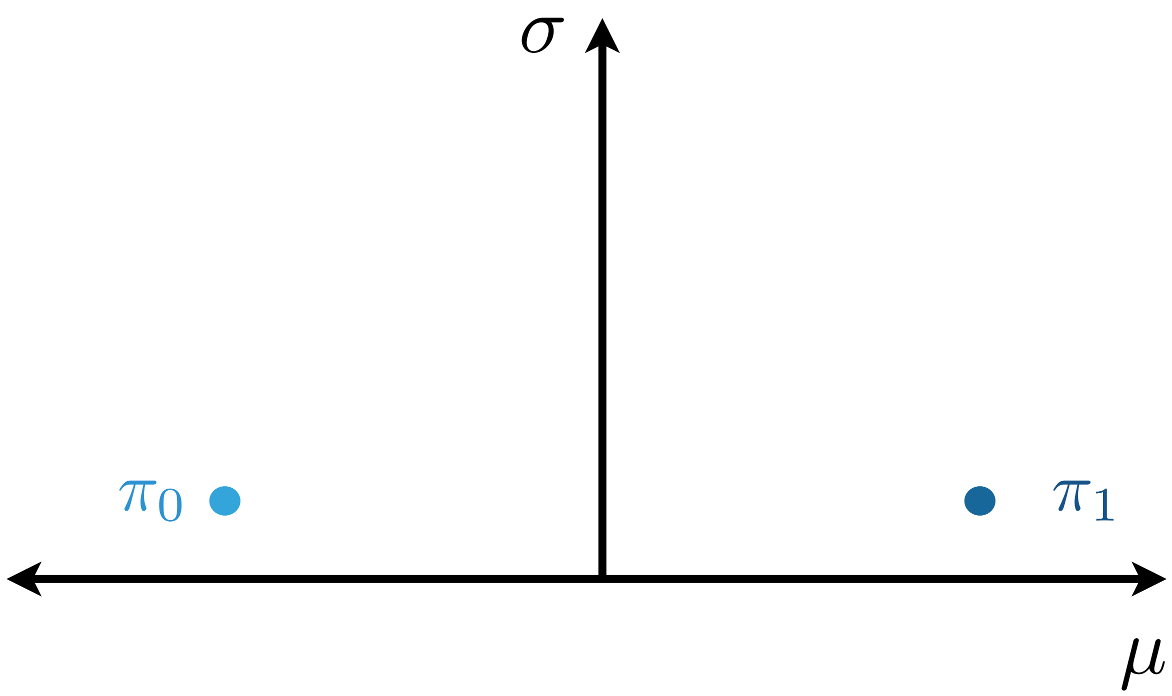

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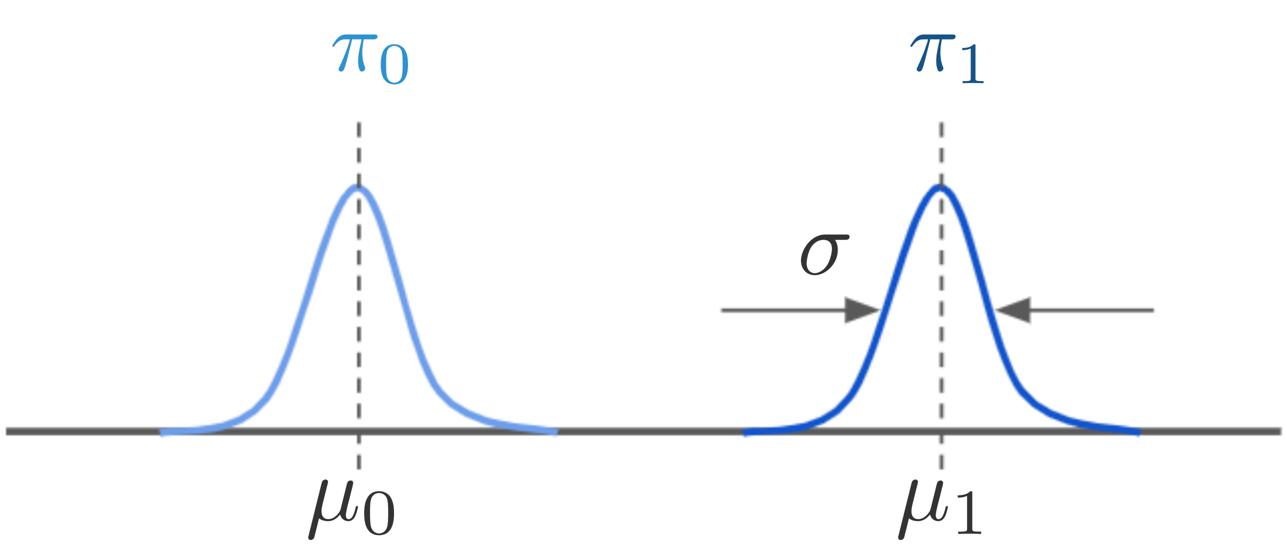

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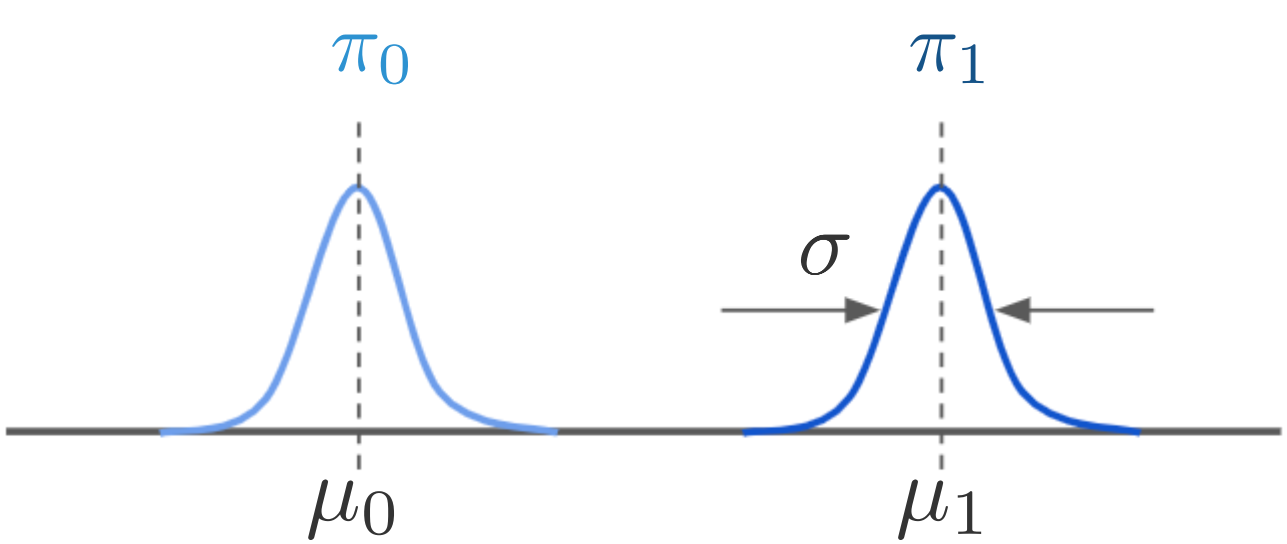

