LECTURE 8

INTRODUCTION TO PARALLEL ANNEALING

Saifuddin Syed

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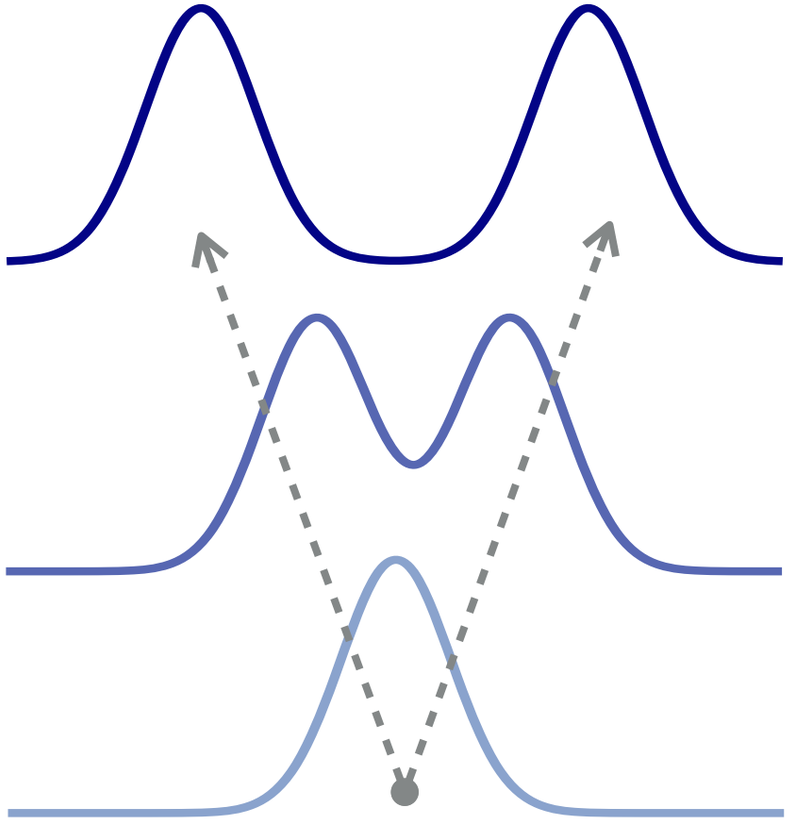
- **Algorithmic:** Single chain tries to simultaneously efficiently explore & be accurate
- **Solution:** Build an interacting particle system
  - Delegate exploration to tractable **reference** chain
  - Communicate to **target** through the **interpolating distributions**



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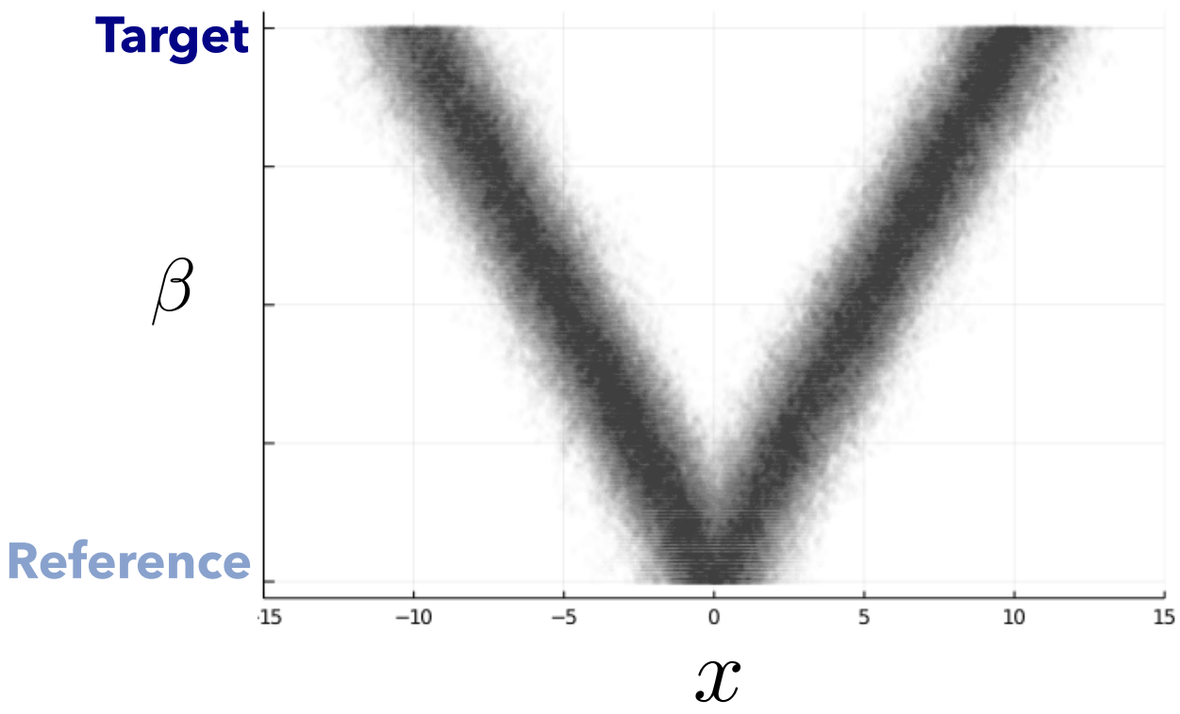

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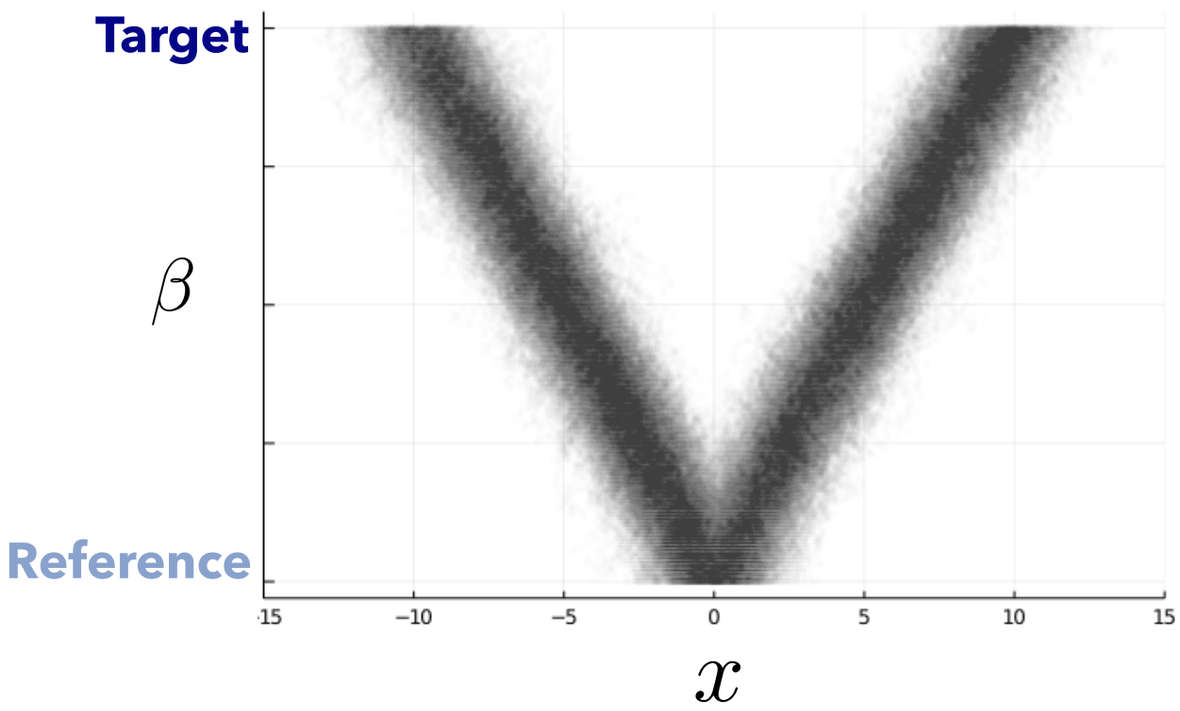

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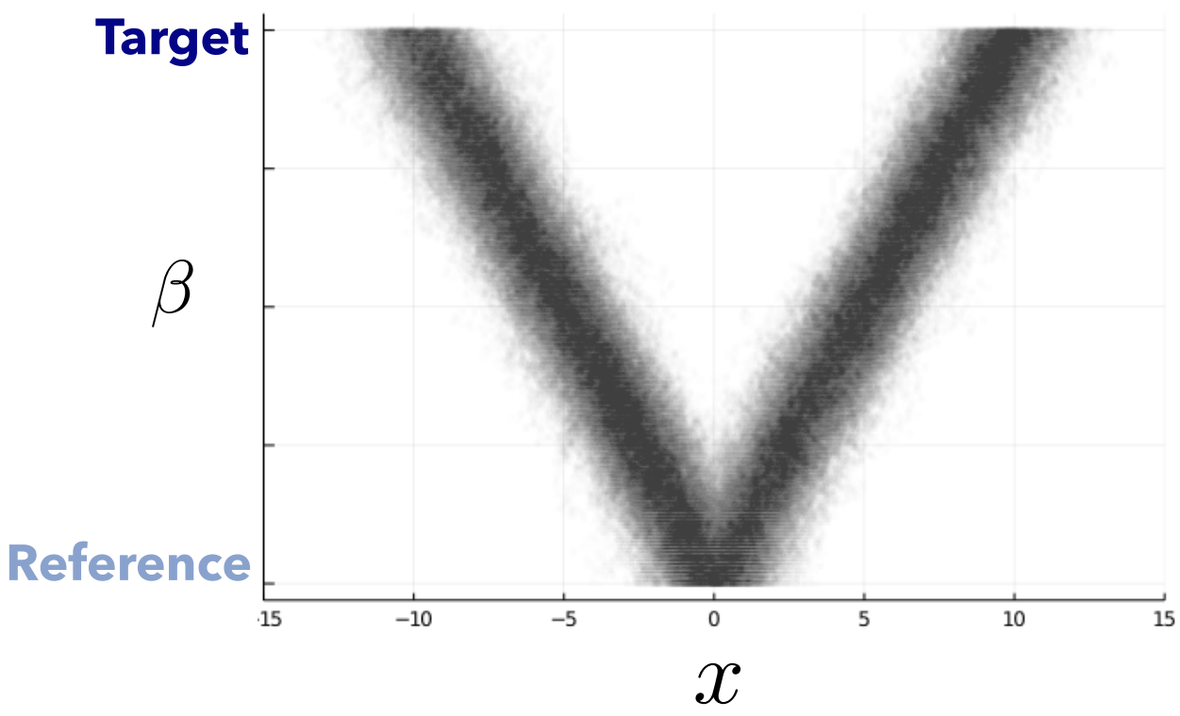

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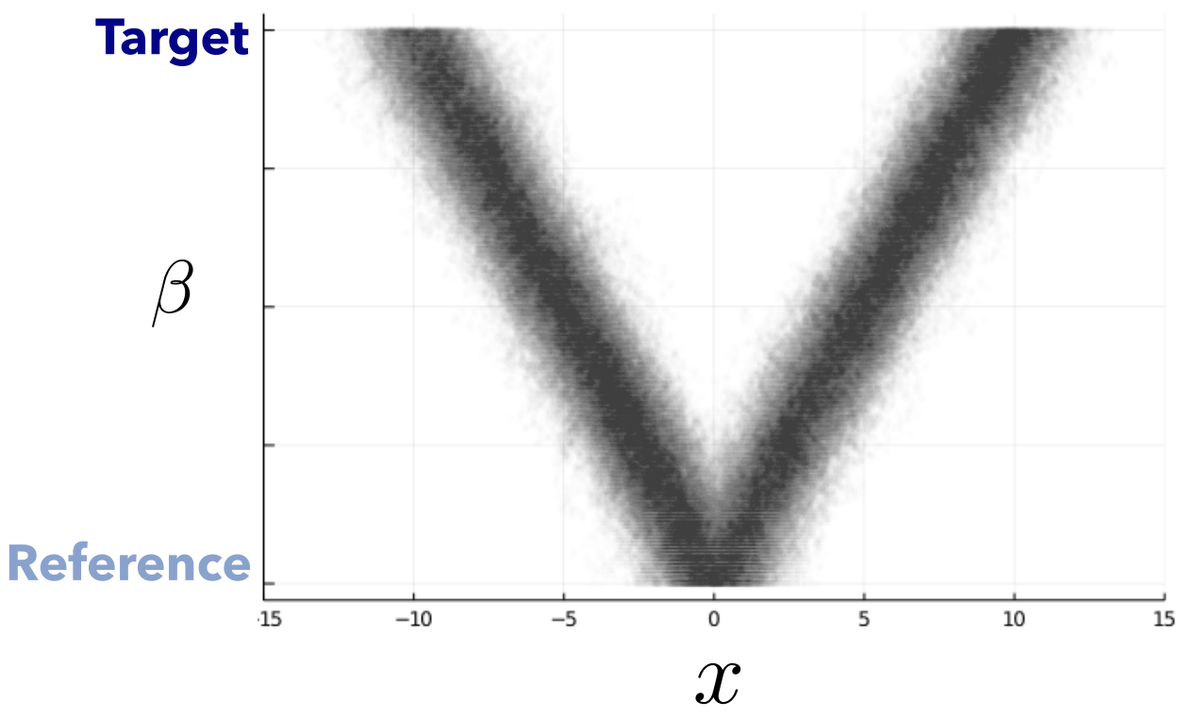

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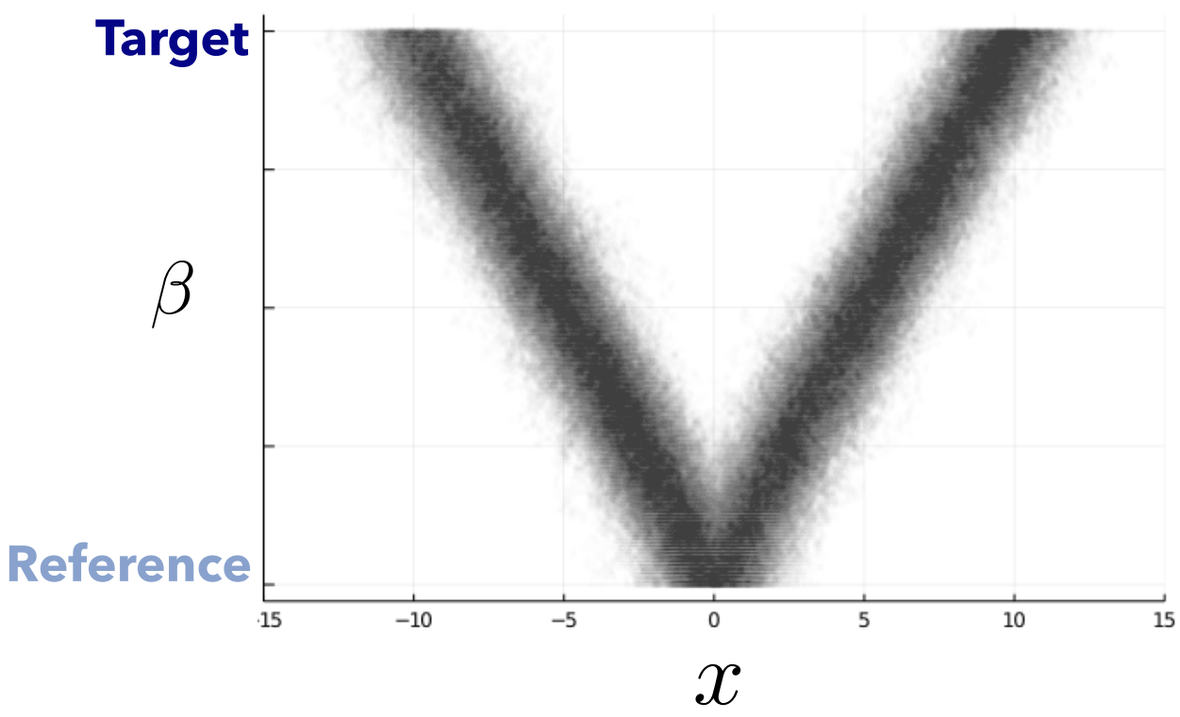

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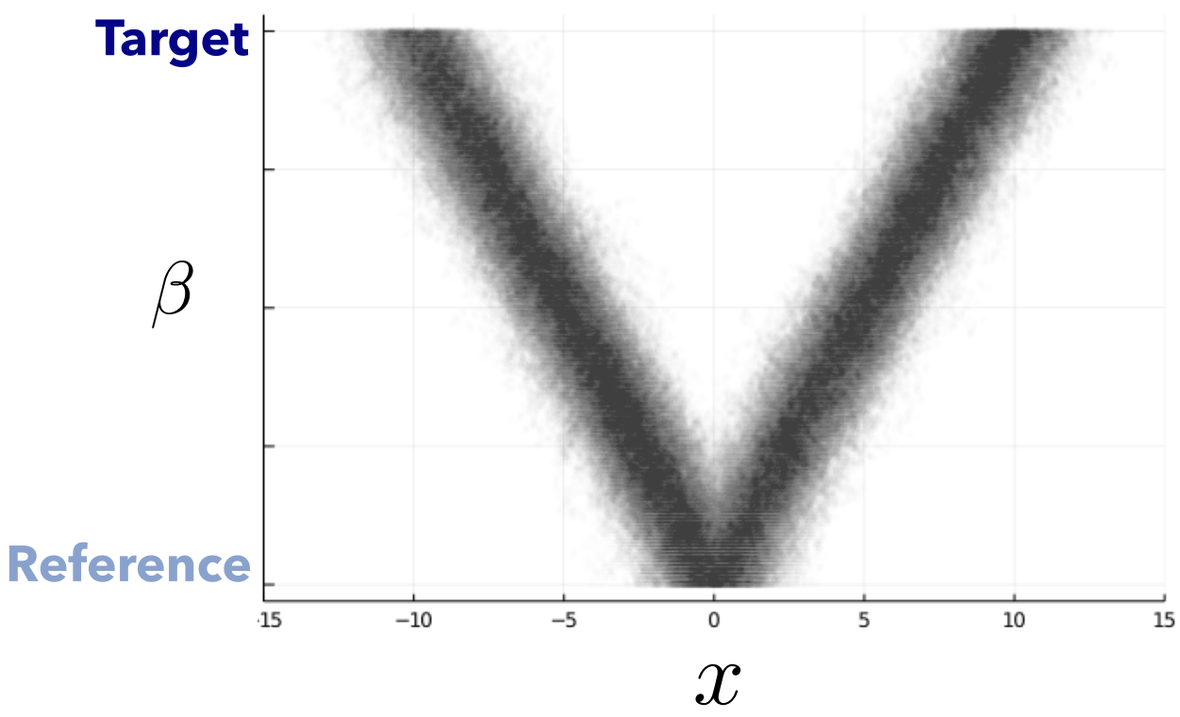