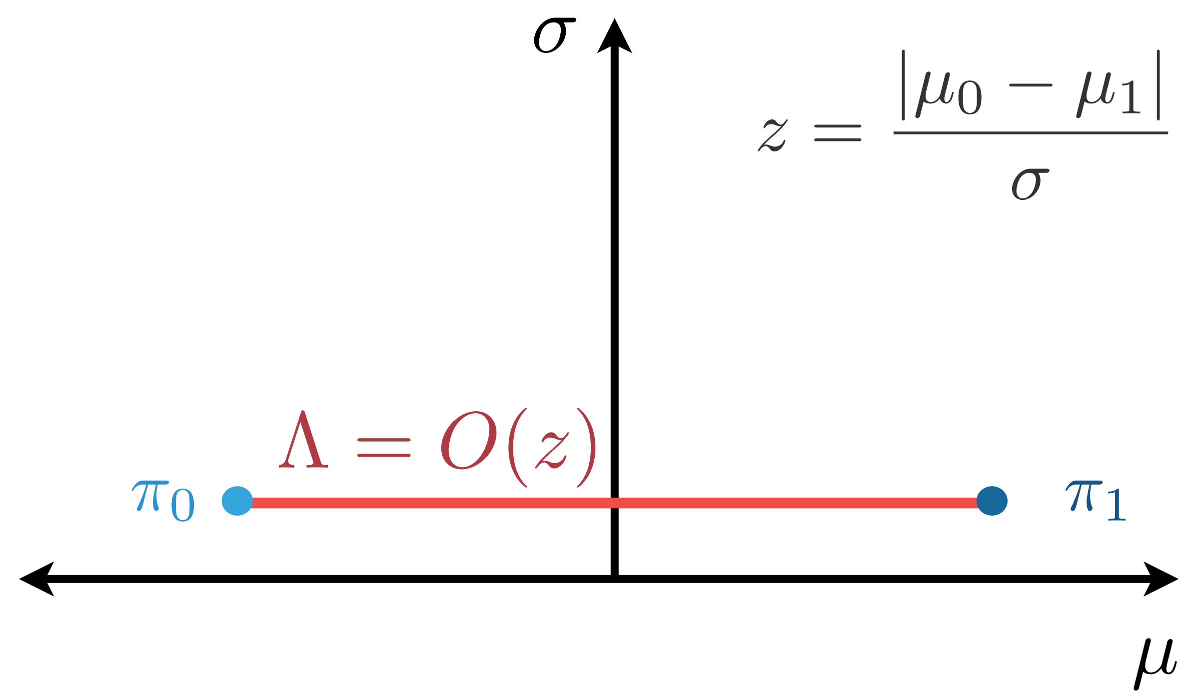

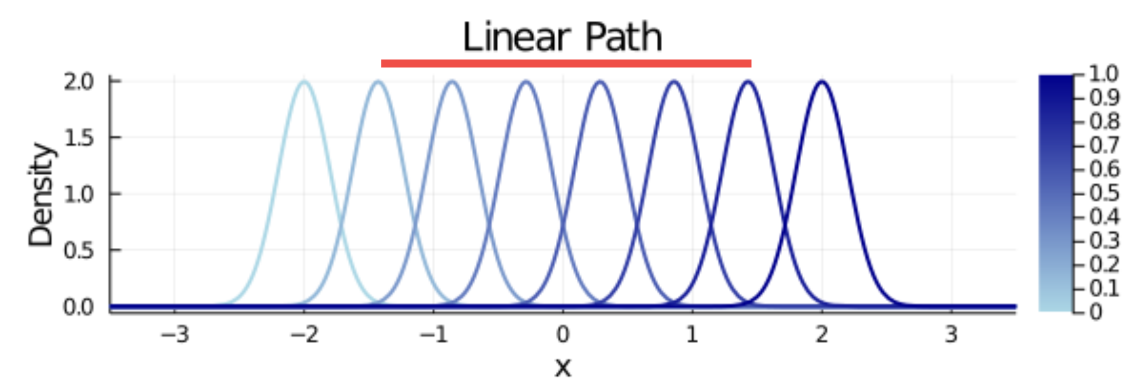

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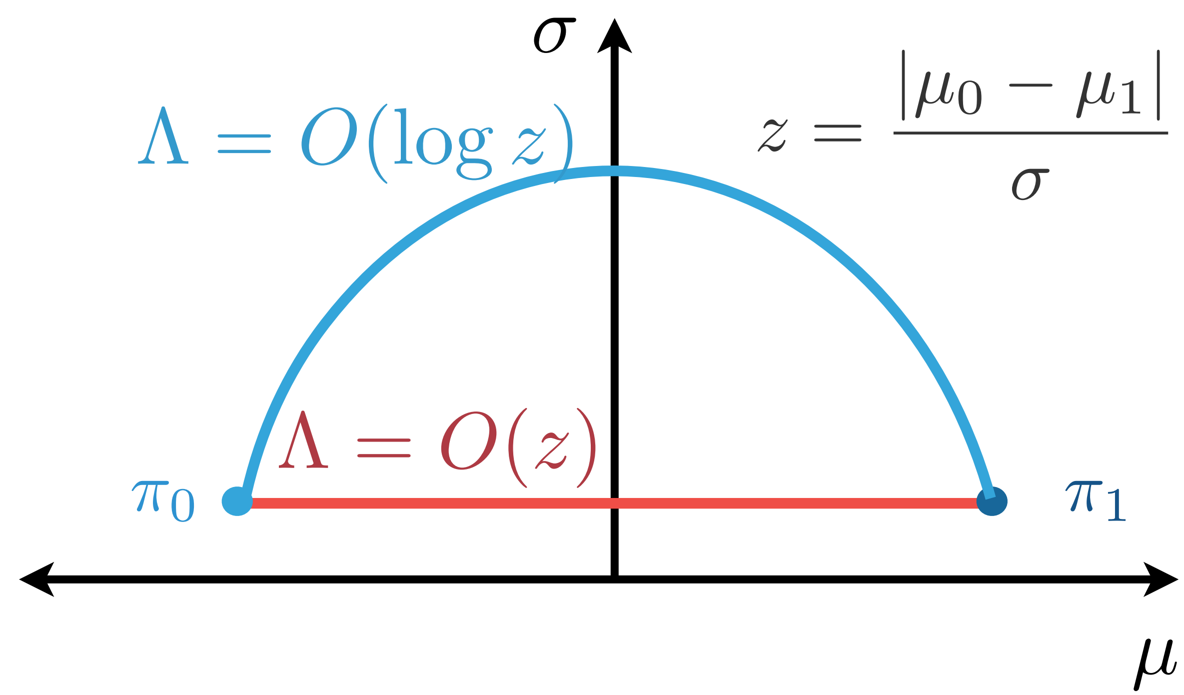

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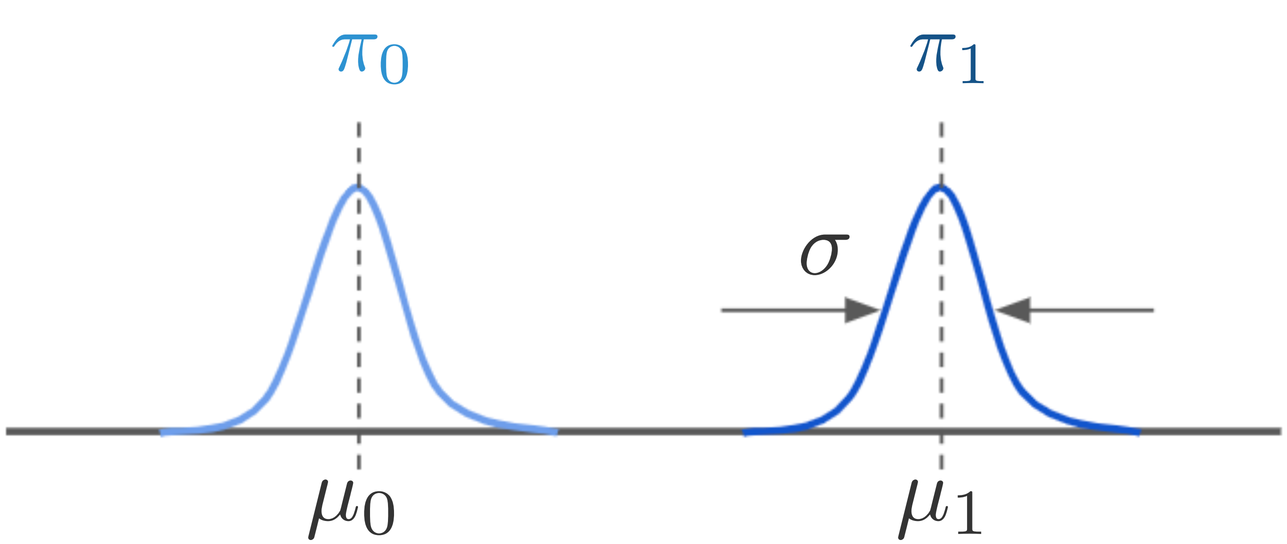