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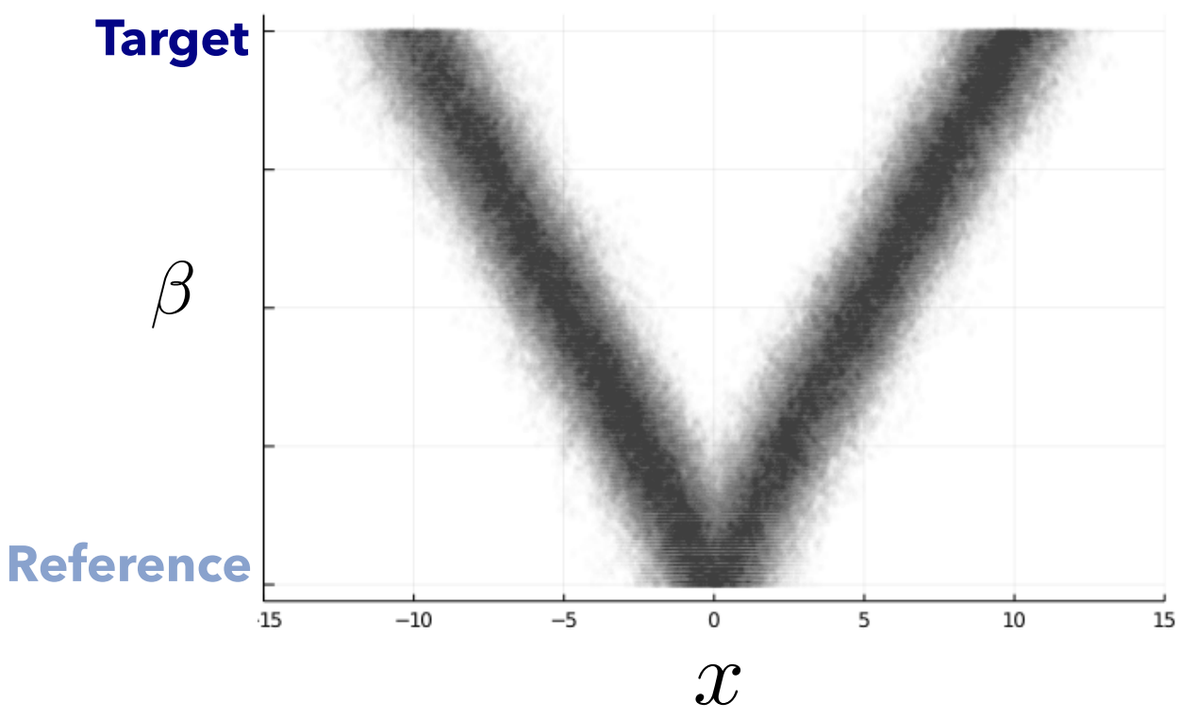
- Can use the reference to assess the quality and ensure robustness



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$$0 = \beta_0 < \beta_1 < \cdots < \beta_N = 1$$

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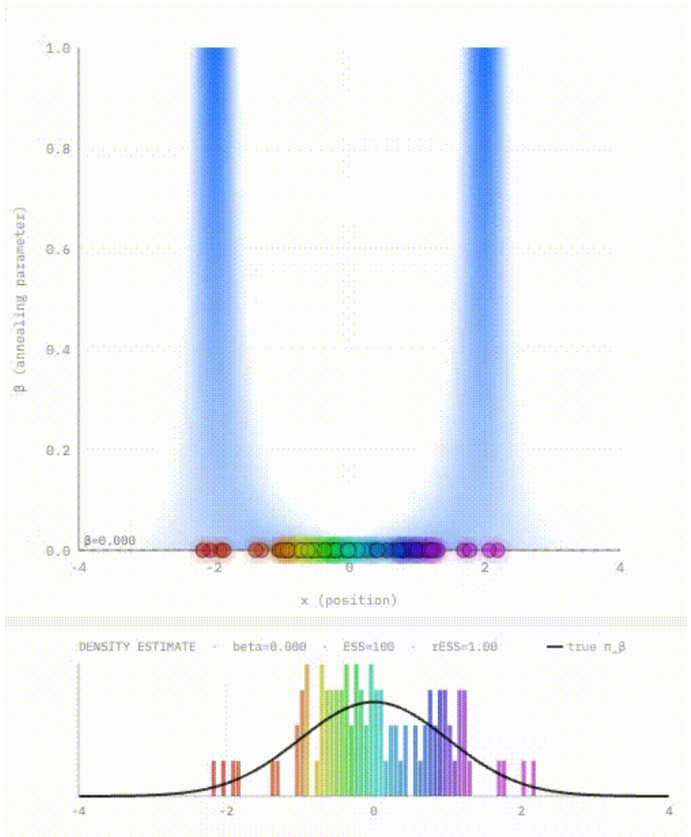
Sequential Annealing



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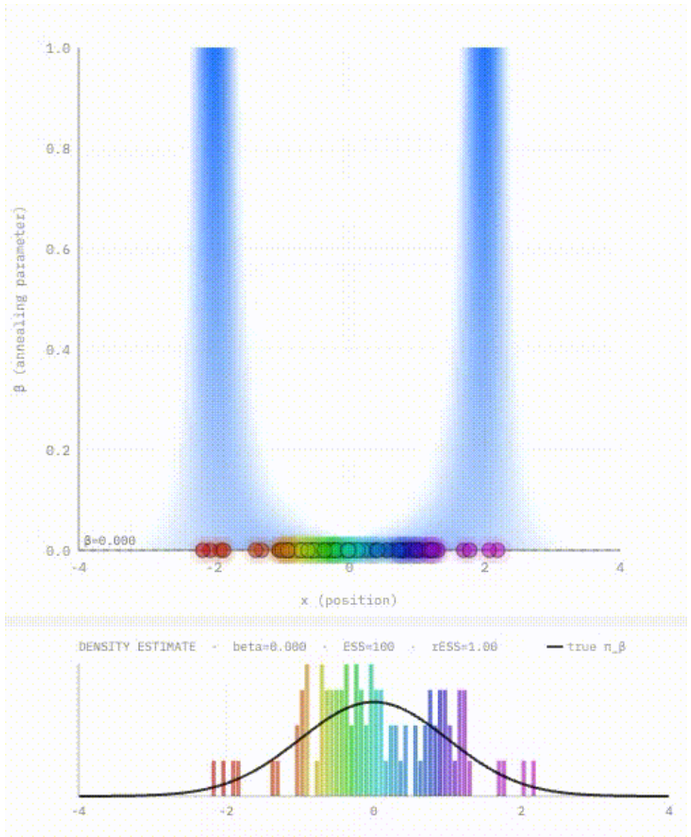
- We simultaneously evolve a system of particles to approximation the annealing path

Sequential Annealing

- Construct path sequentially



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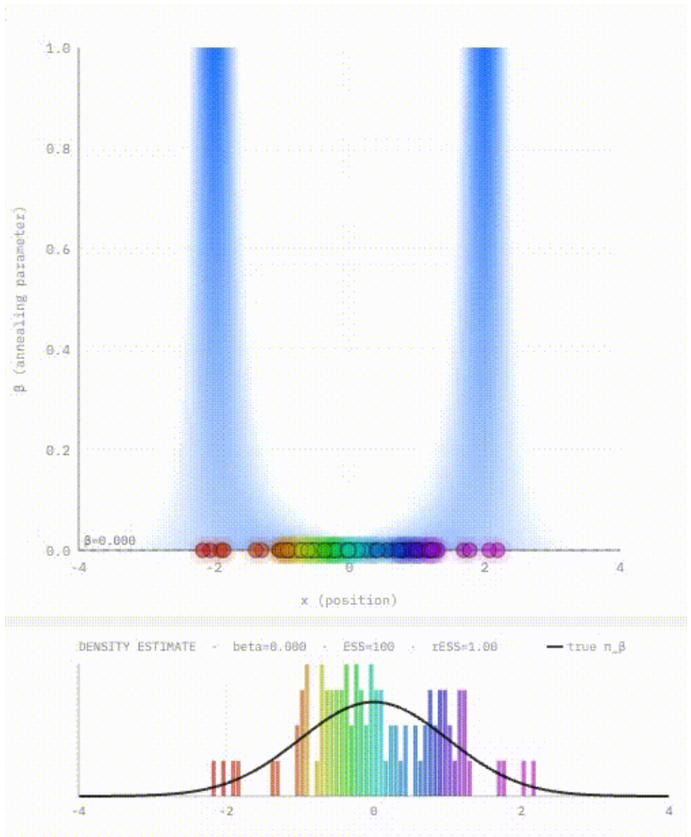
Sequential Annealing

- Construct path sequentially
- Samples generated in parallel



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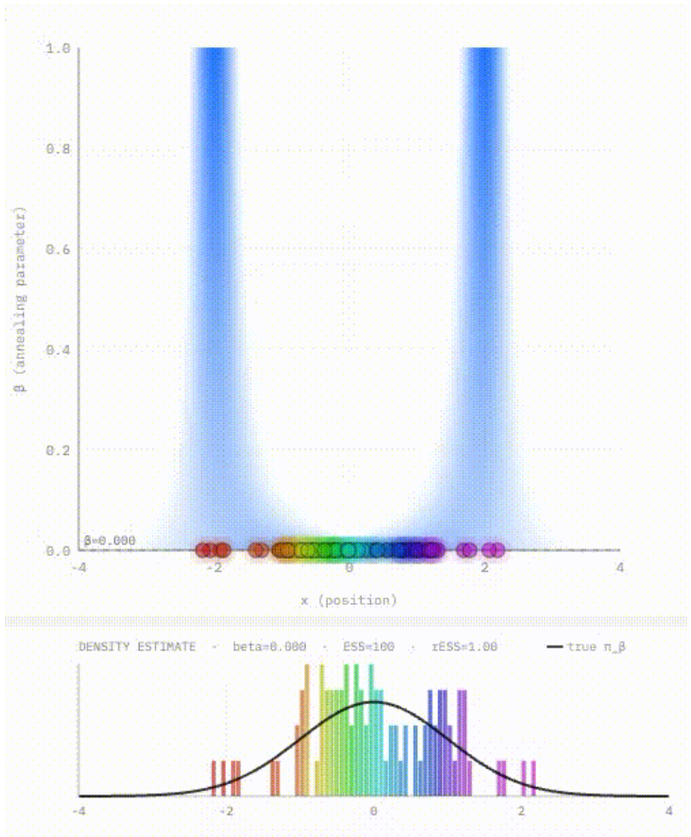
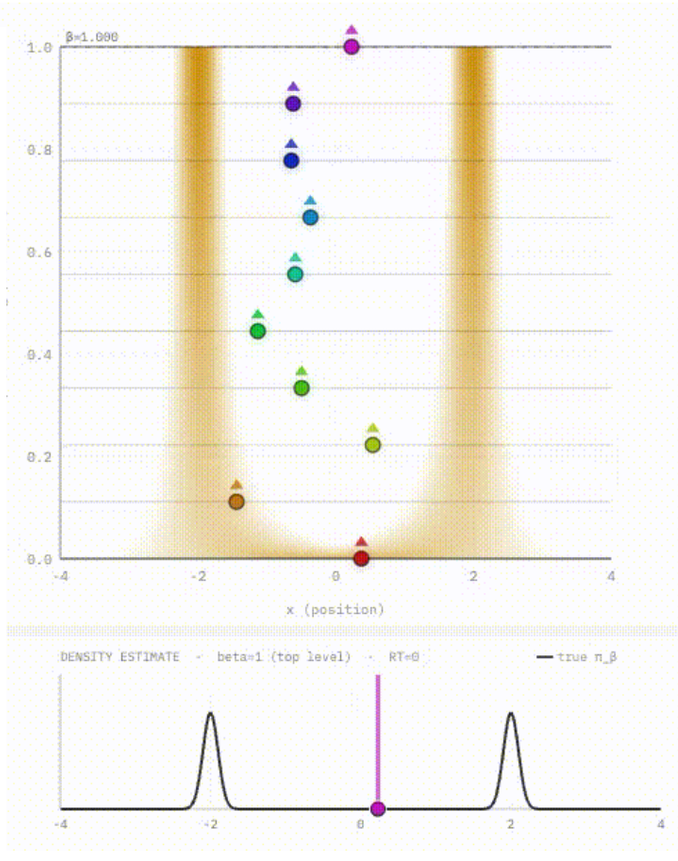


Parallel Annealing



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Parallel Annealing

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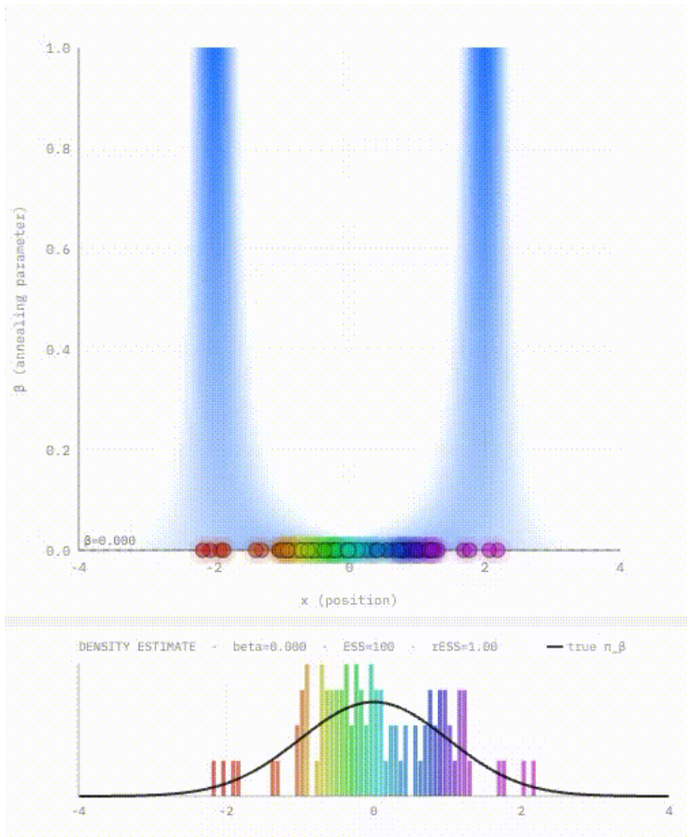

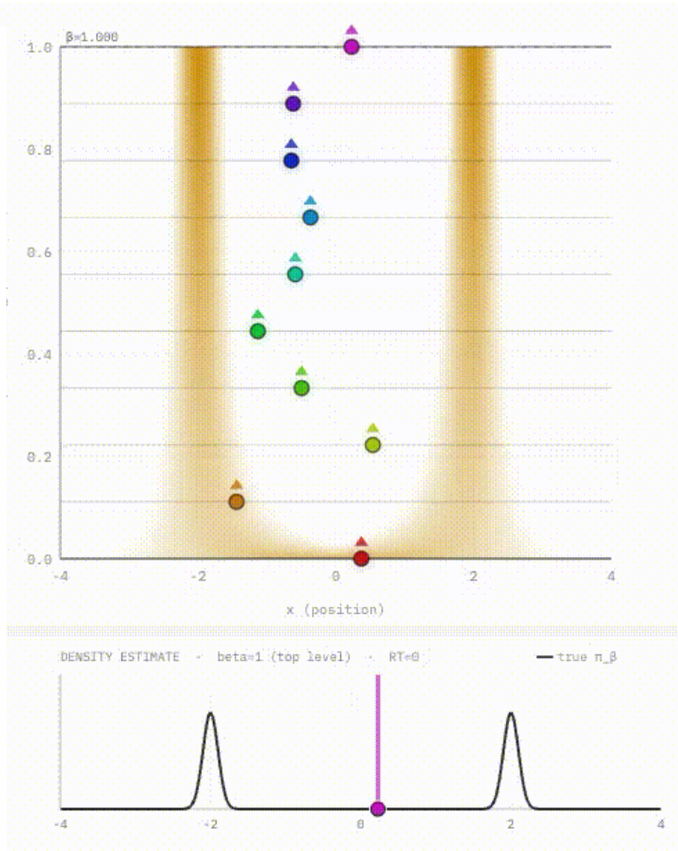

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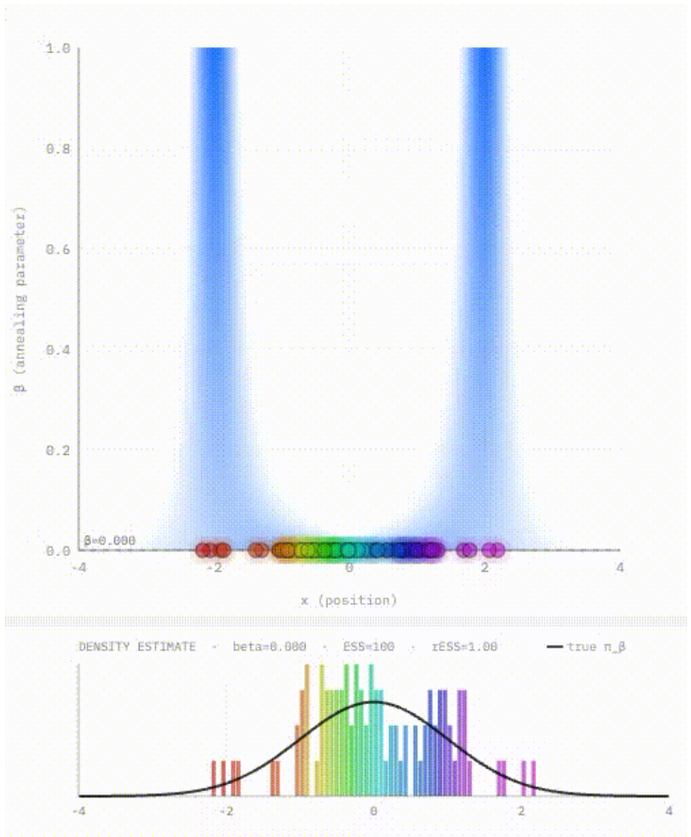
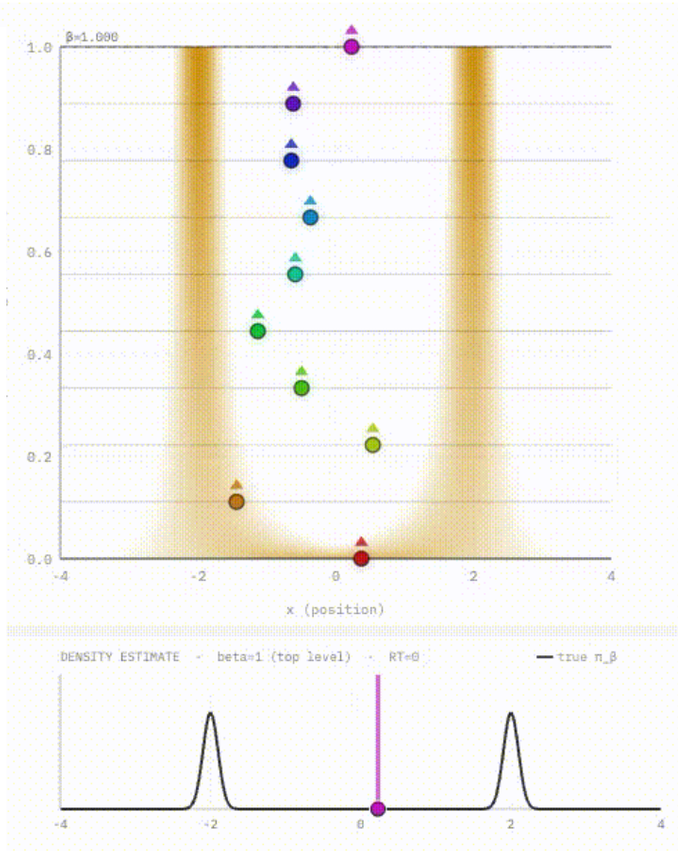