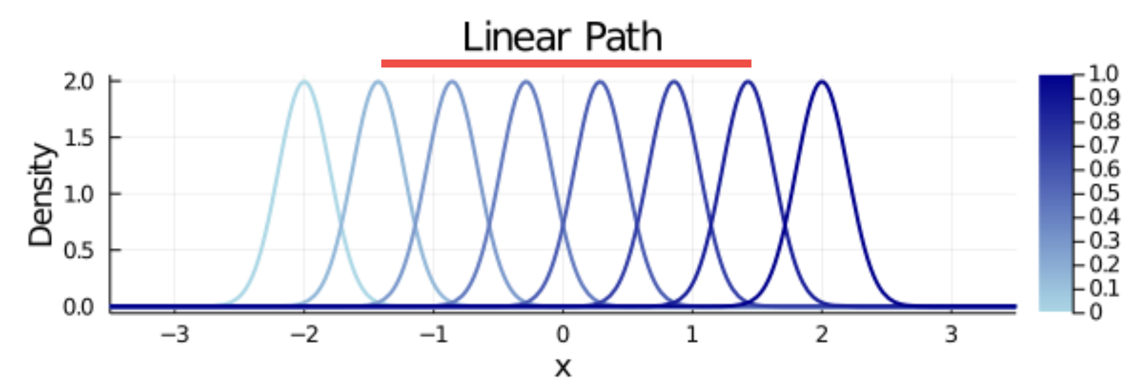

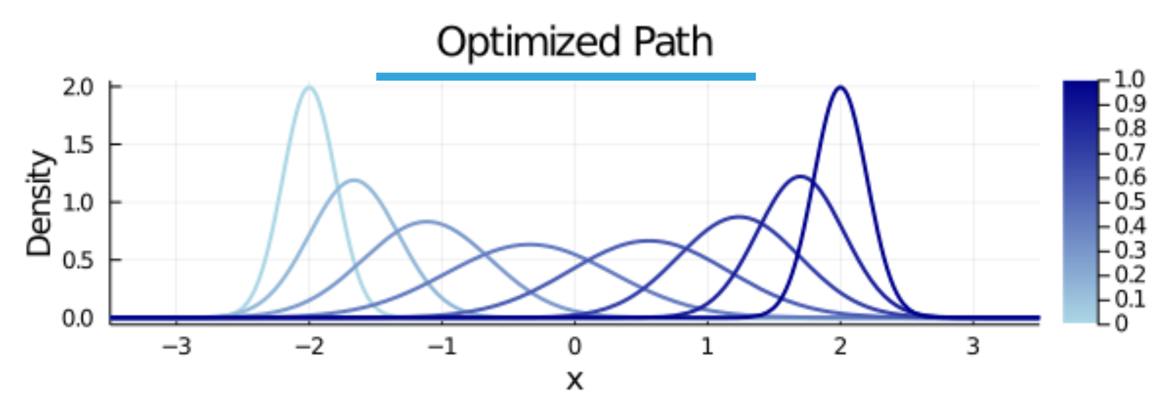

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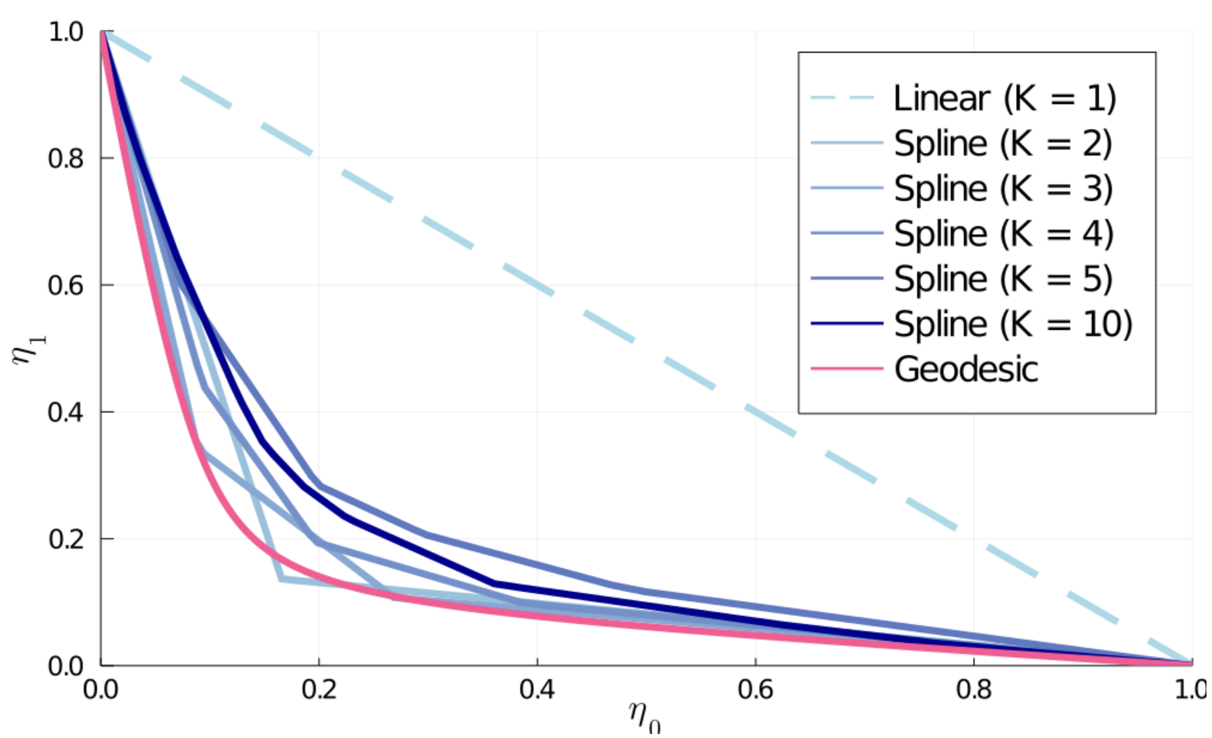

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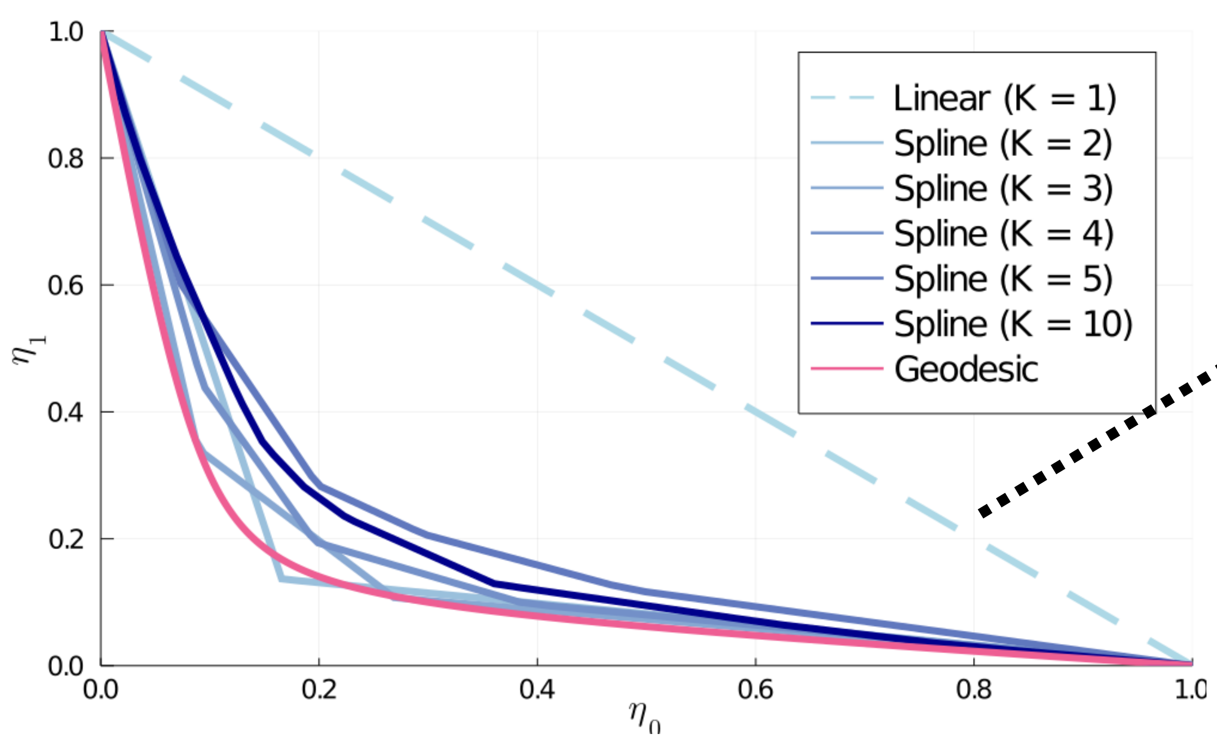