SEQUENTIAL VERSUS PARALLEL ANNEALING

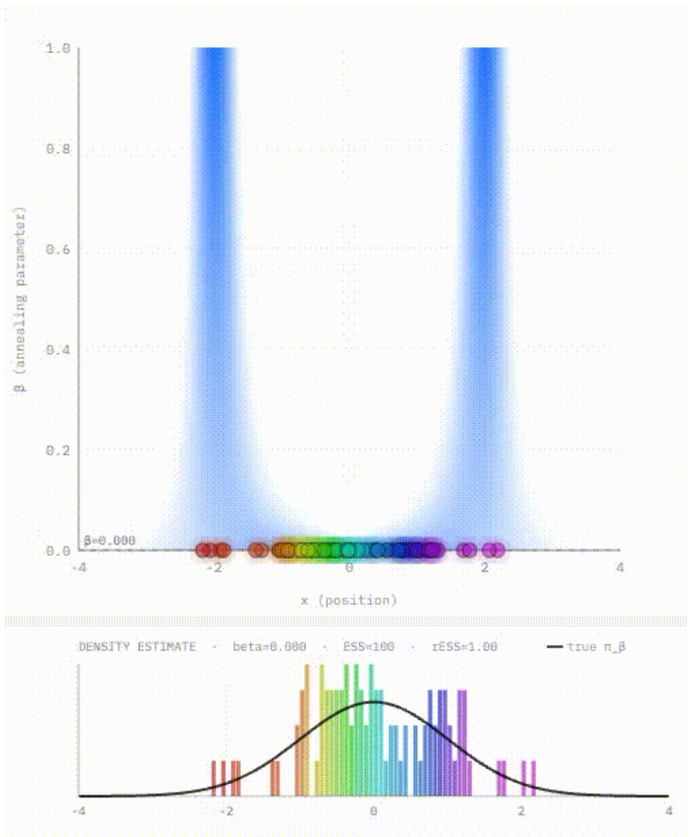
- We simultaneously evolve a system of particles to approximation the annealing path

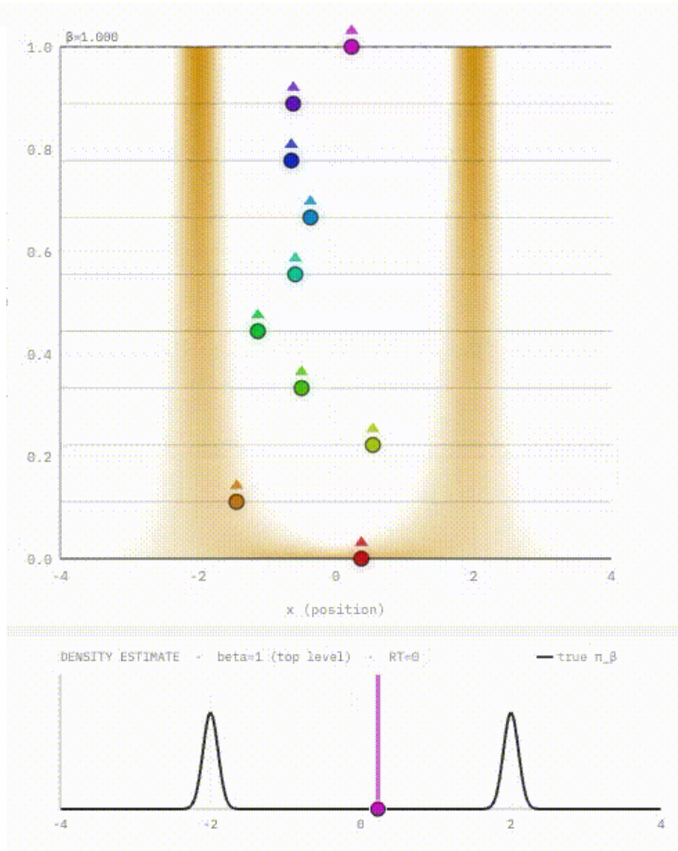
Sequential Annealing

- Construct path sequentially
- Samples generated in parallel
- Built using importance sampling

Parallel Annealing

- Construct path in parallel
- Samples generated in sequentially





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Parallel Annealing

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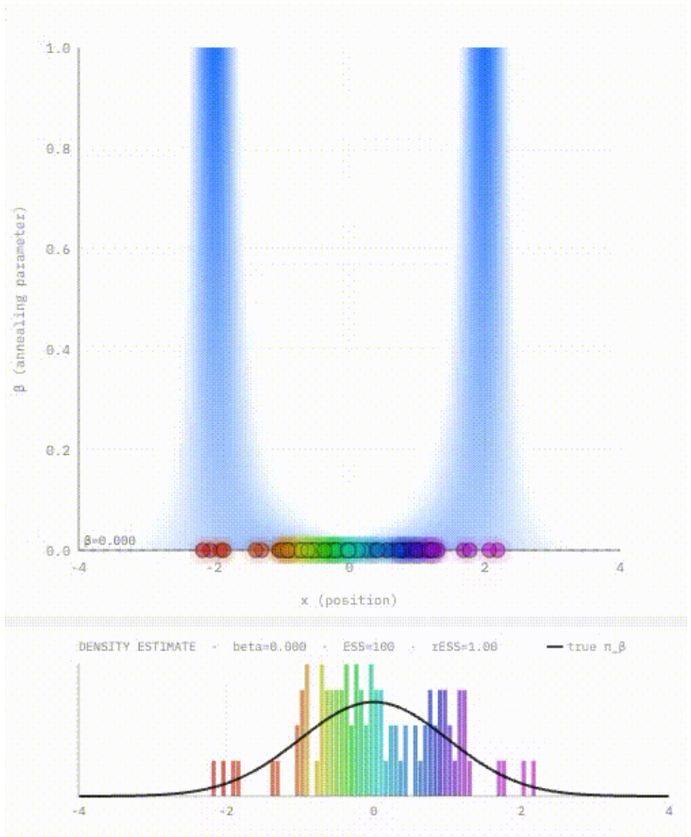
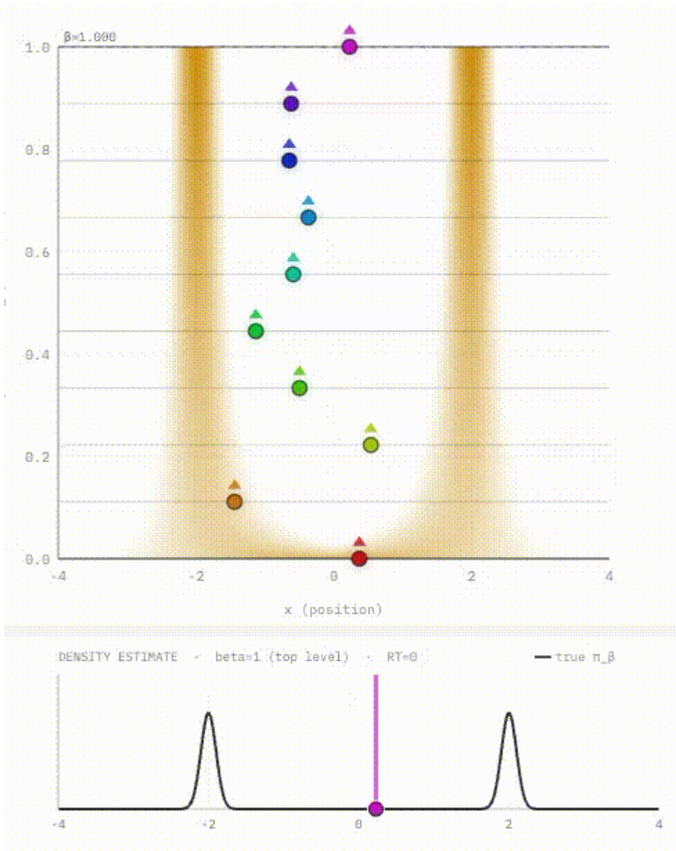
- Samples generated in sequentially
- Built using MCMC





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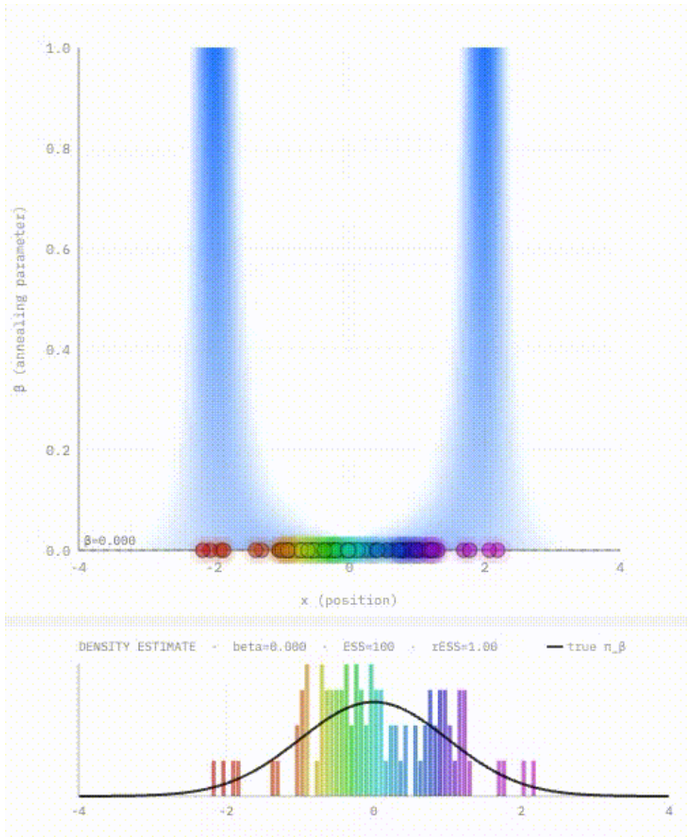
- We simultaneously evolve a system of particles to approximation the annealing path

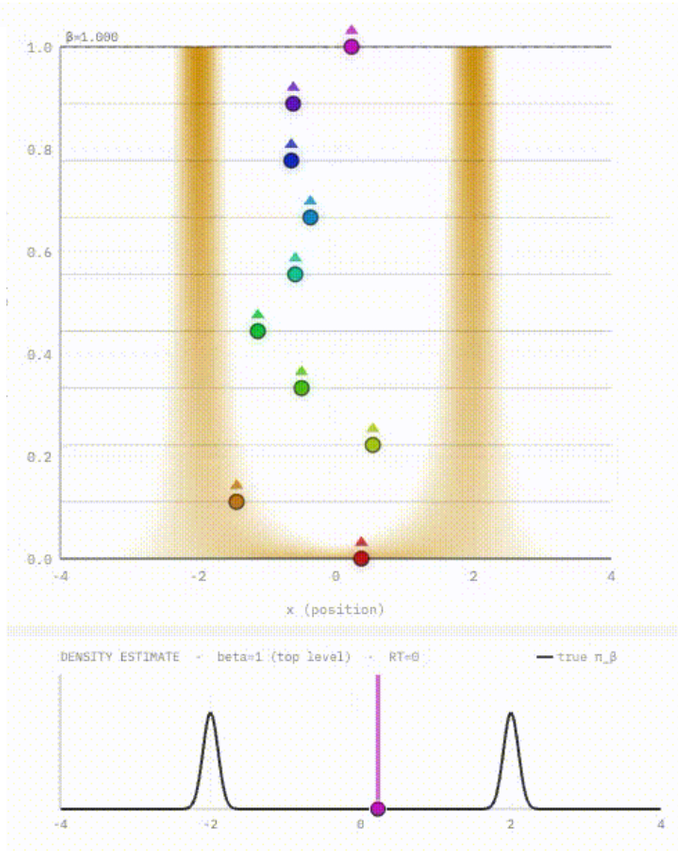
Sequential Annealing

- Construct path sequentially
- Samples generated in parallel
- Built using importance sampling
- Interacting → Sequential Monte Carlo Samplers

Parallel Annealing

- Construct path in parallel
- Samples generated in sequentially
- Built using MCMC





SEQUENTIAL VERSUS PARALLEL ANNEALING

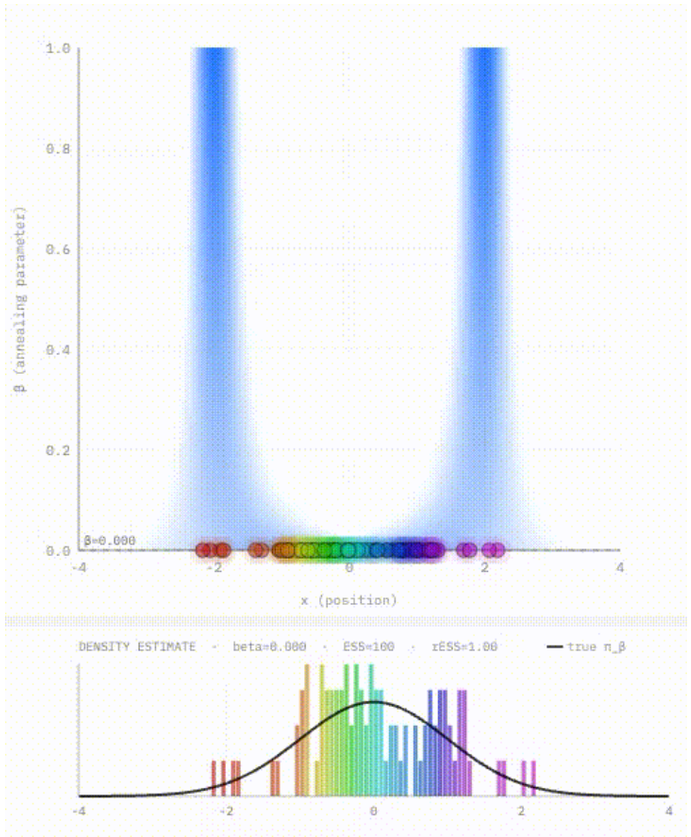
- We simultaneously evolve a system of particles to approximation the annealing path

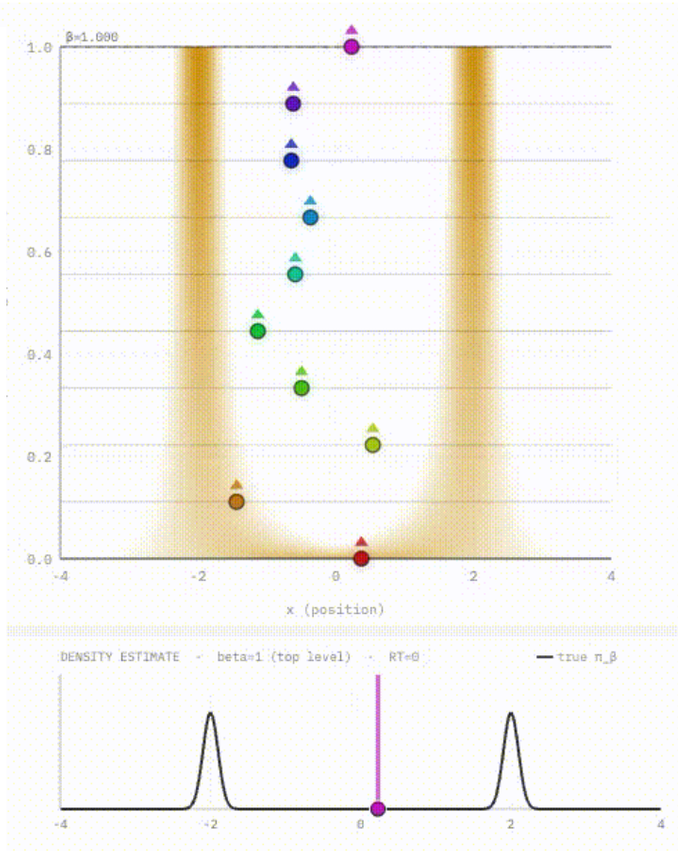
Sequential Annealing

- Construct path sequentially
- Samples generated in parallel
- Built using importance sampling
- Interacting → Sequential Monte Carlo Samplers

Parallel Annealing

- Construct path in parallel
- Samples generated in sequentially
- Built using MCMC
- Interacting → Parallel Tempering





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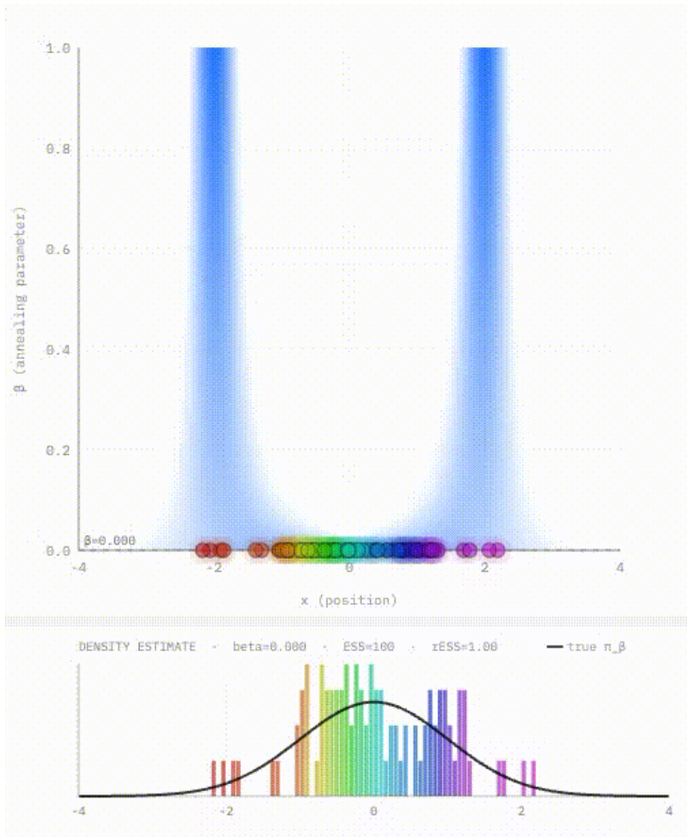
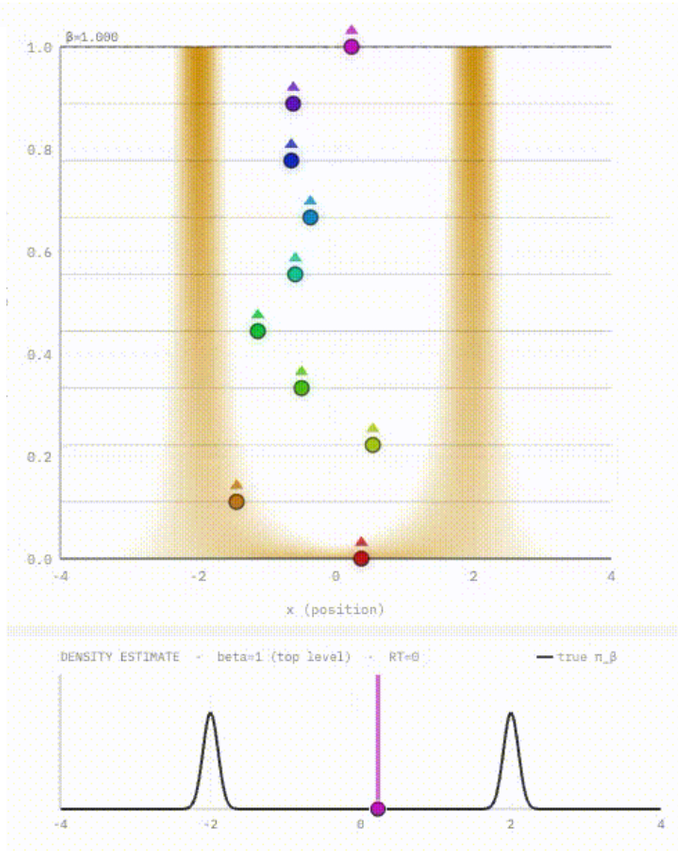
Sequential Annealing