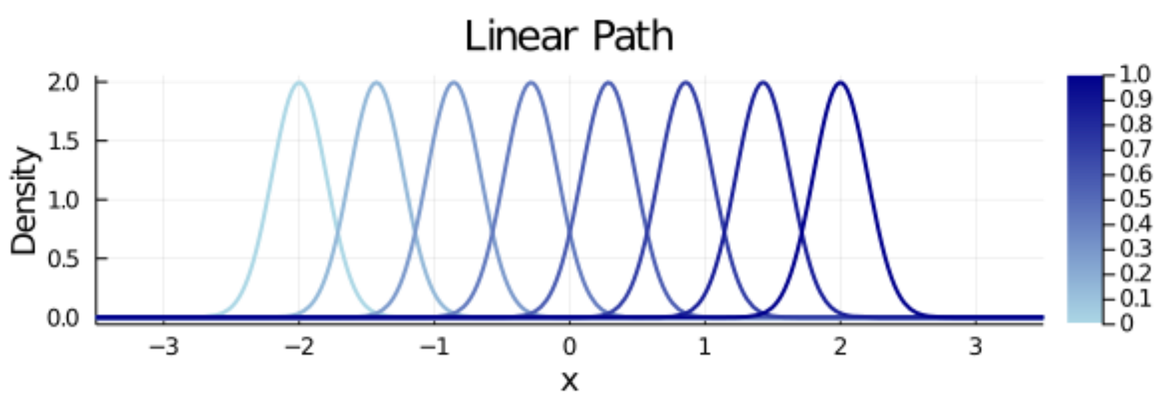

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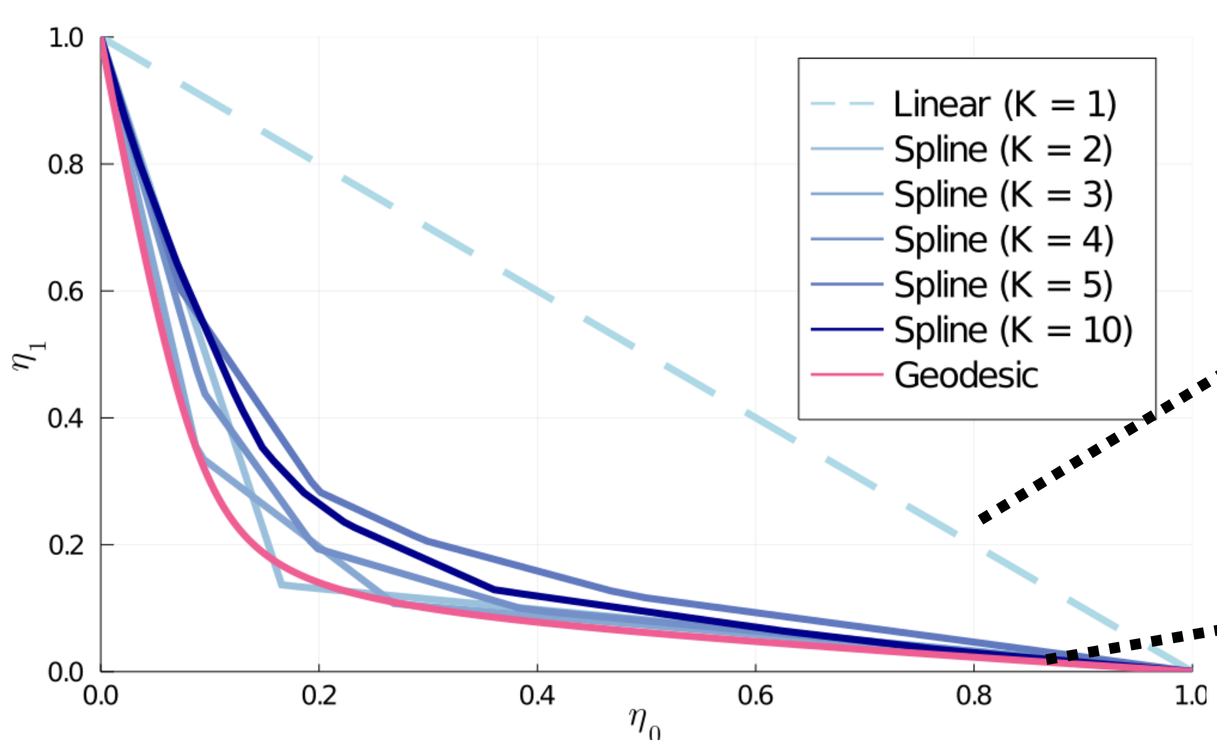
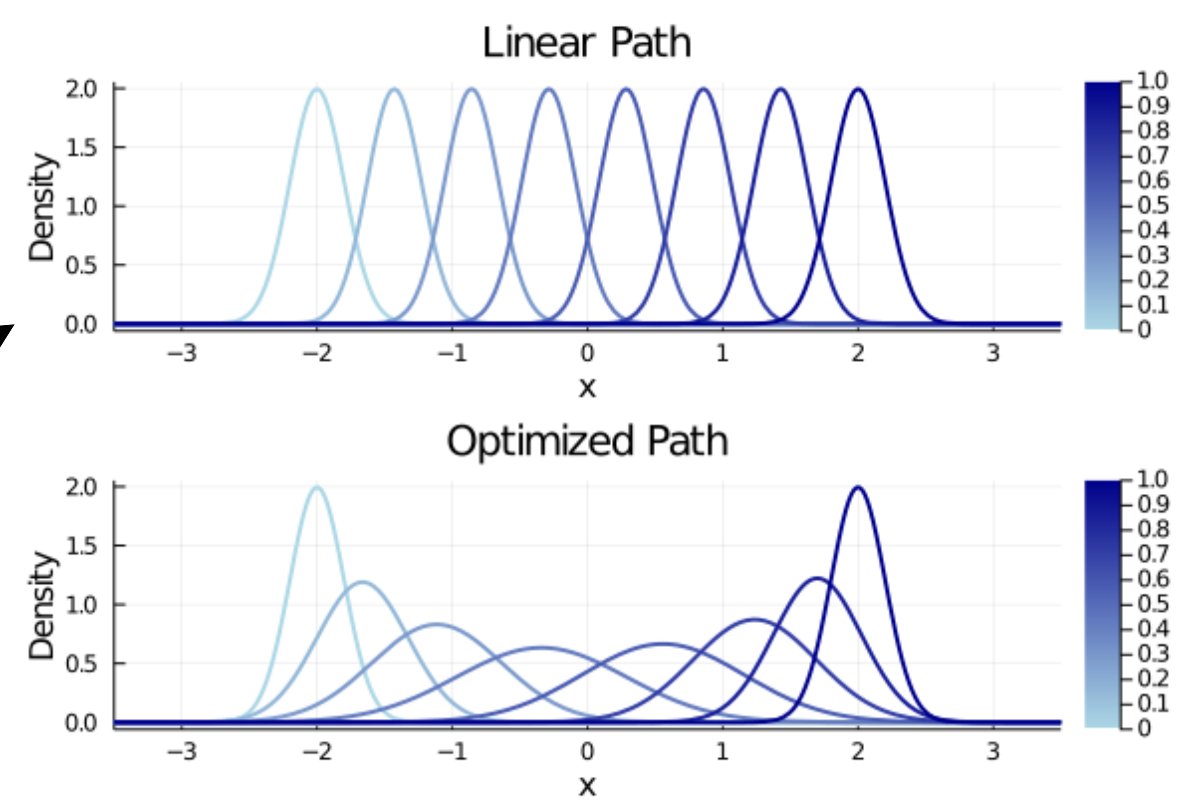
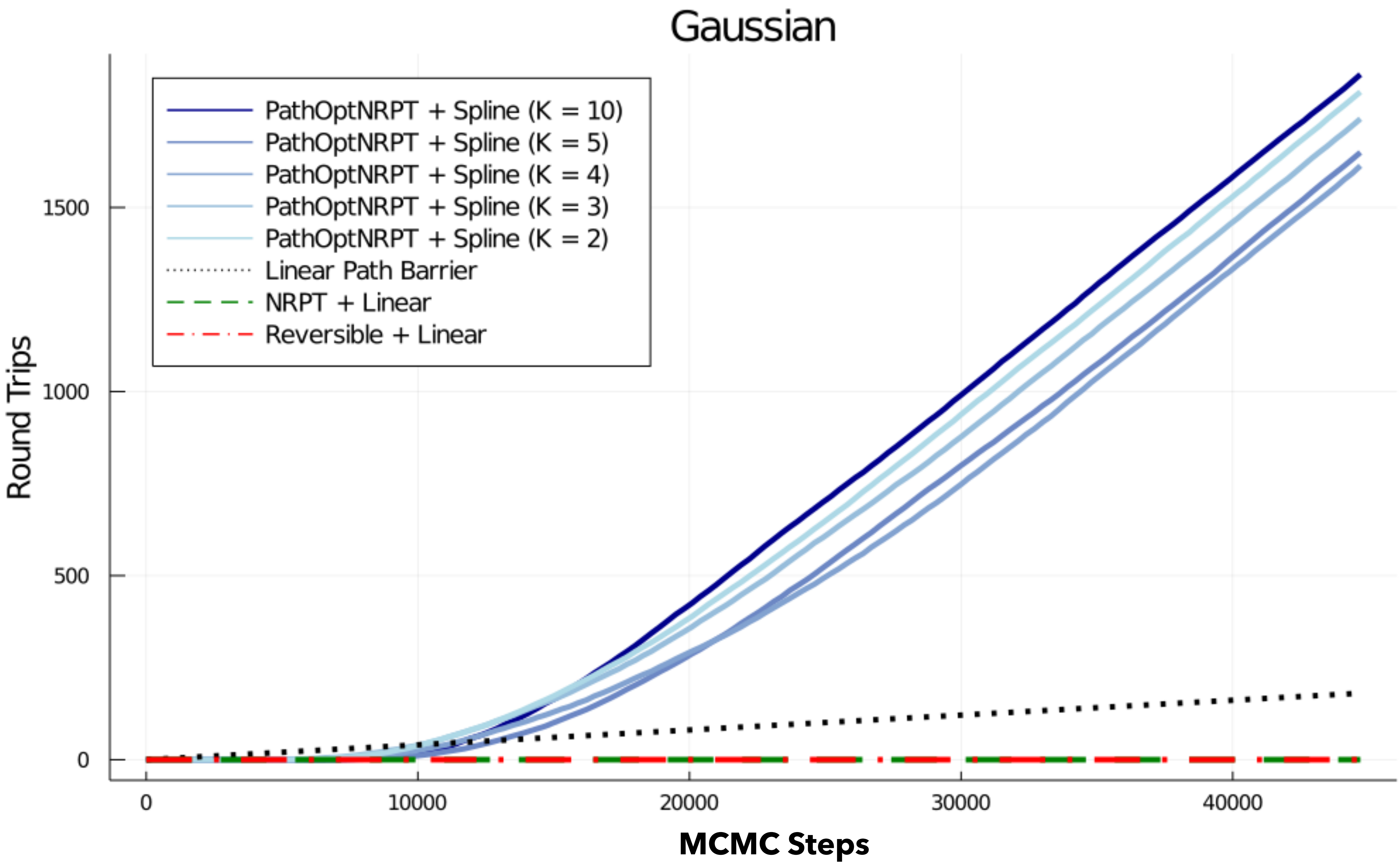