- Construct path sequentially
- Samples generated in parallel
- Built using importance sampling
- Interacting → Sequential Monte Carlo Samplers
- Distributed → Simulated sampling

Parallel Annealing

- Construct path in parallel
- Samples generated in sequentially
- Built using MCMC
- Interacting → Parallel Tempering





SEQUENTIAL VERSUS PARALLEL ANNEALING

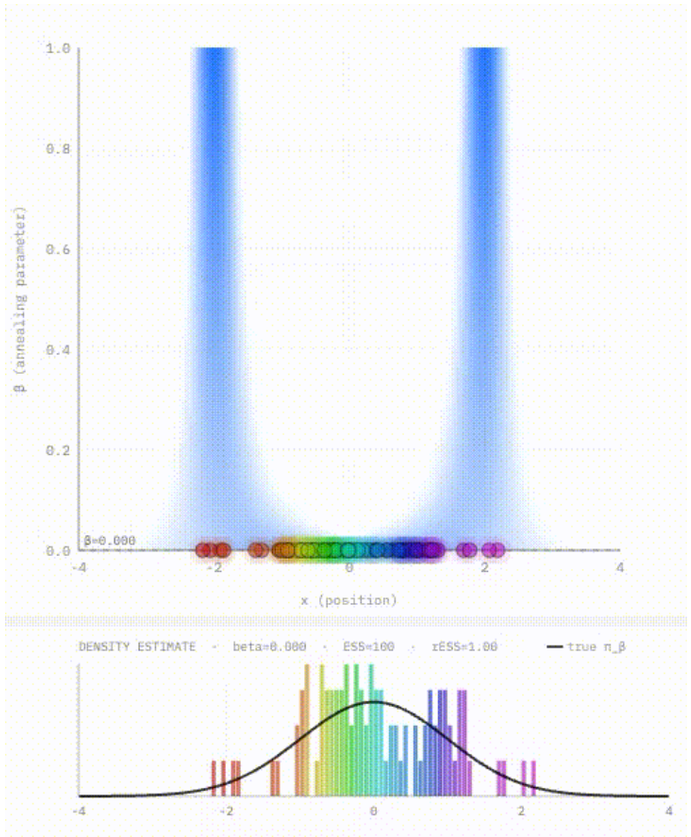
- We simultaneously evolve a system of particles to approximation the annealing path

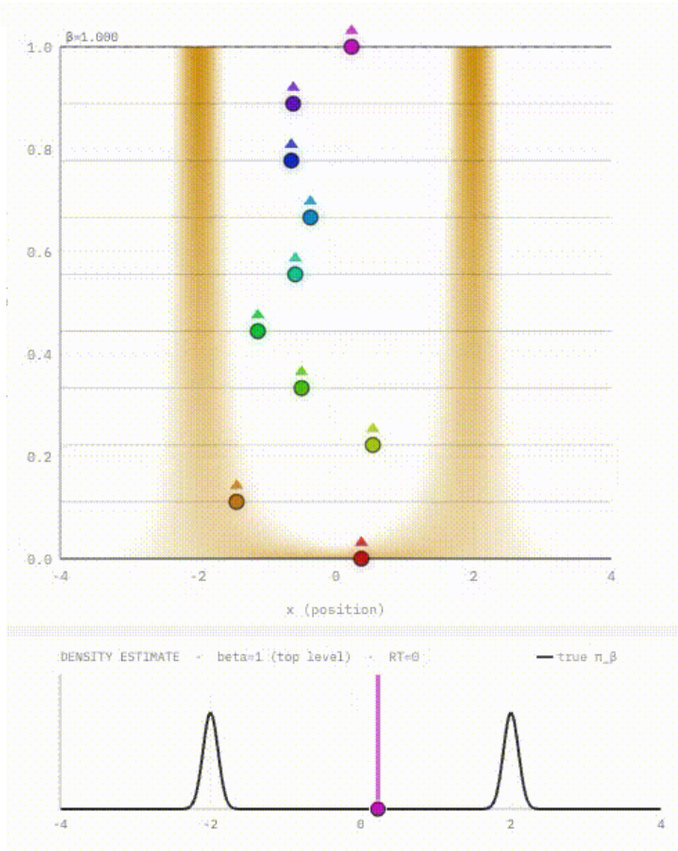
Sequential Annealing

- Construct path sequentially
- Samples generated in parallel
- Built using importance sampling
- Interacting → Sequential Monte Carlo Samplers
- Distributed → Simulated sampling

Parallel Annealing

- Construct path in parallel
- Samples generated in sequentially
- Built using MCMC
- Interacting → Parallel Tempering
- Distributed → Annealed Importance Sampling





PLAN FOR TERM

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- For the next 5 lectures we will do the following:

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  - **Parallel Annealing:**

PLAN FOR TERM

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PLAN FOR TERM

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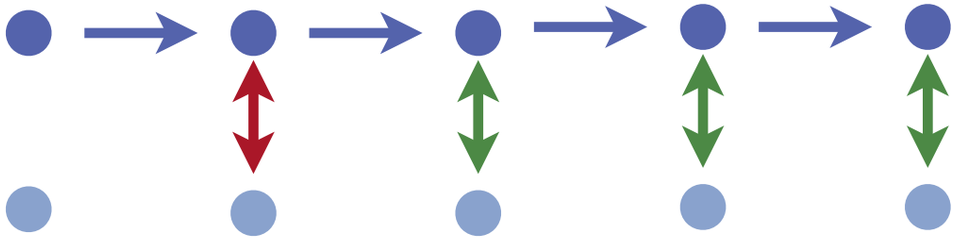
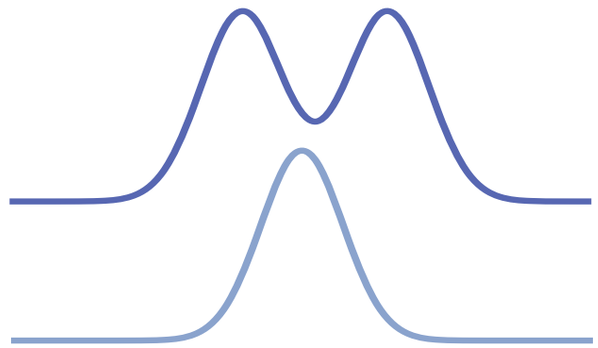
  - **Tuning annealing algorithms**
  - **Normalising constant estimation**

RECALL STABILISED MCMC

- Referenced stabilised MCMC is **stable** when reference is close to target
  - Acceptance rate is stable





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- Referenced stabilised MCMC is **stable** when reference is close to target
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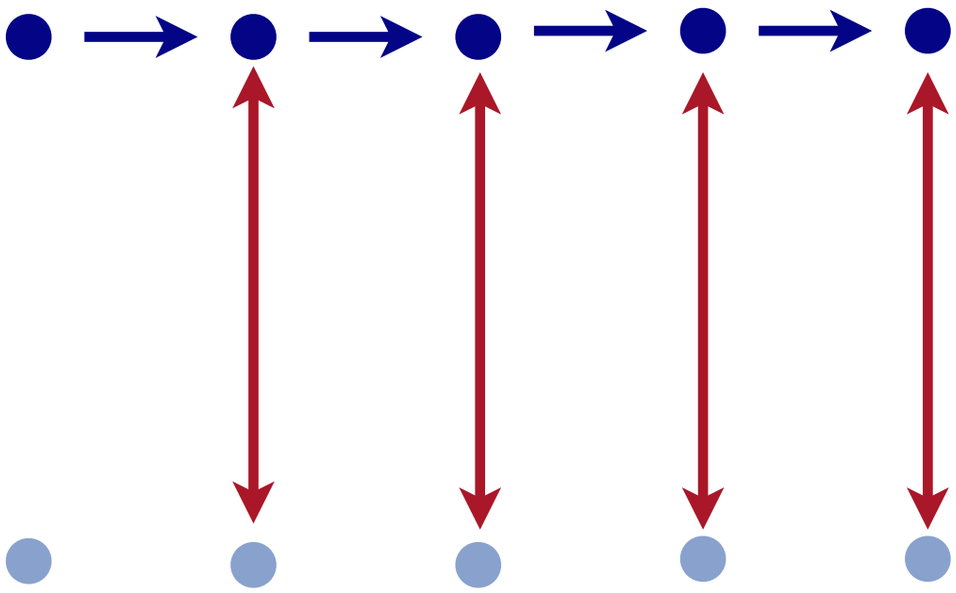
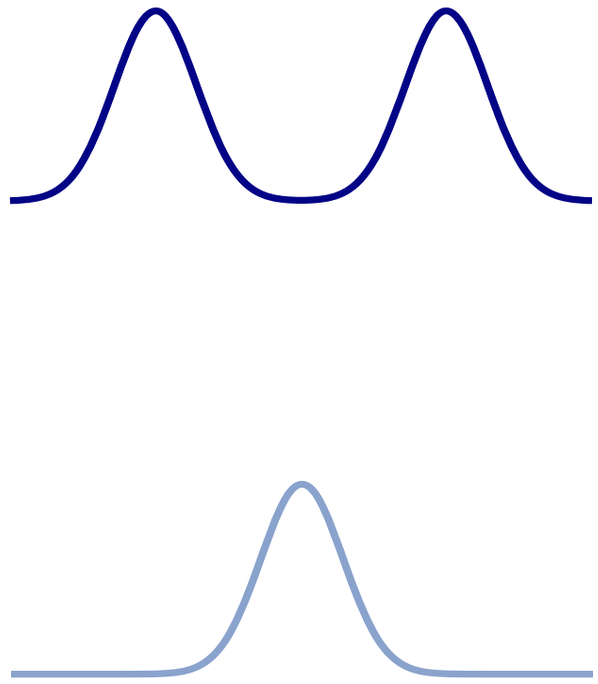
- Referenced stabilised MCMC is **fragile** when the reference share little support with target
  - Most proposed refernce samples are rejected





RECALL STABILISED MCMC

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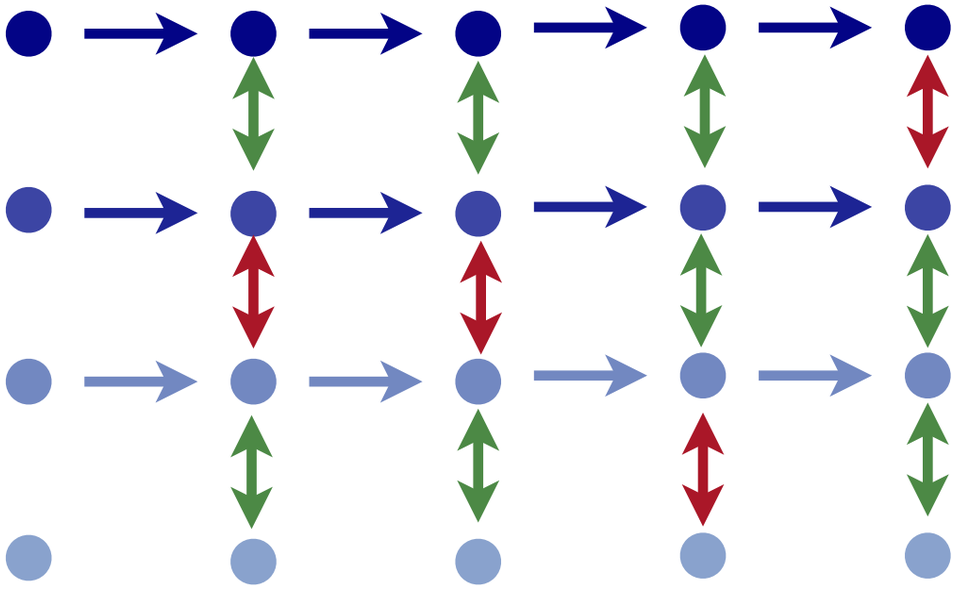
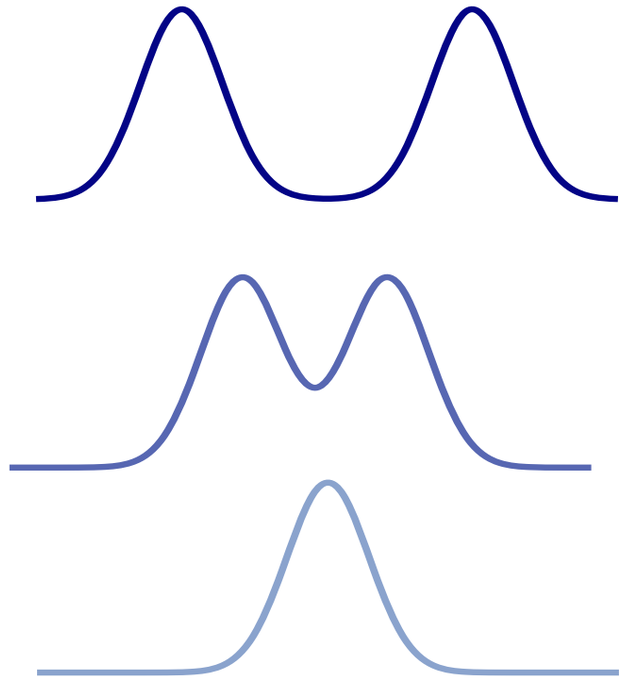
  - Most proposed refernce samples are rejected
- Introduce multiple interpolating distributions with enough overlap to maintain stability





PARALLEL TEMPERING

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- Uses stabilised MCMC to target annealing distributions in **parallel**

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Target X_t^N

$\vdots$

X_t^1

Reference X_t^0

PARALLEL TEMPERING

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Target X_t^N ●

⋮ ●

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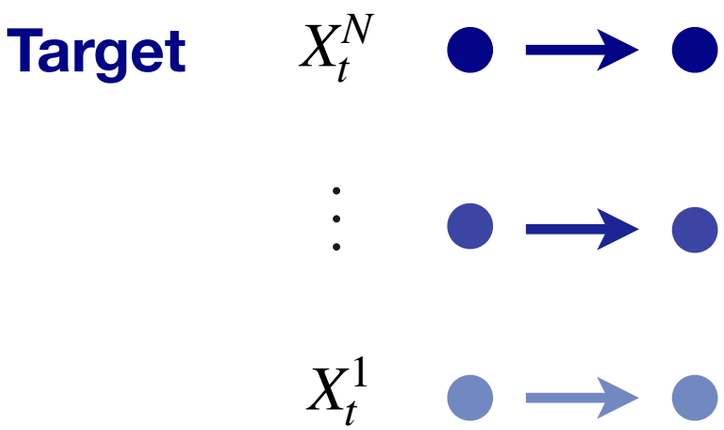

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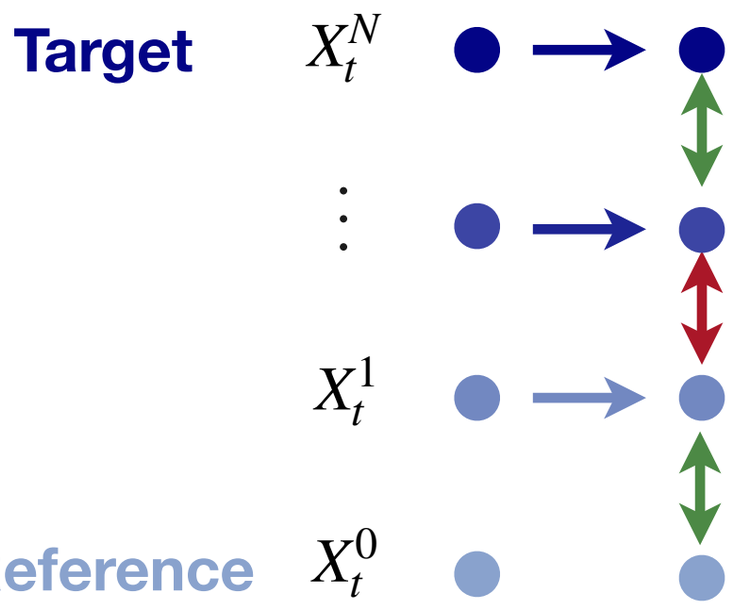

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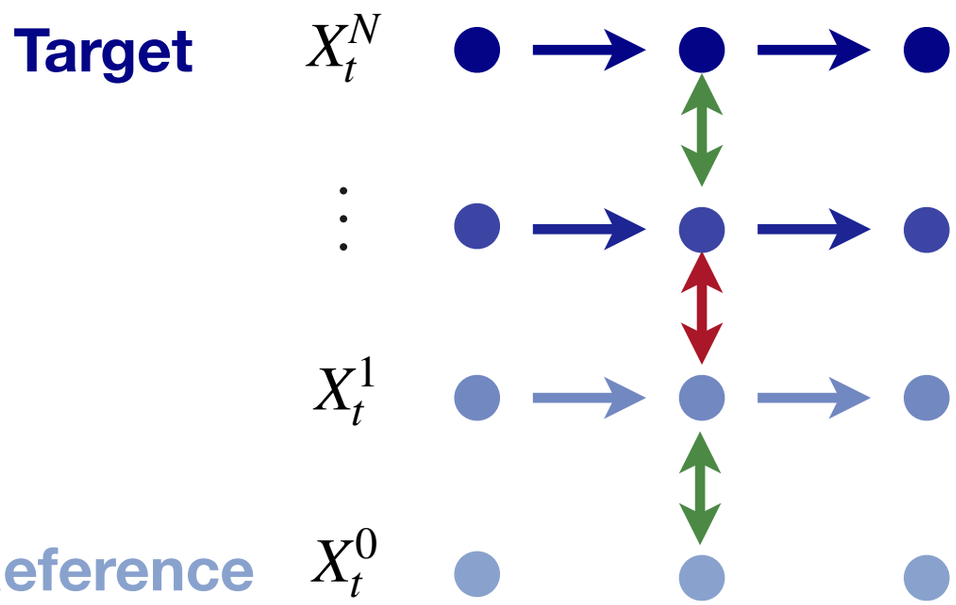