EXAMPLES



Gaussian
PathOptNRPT + Spline (K = 10)
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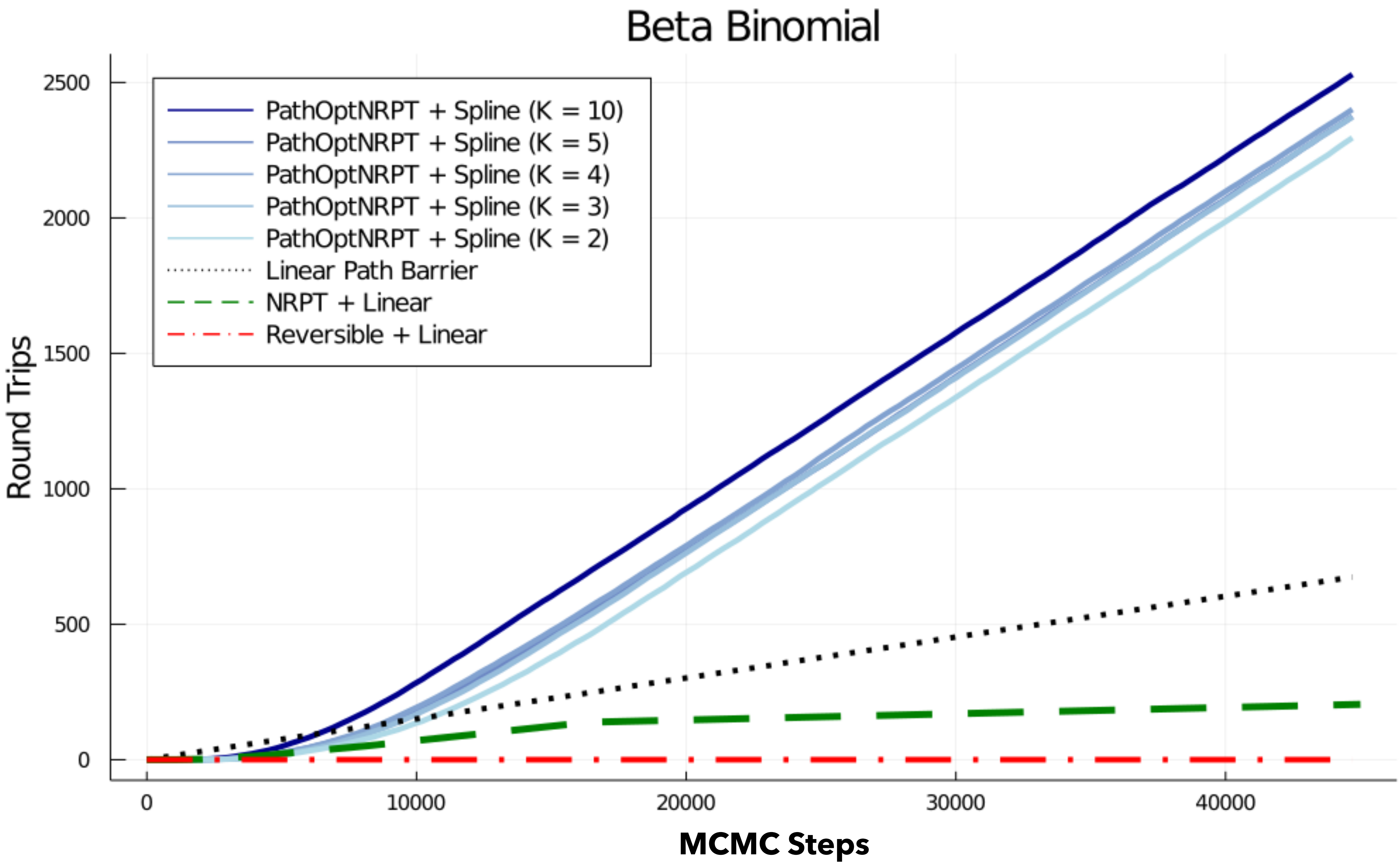
PathOptNRPT + Spline (K = 2)
Linear Path Barrier
NRPT + Linear
Reversible + Linear
Round Trips
1500
1000
500
0
0
10000
20000
30000
40000
MCMC Steps

EXAMPLES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2500
2000
1500
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20000
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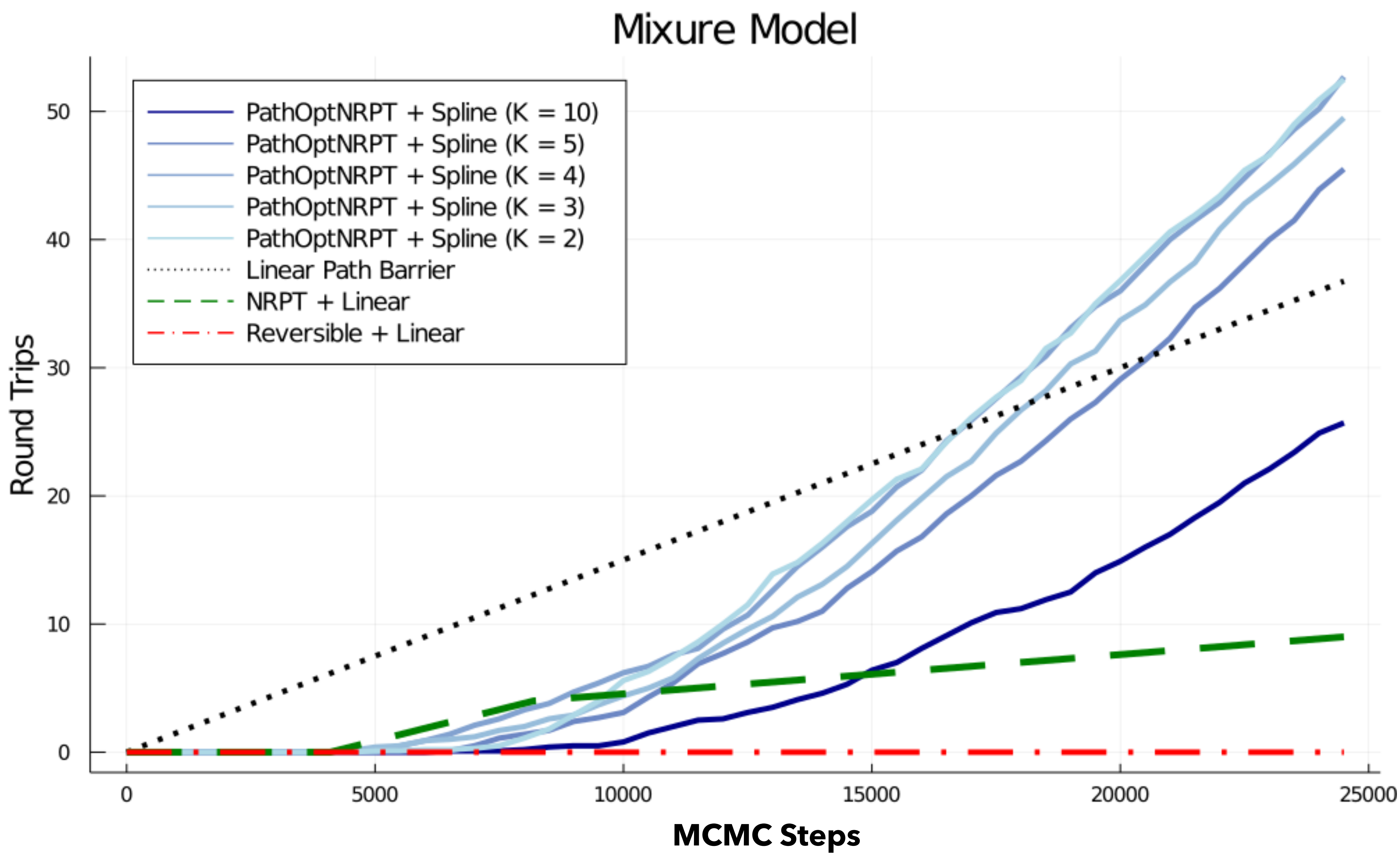
EXAMPLES



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20
30
40
50
0
5000
10000
15000
20000
25000
MCMC Steps

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THANK YOU!