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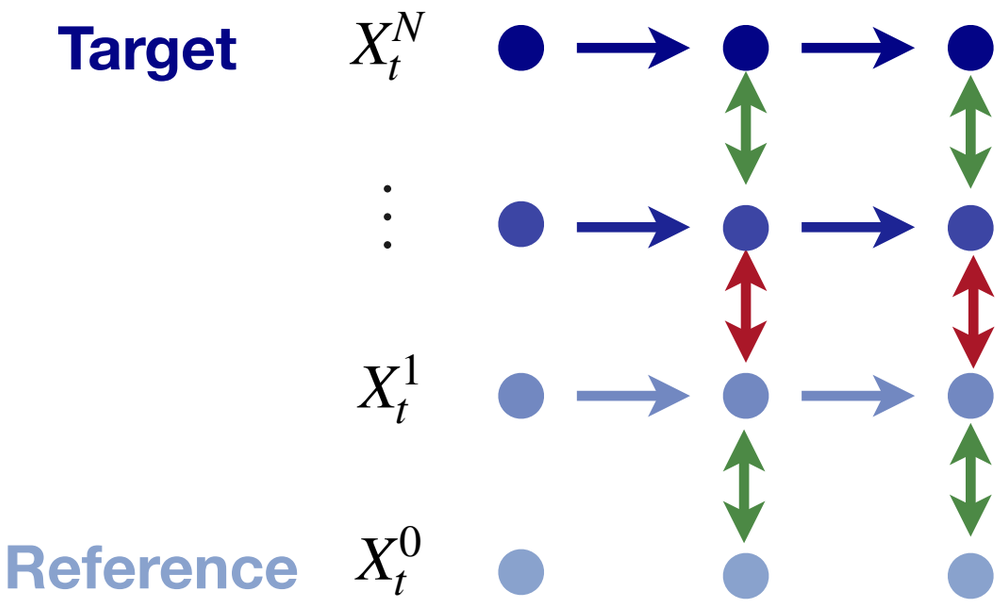

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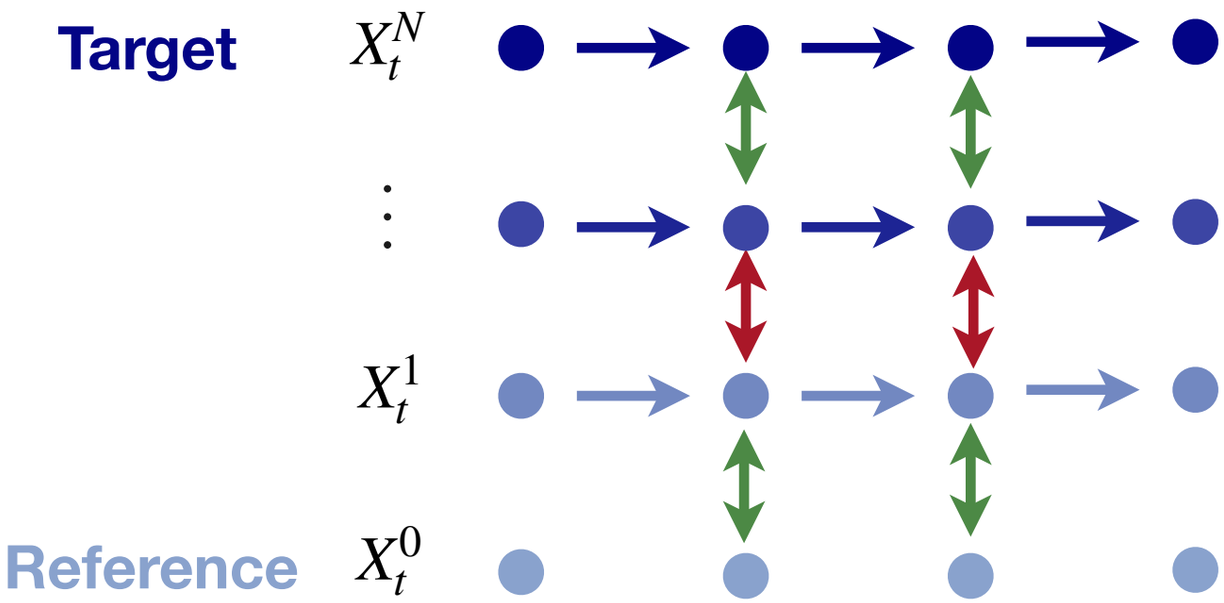

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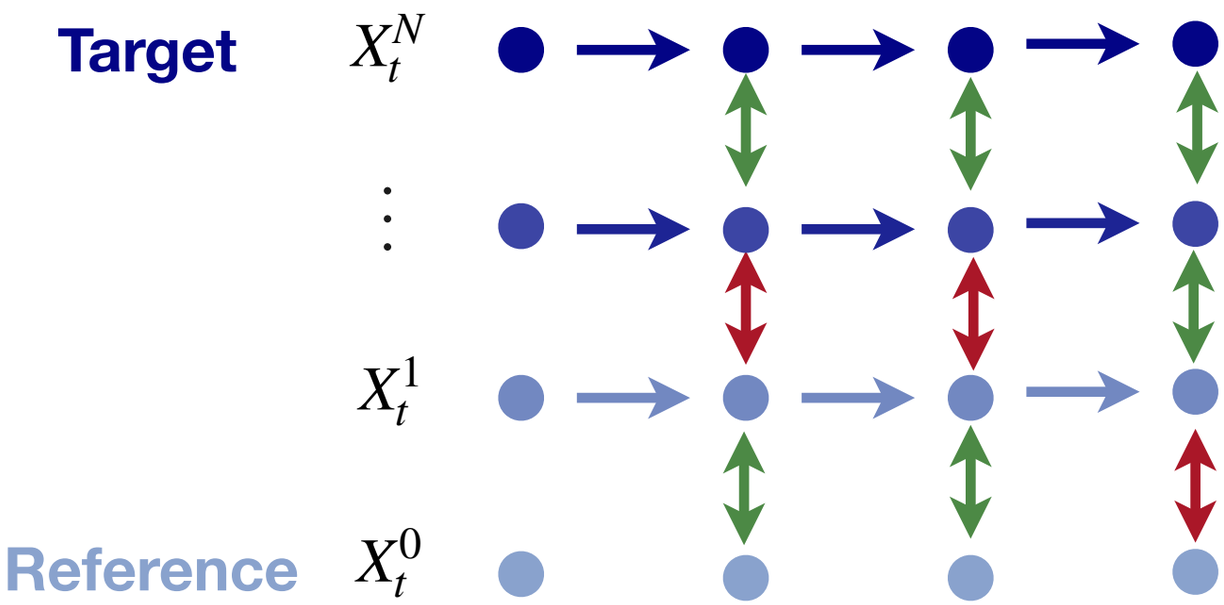

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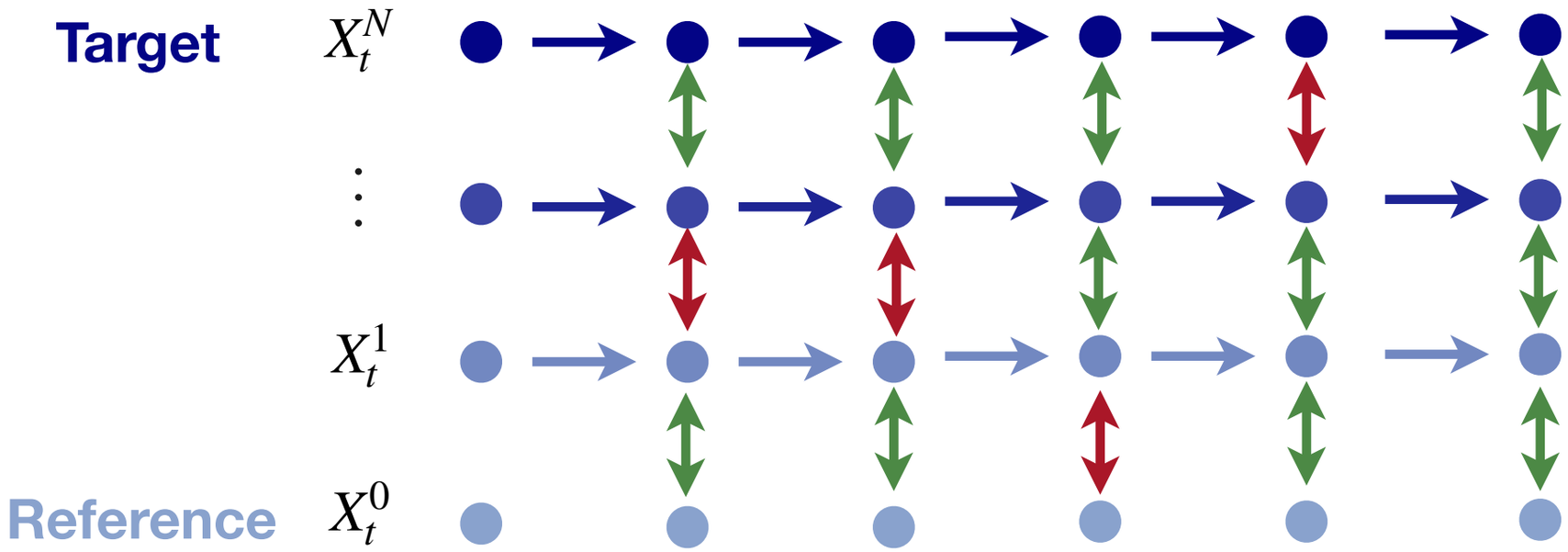

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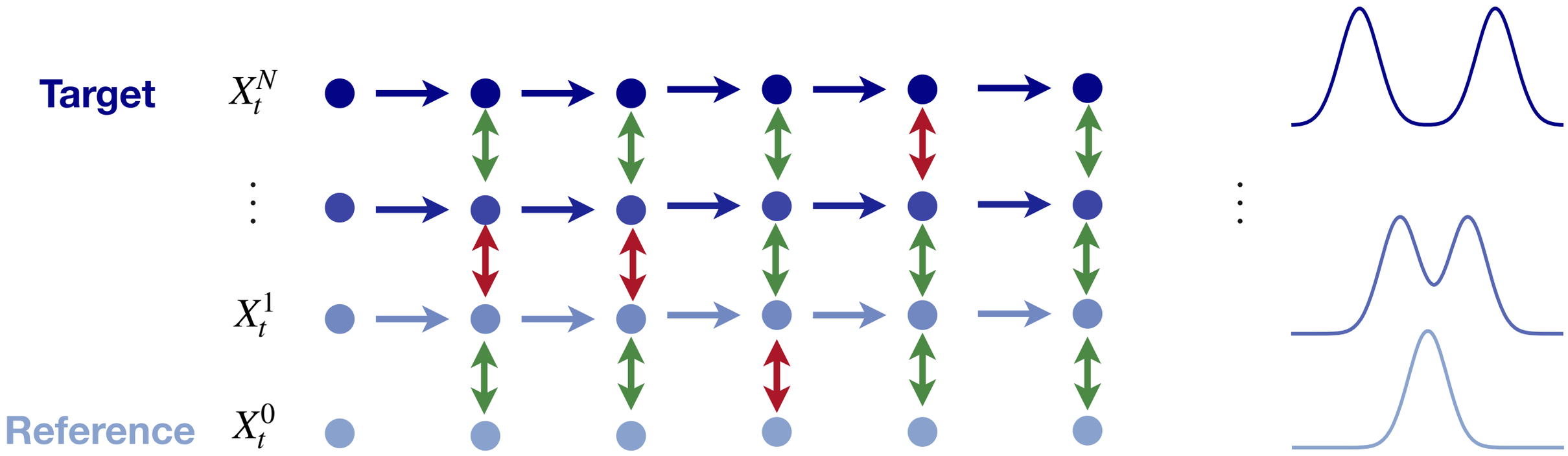

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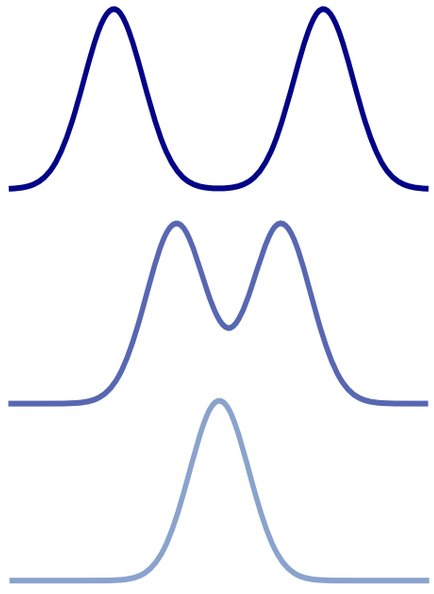
- Parallel tempering constructs MCMC chain $\mathbf{X}_t$ on $\mathbb{X}^{N+1}$ targetting $\pi_{\beta_0} \otimes \cdots \otimes \pi_{\beta_N}$

$$\mathbf{X}_t = \begin{pmatrix} X_t^N \\ \vdots \\ X_t^n \\ \vdots \\ X_t^0 \end{pmatrix} \begin{matrix} \sim \pi_{\beta_N} \\ \\ \sim \pi_{\beta_n} \\ \\ \sim \pi_{\beta_0} \end{matrix}$$

Target States

Interpolating States

Reference States



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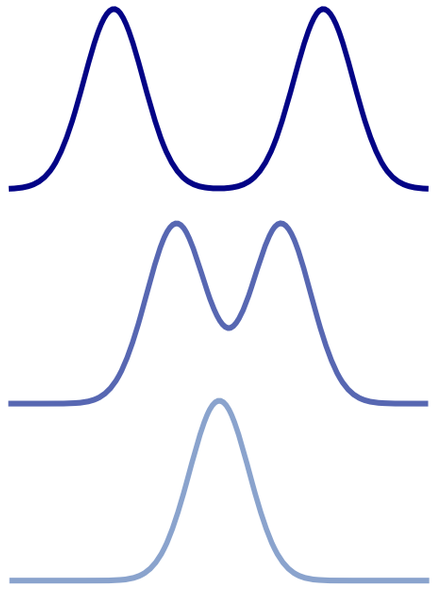

- Generate $\mathbf{X}_t$ from $\mathbf{X}_{t-1}$ using by applying the local exploration and communication moves

$$\mathbf{X}_t \sim \mathbf{K}_{\mathrm{PT}}(\mathbf{X}_{t-1}, \mathrm{d}\mathbf{x}') \qquad \mathbf{K}_{\mathrm{PT}} = \mathbf{K}_{\mathrm{expl}}\mathbf{K}_{\mathrm{comm}}$$

LOCAL EXPLORATION

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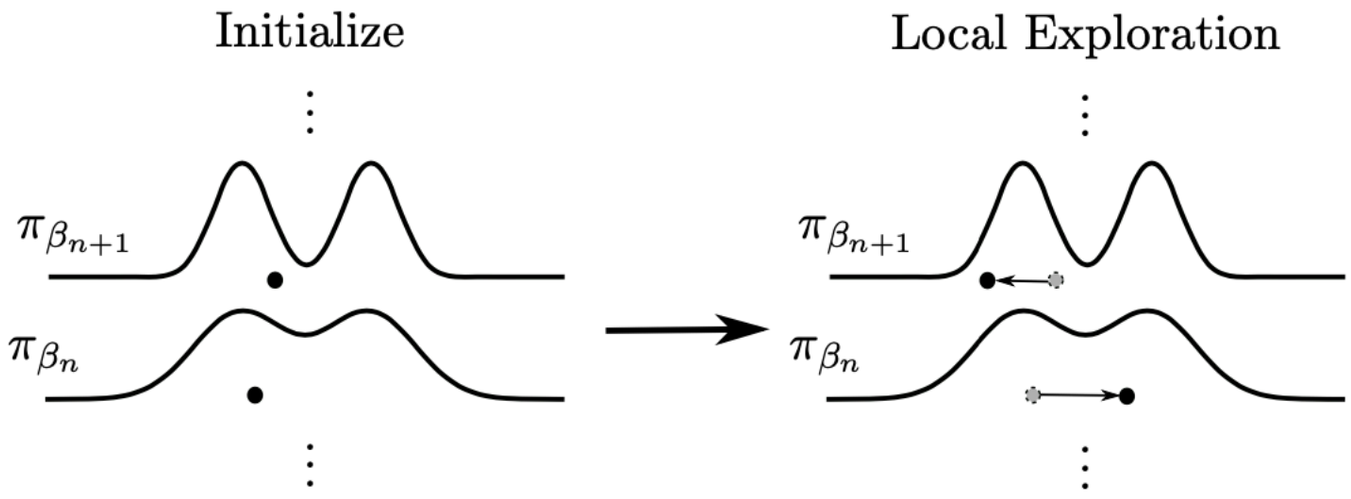

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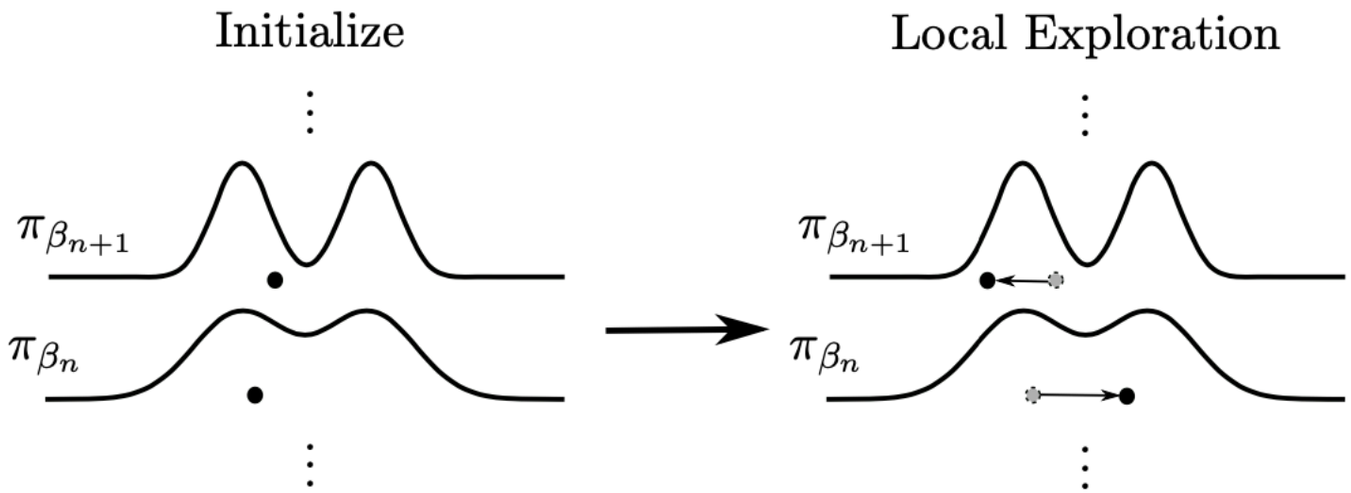
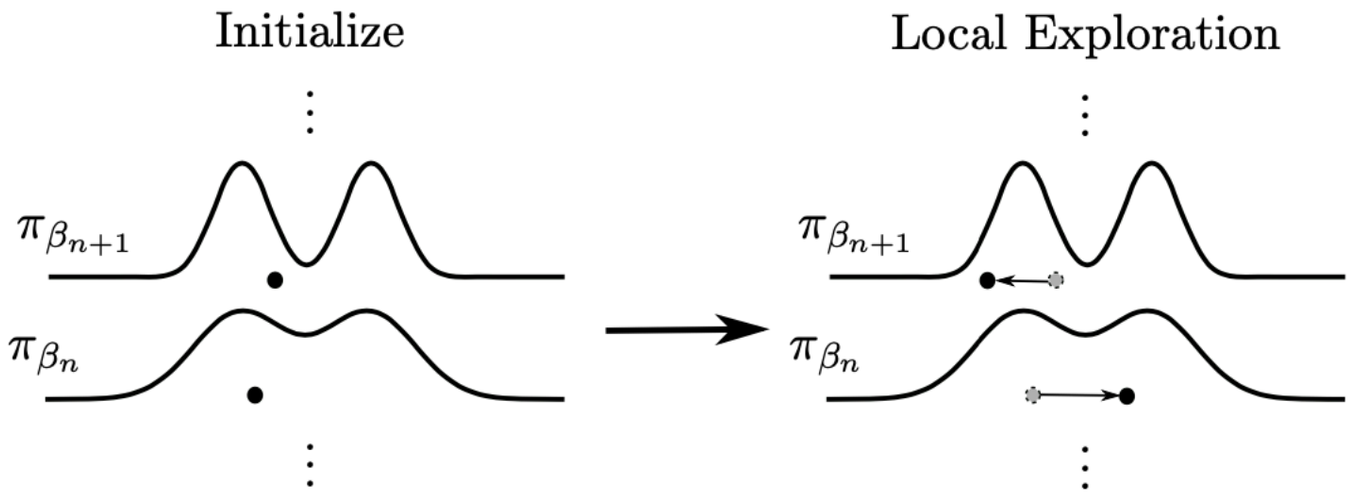


- **Exploration:** Update components of $\mathbf{x} = (x^0, \ldots, x^N)$ in parallel using MCMC

LOCAL EXPLORATION



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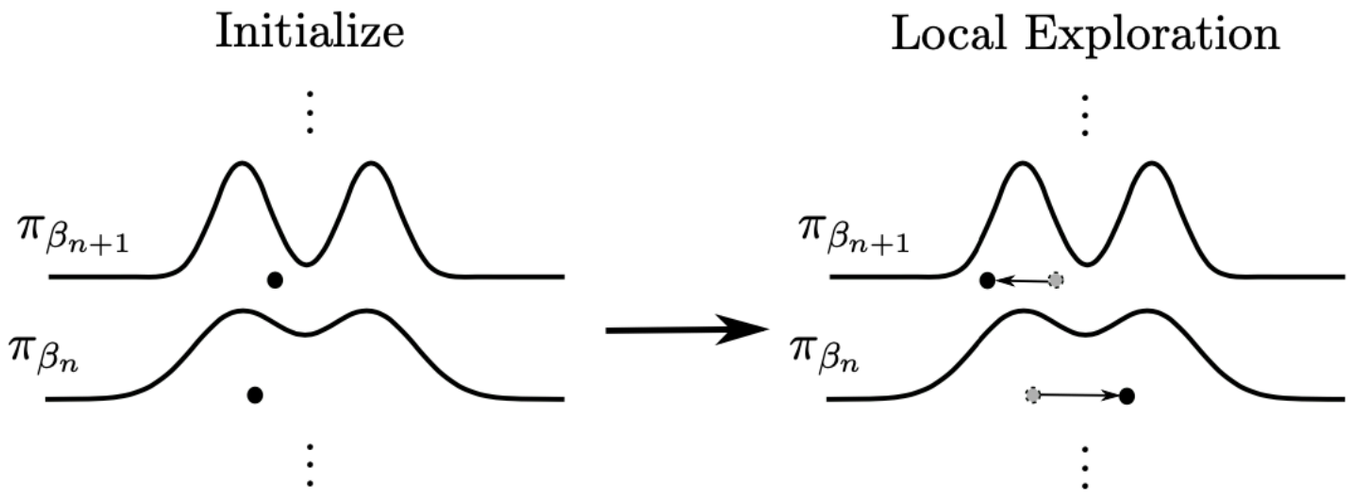
- Update the x^n using the local move K_{β_n} targeting π_{β_n}

$$K_{\text{expl}}(\mathbf{x}, \mathrm{d}\mathbf{x}') = K_{\beta_0} \otimes \cdots \otimes K_{\beta_N}(\mathbf{x}, \mathrm{d}\mathbf{x}')$$

LOCAL EXPLORATION



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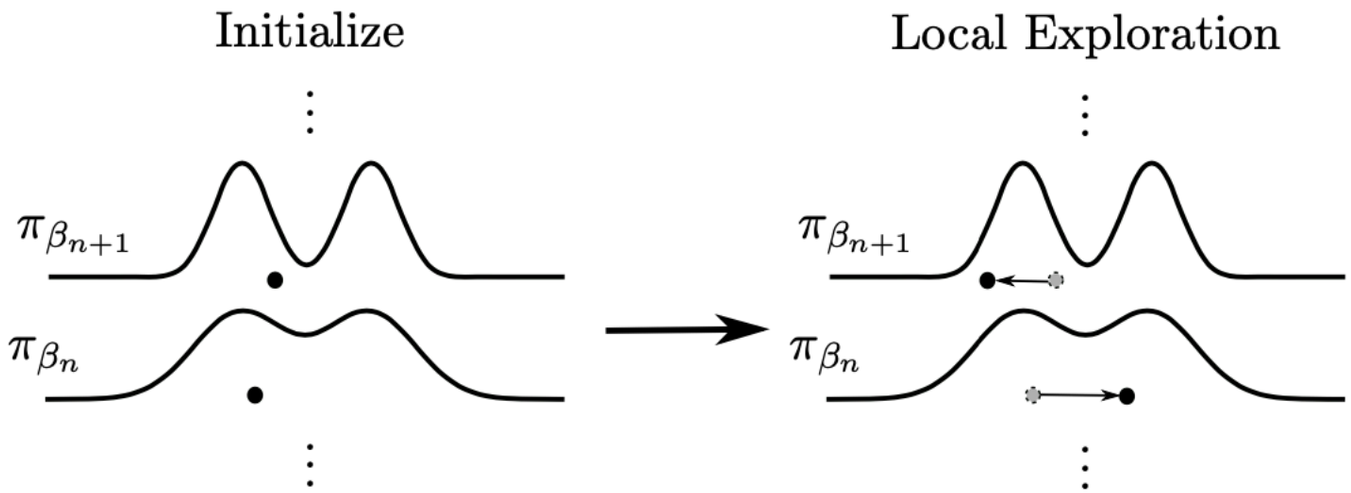
LOCAL EXPLORATION



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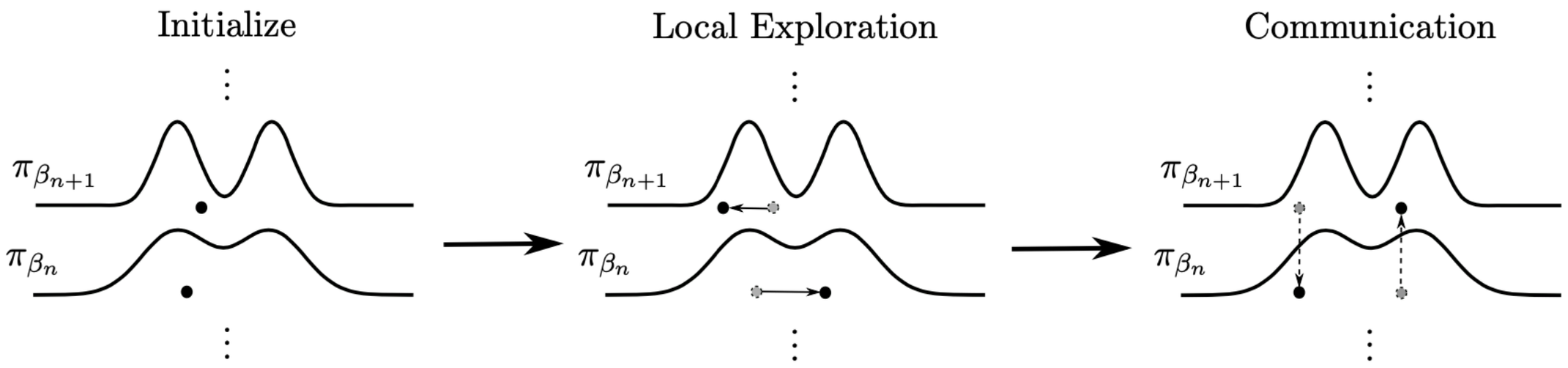
  - Assume that an independent sample from reference

$$K_{\text{expl}}(\mathbf{x}, \mathrm{d}\mathbf{x}') = K_{\beta_0} \otimes \cdots \otimes K_{\beta_N}(\mathbf{x}, \mathrm{d}\mathbf{x}')$$

$$= \eta(\mathrm{d}x'^0) \prod_{n=1}^{N} K_{\beta_n}(x^n, \mathrm{d}x'^n)$$

SWAP MOVE


Initialize
Local Exploration
Communication
$\pi_{\beta_{n+1}}$
π_{β_n}
$\pi_{\beta_{n+1}}$
π_{β_n}
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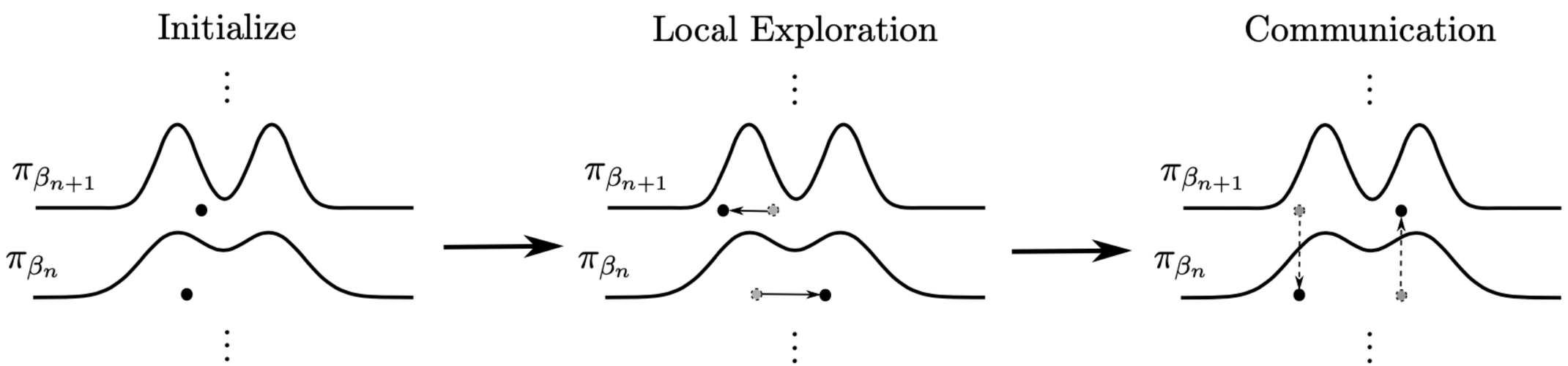
π_{β_n}

SWAP MOVE



- The n-th swap move takes the state $\mathbf{x}$ proposes $\mathbf{x}^{(n,n+1)}$ swapping components n and $n+1$

$$\mathbf{x}^{(n,n+1)} = (x^0, \ldots, x^{n-1}, x^{n+1}, x^n, x^{n+2}, \ldots, x^N)$$

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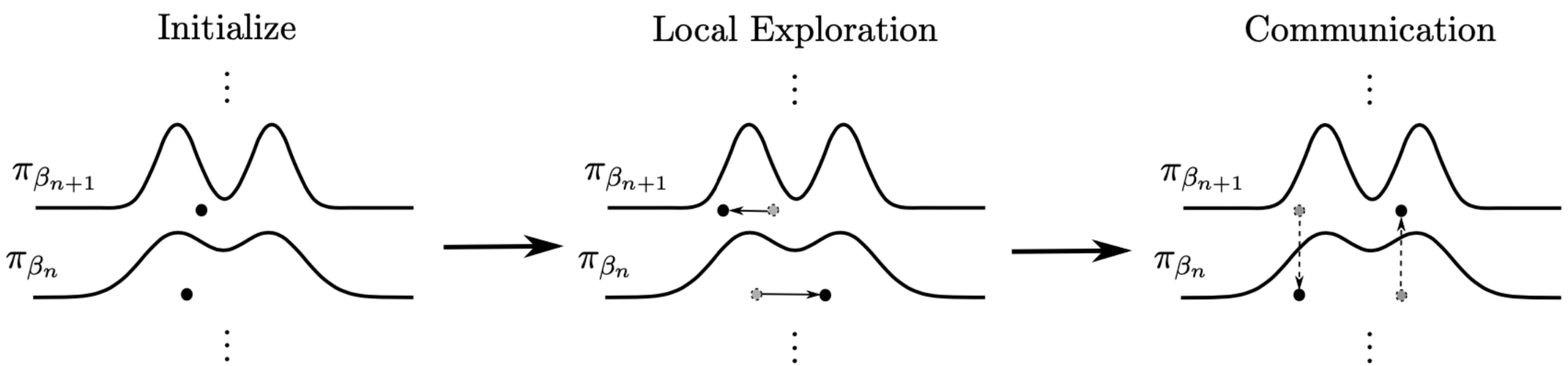

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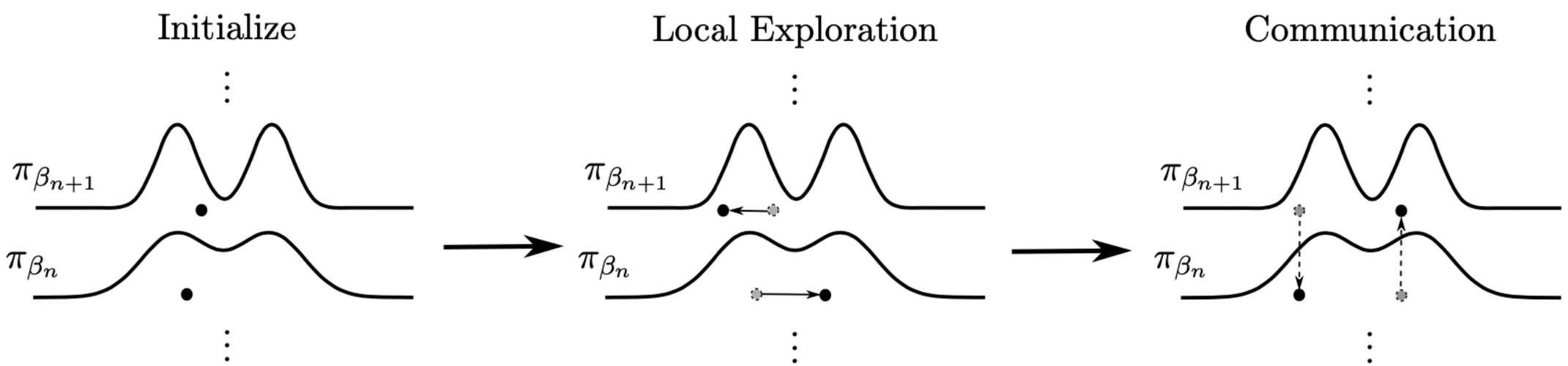
$$\mathbf{K}^{(n,n+1)}(\mathbf{x}, \mathrm{d}\mathbf{x}') = \alpha^{(n,n+1)}(\mathbf{x})\delta_{\mathbf{x}^{(n,n+1)}}(\mathrm{d}\mathbf{x}') + (1 - \alpha^{(n,n+1)}(\mathbf{x})\delta_{\mathbf{x}}(\mathrm{d}\mathbf{x}')$$

SWAP MOVE



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$$\alpha^{(n,n+1)}(\mathbf{x}) = 1 \wedge \frac{\boldsymbol{\pi}(\mathbf{x}^{(n,n+1)})}{\boldsymbol{\pi}(\mathbf{x})}$$

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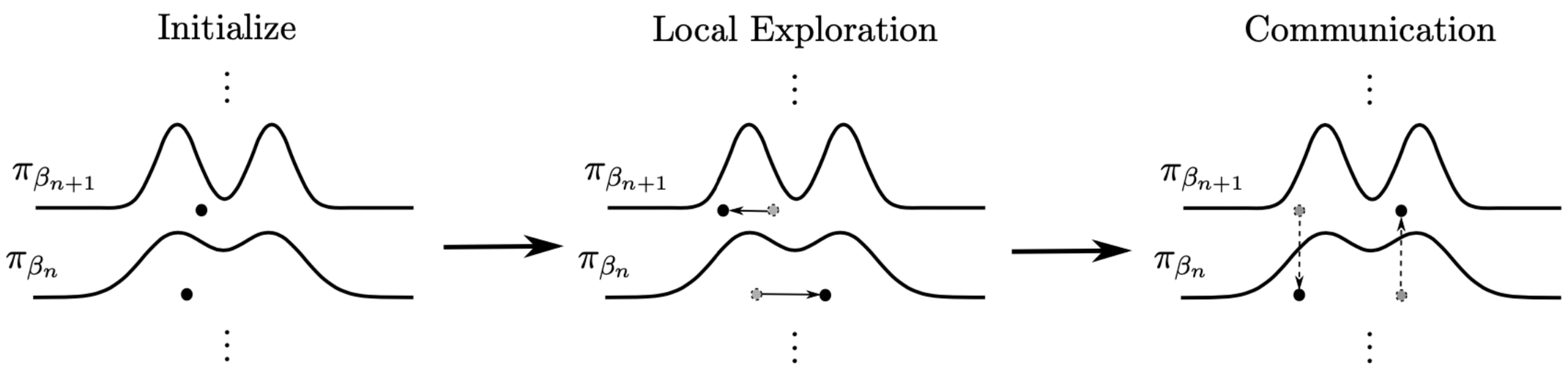

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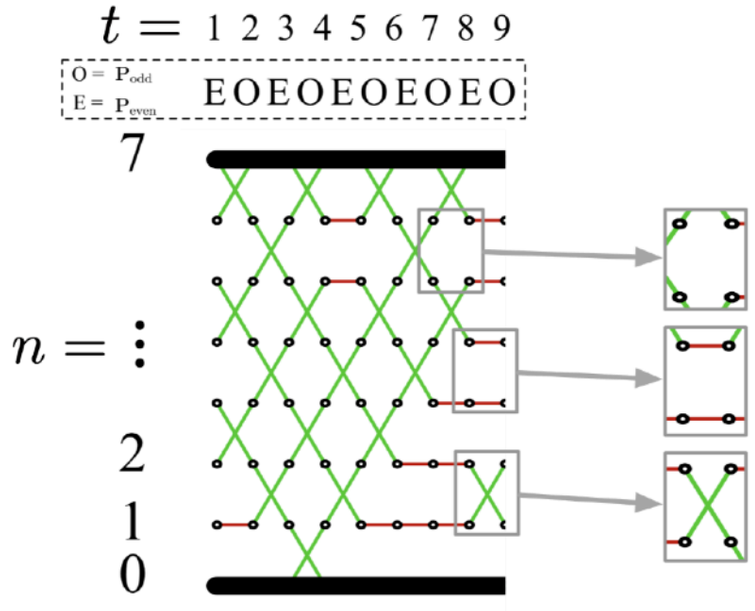
COMMUNICATION