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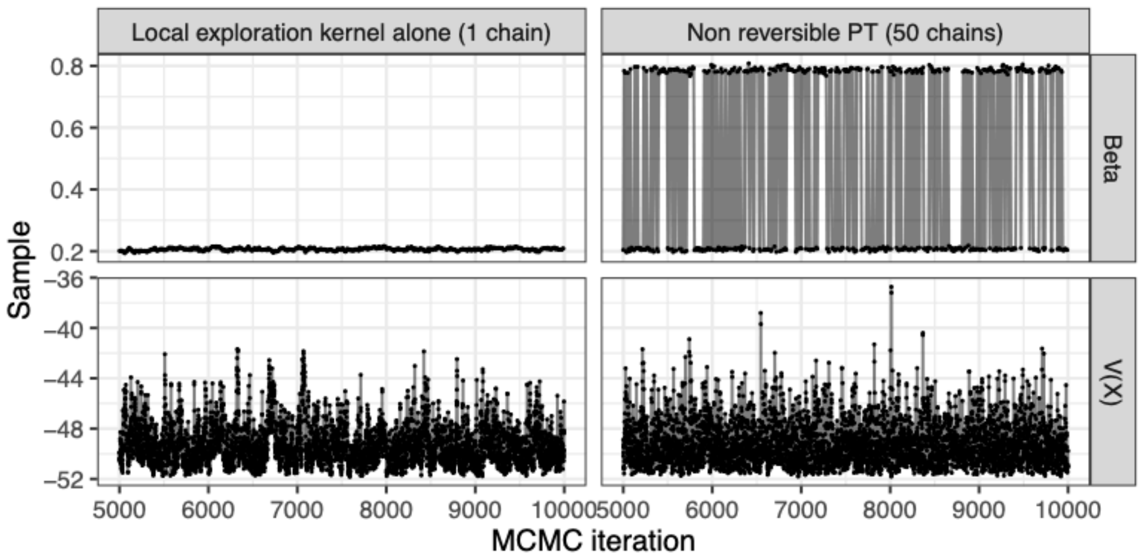
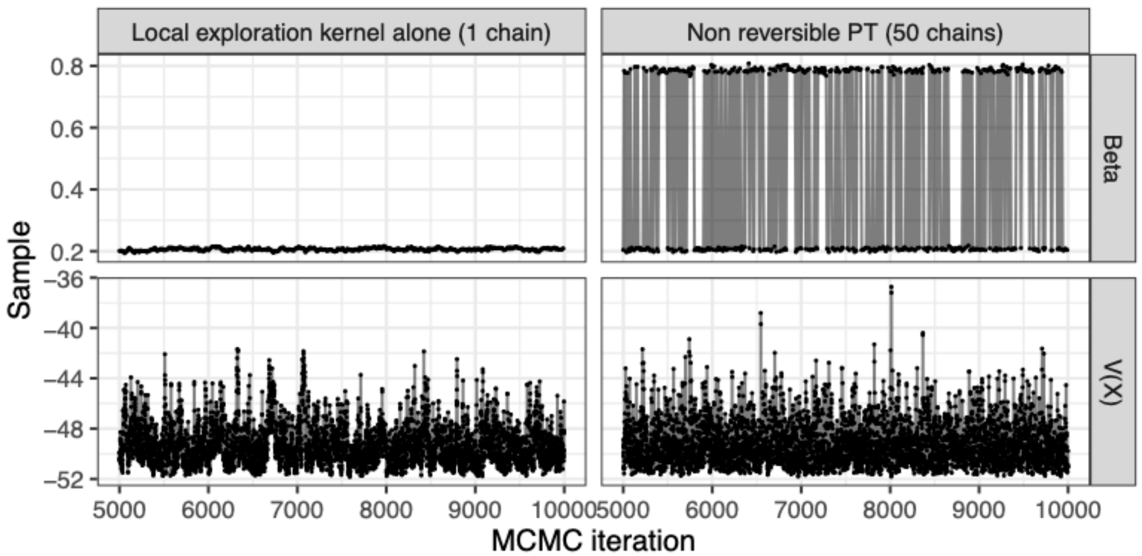
VIOLATION OF ELE

ODE parameter estimation

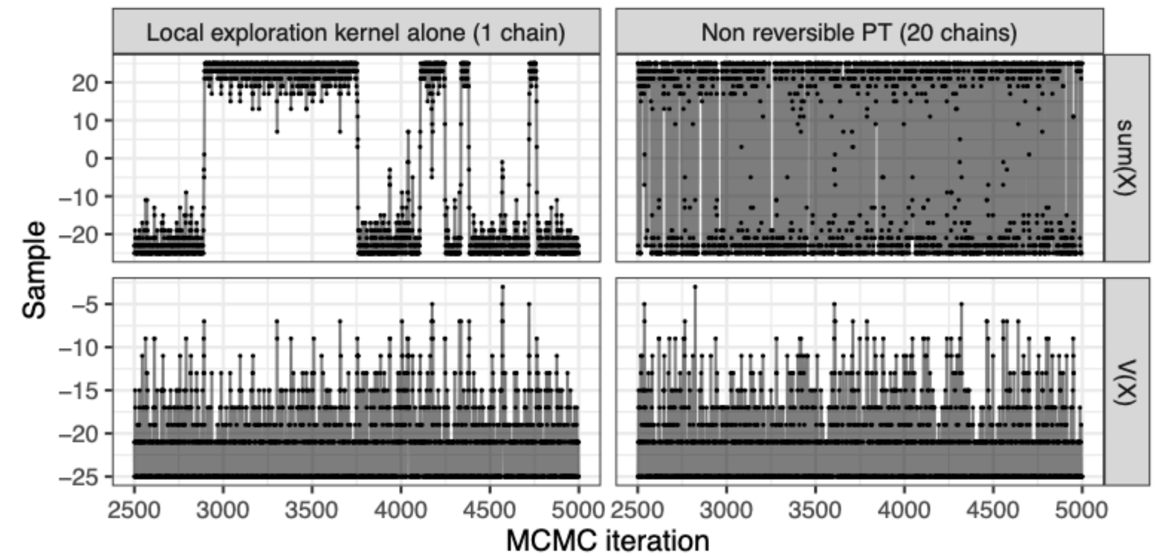


VIOLATION OF ELE

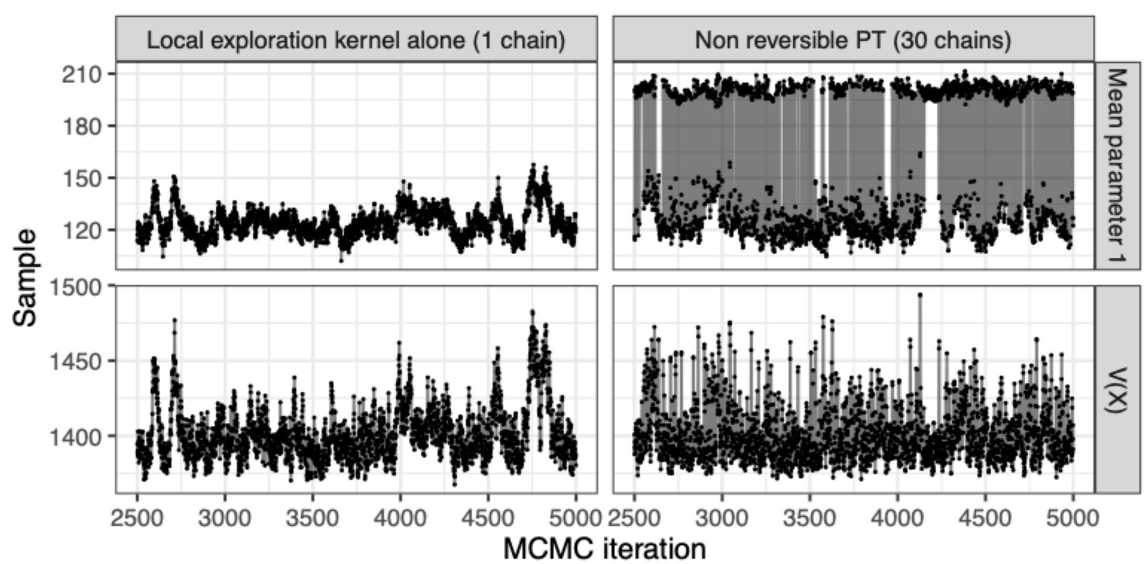
ODE parameter estimation



Ising model



Bayesian Mixture Model



Copy-number inference