COMMUNICATION

- **Communication move**

$$\mathbf{K}_{\text{comm}} = \prod_{n=1}^{N} K^{(n,n+1)} P_t^{(n,n+1)}$$



Proposal indicators

$P_7^{(5,6)} = 0$

$P_8^{(3,4)} = 1$

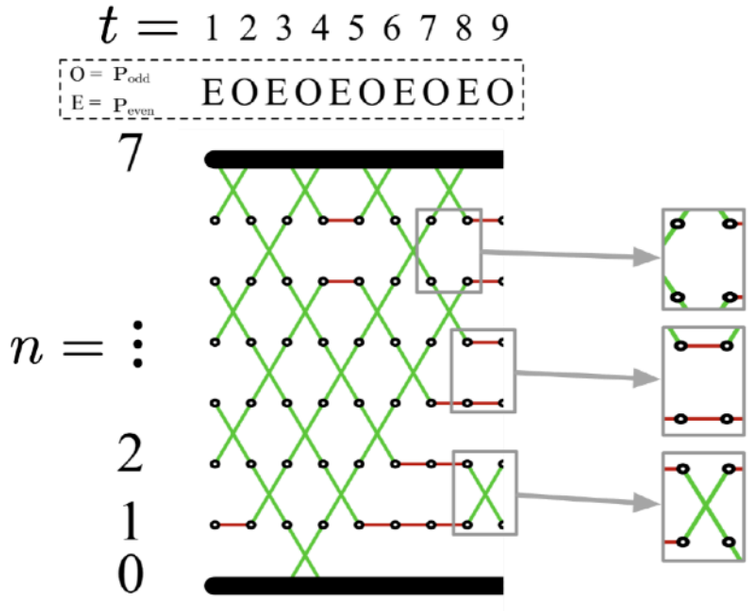
$P_8^{(1,2)} = 1$

COMMUNICATION

- **Communication move**

$$\mathbf{K}_{\text{comm}} = \prod_{n=1}^{N} K^{(n,n+1)} P_t^{(n,n+1)}$$

  - $P_t^{(n,n+1)} \in \{0,1\}$ indicated if the n-th swap is proposed



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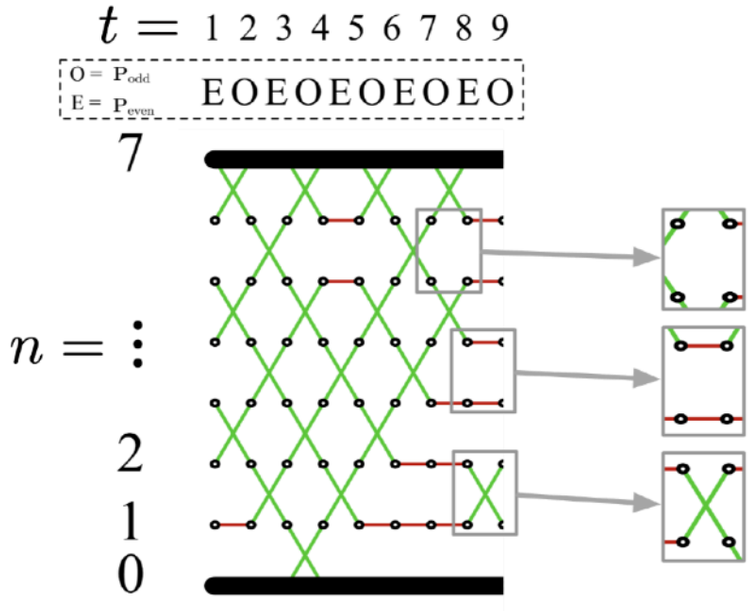

Proposal indicators

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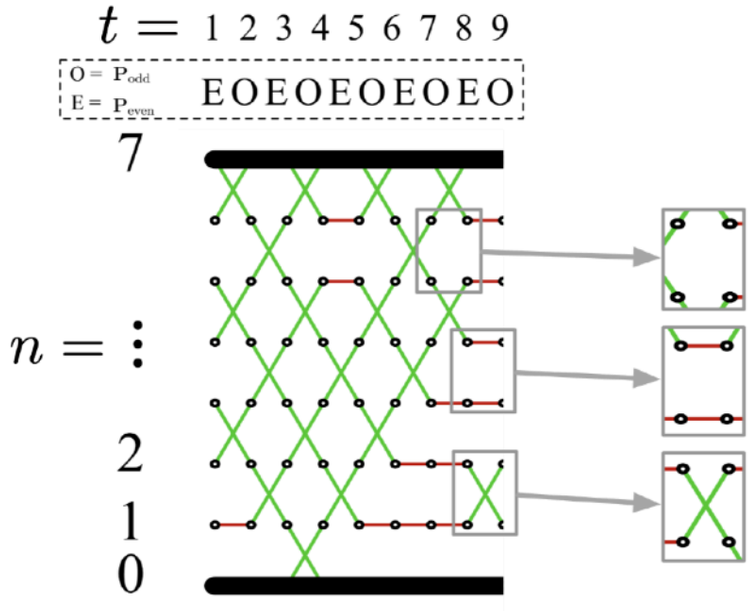

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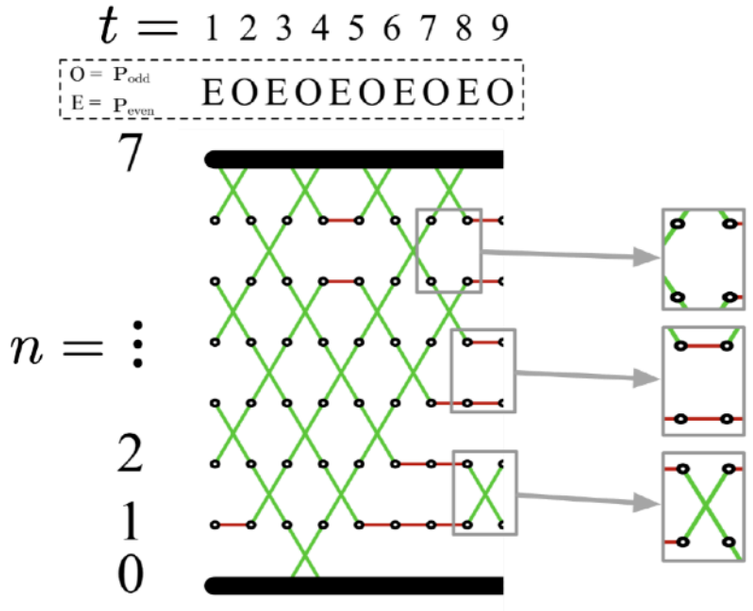

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  - These are the largest collection of swap moves in parallel
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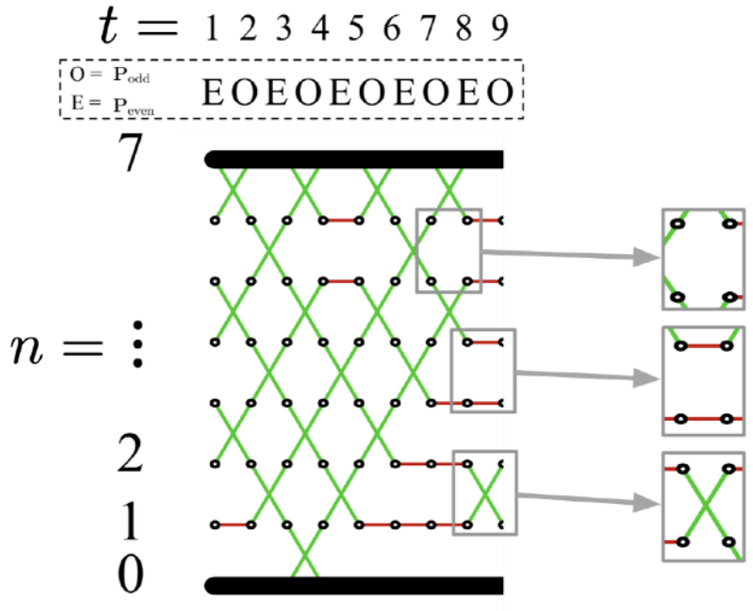

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PARALLEL TEMPERING

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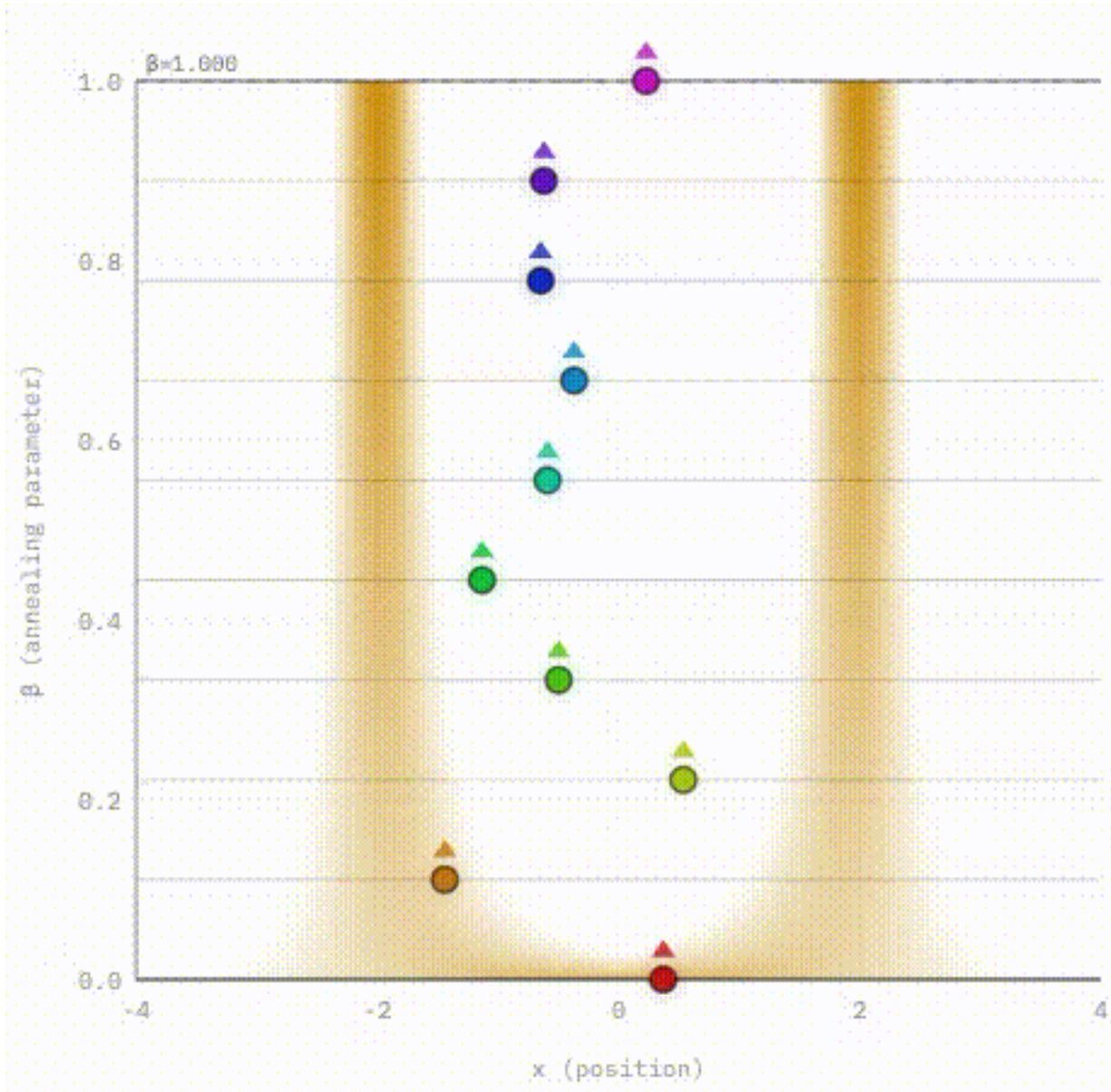
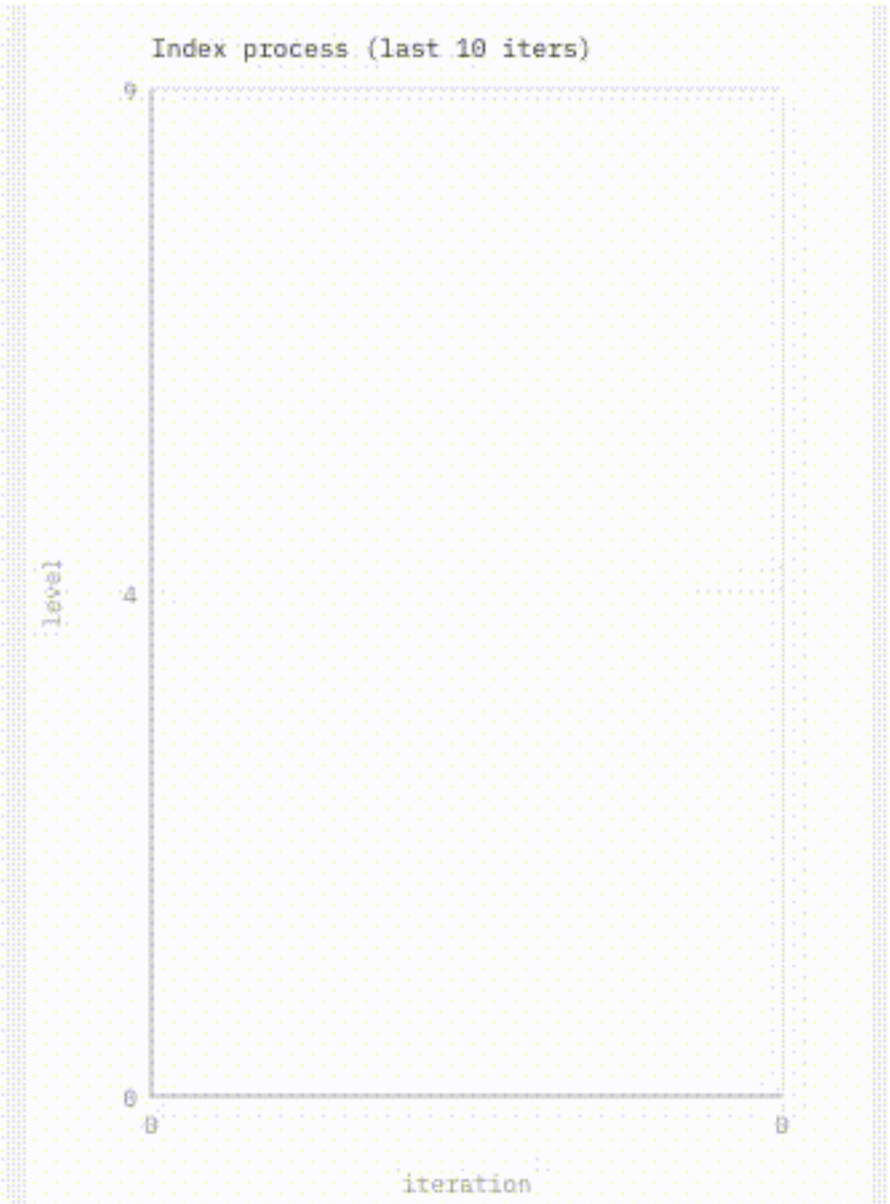
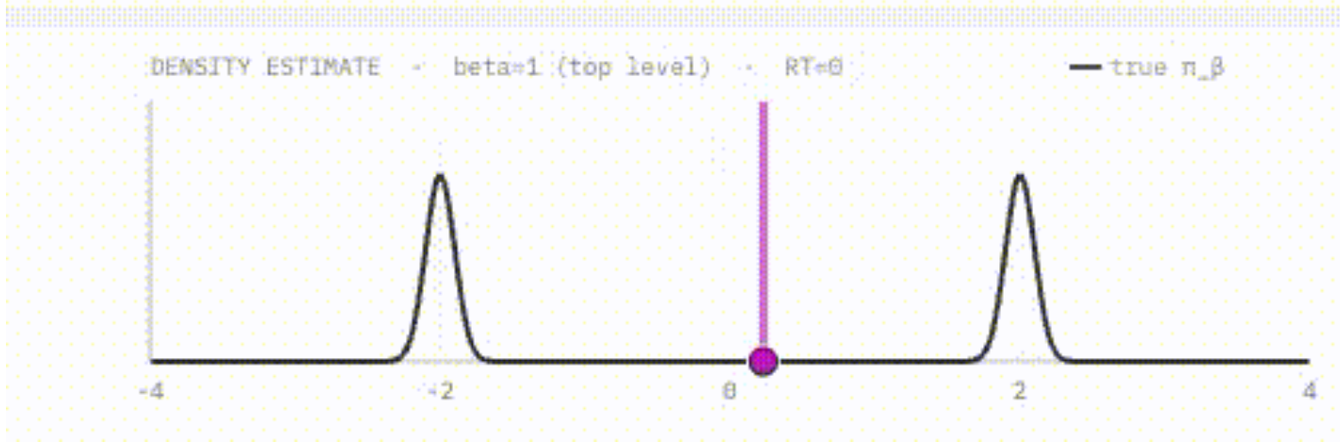


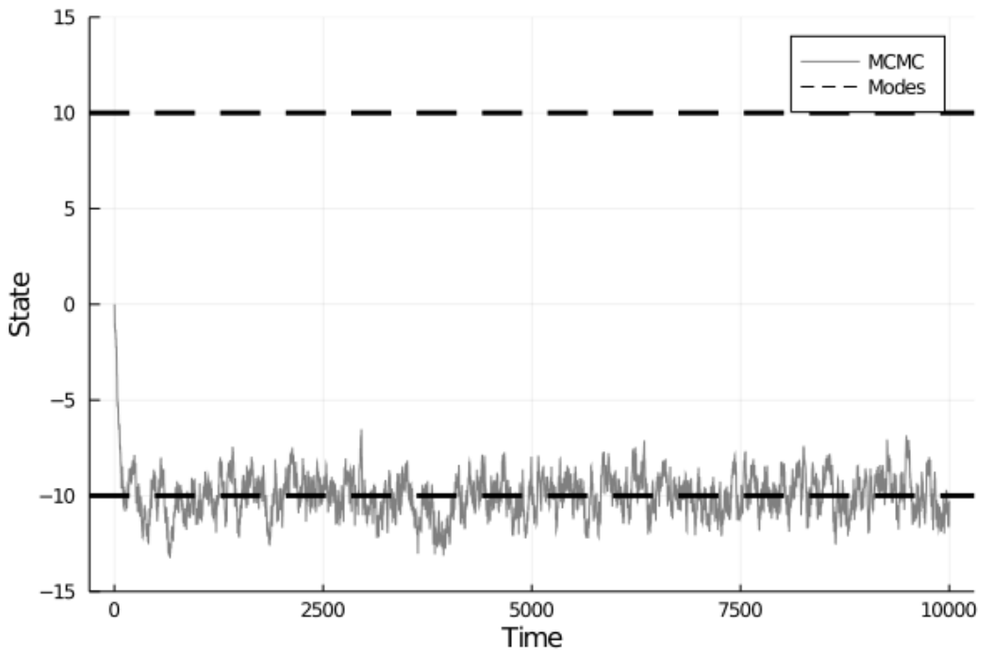


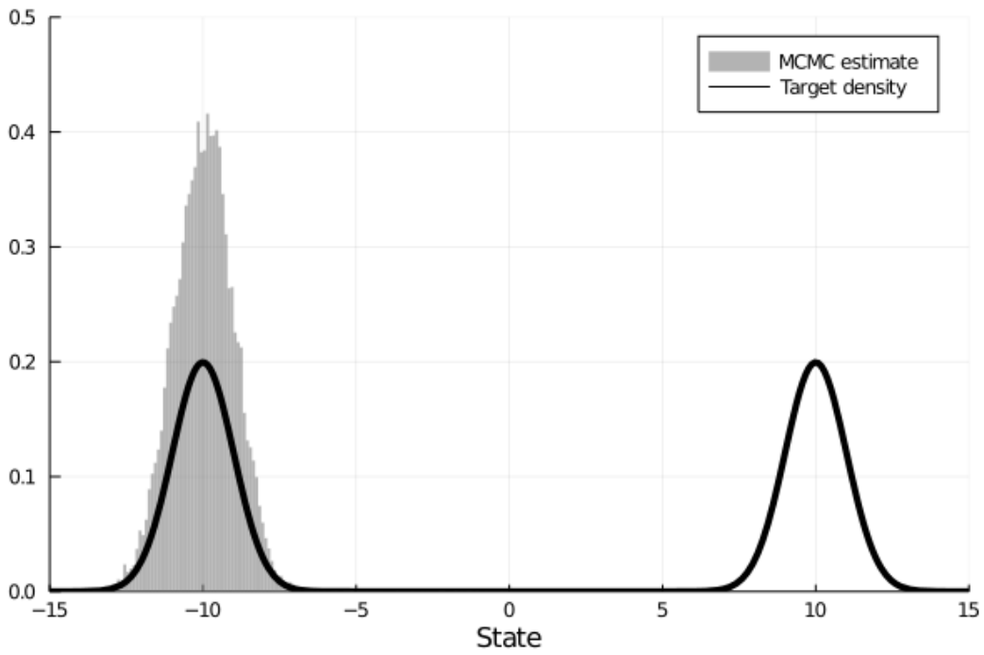


MCMC VS PARALLEL TEMPERING

MCMC VS PARALLEL TEMPERING

Single Chain MCMC





MCMC VS PARALLEL TEMPERING

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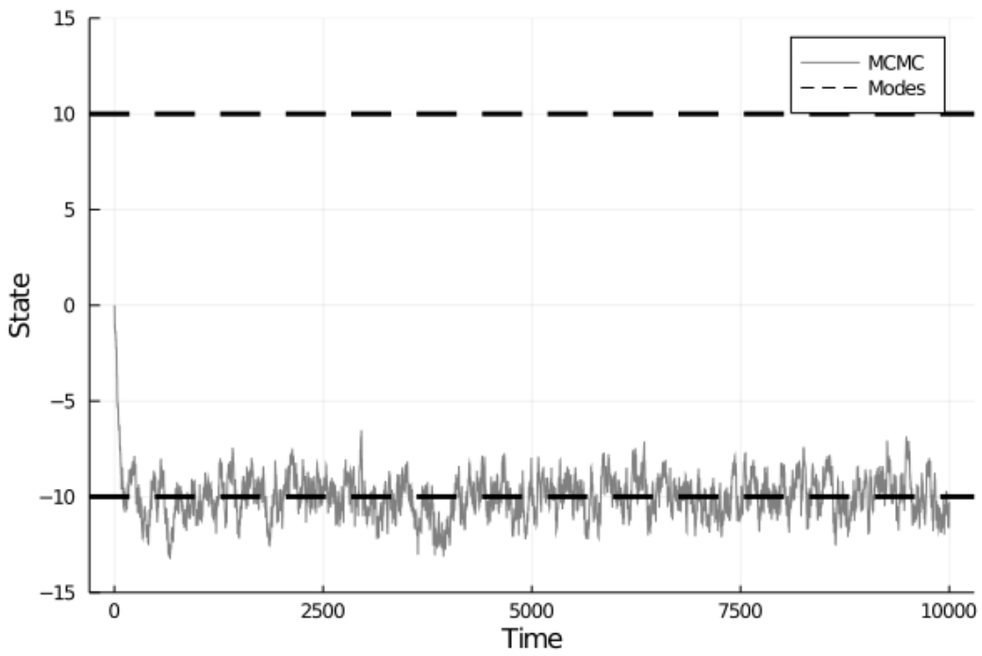
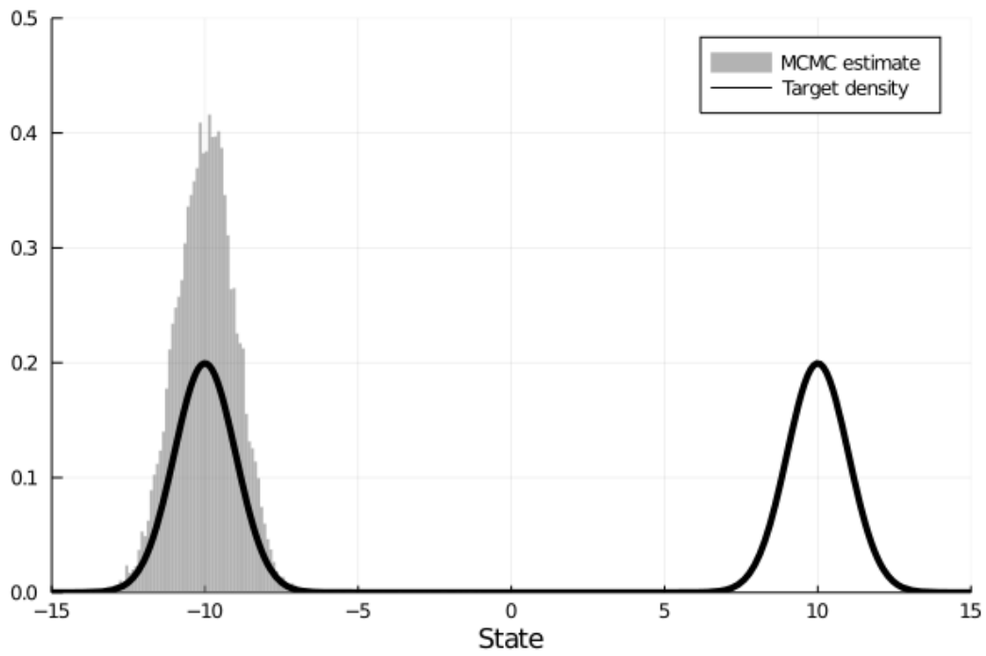
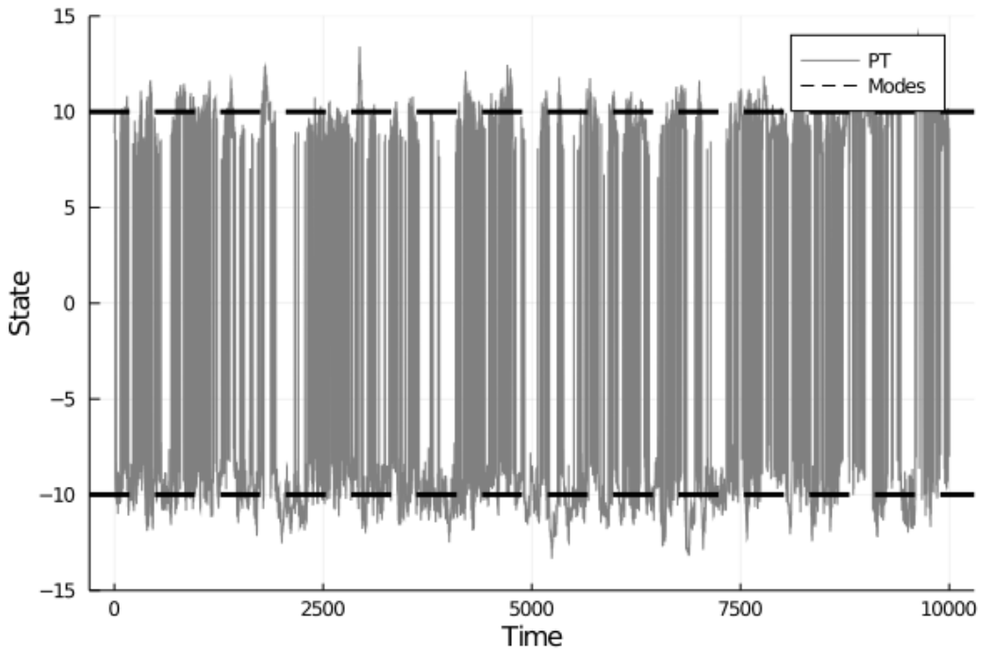
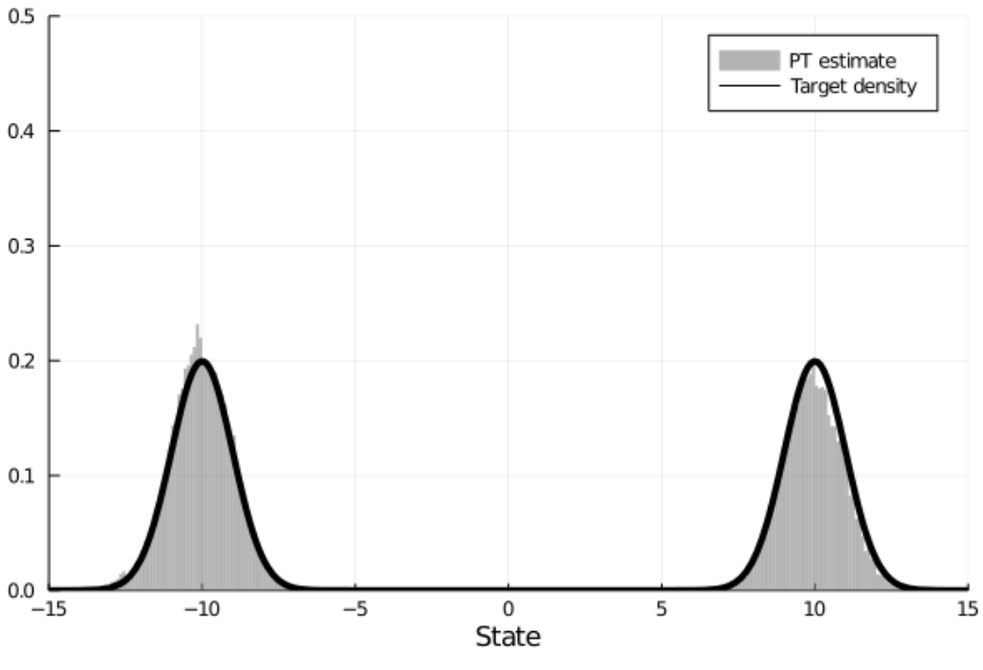




Parallel Tempering (N = 10)

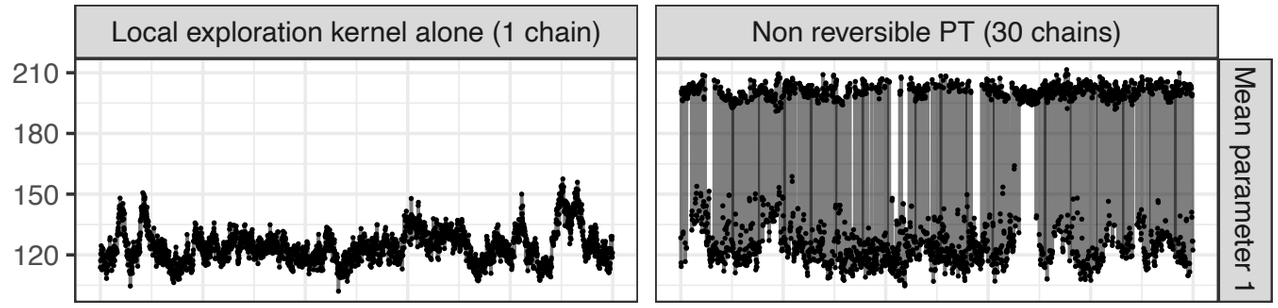




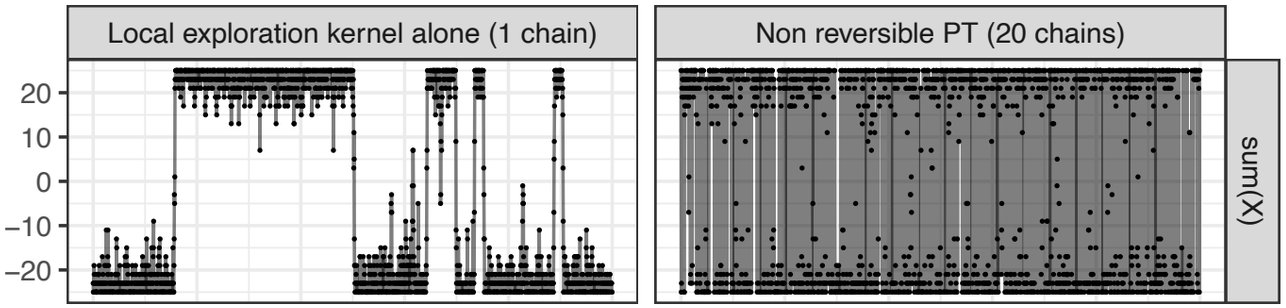
EXAMPLE: MULTIMODAL TARGETS

Single Chain MCMC **Parallel Tempering**

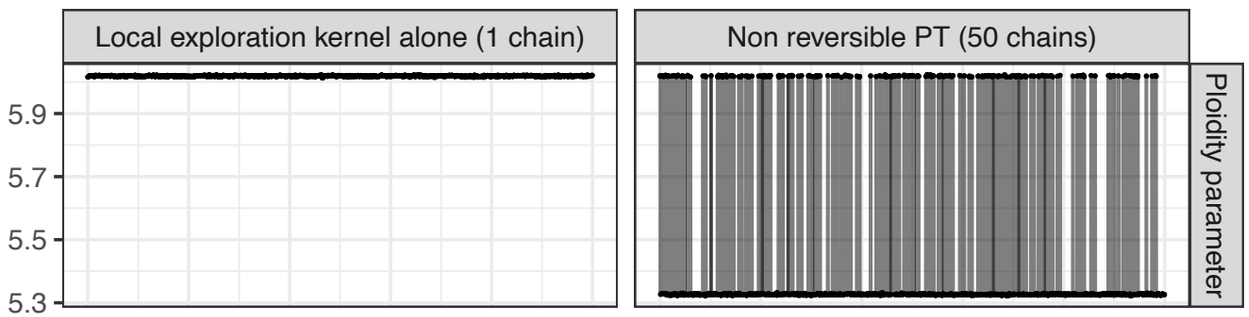
Bayesian Mixture Model
(d = 155)



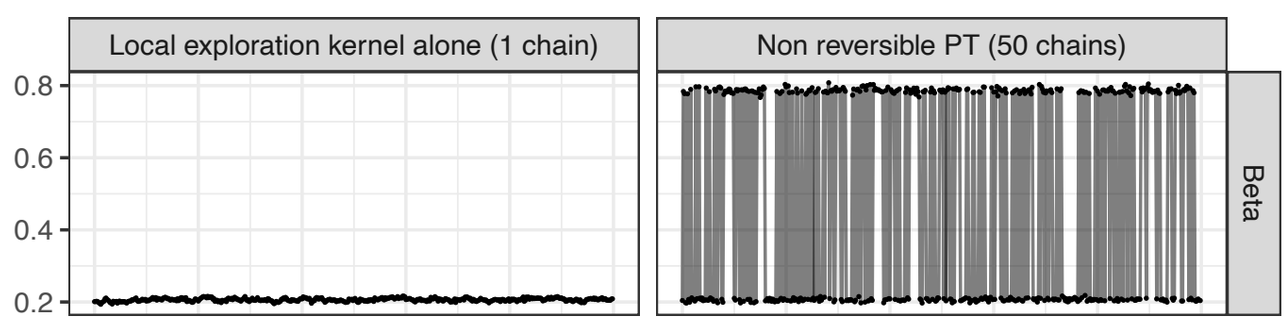
Ising Model
(d = 25)



Copy number inference
w/ whole genome ovarian cancer data
(d = 30)



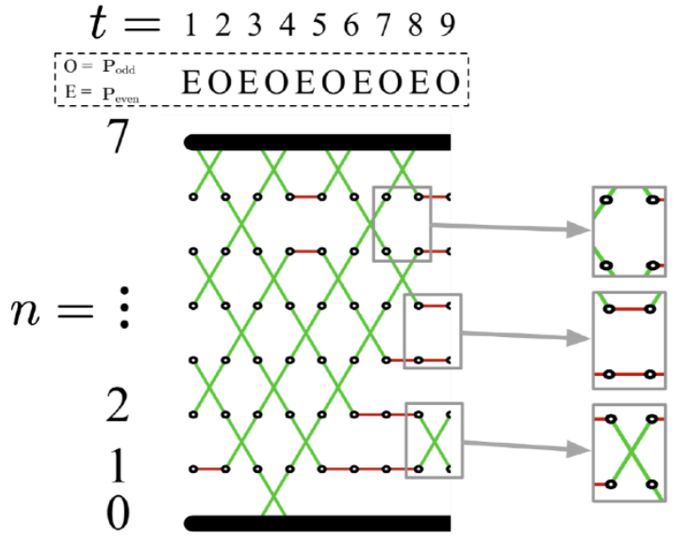
ODE parameter inference
w/ mRNA data
(d = 9)



DISTRIBUTED PT

DISTRIBUTED PT

- **Dual perspective on PT:** Swap annealing parameters not states!



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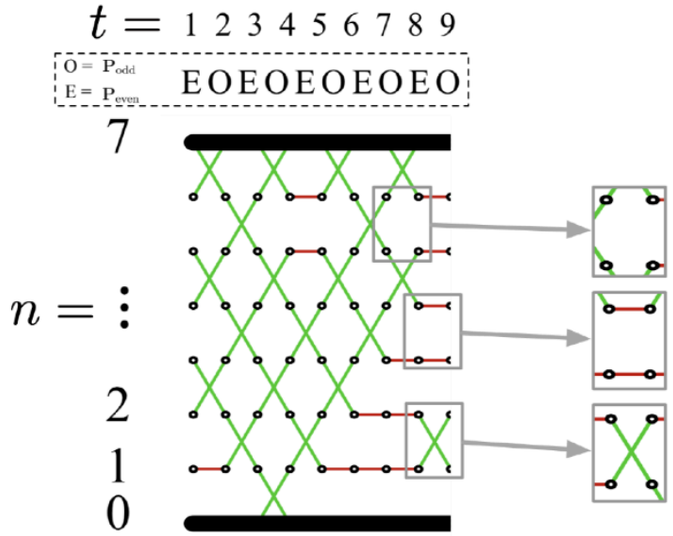
DISTRIBUTED PT

- **Dual perspective on PT:** Swap annealing parameters not states!
  - We can study communication through the dynamics of the permuted annealing parameters



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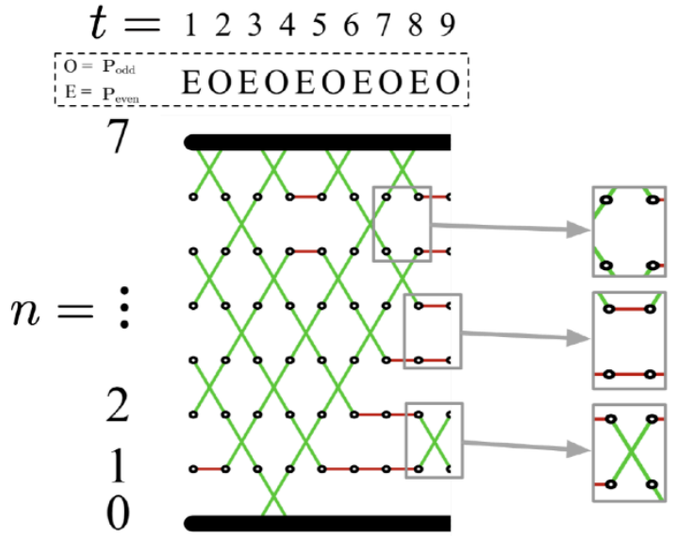

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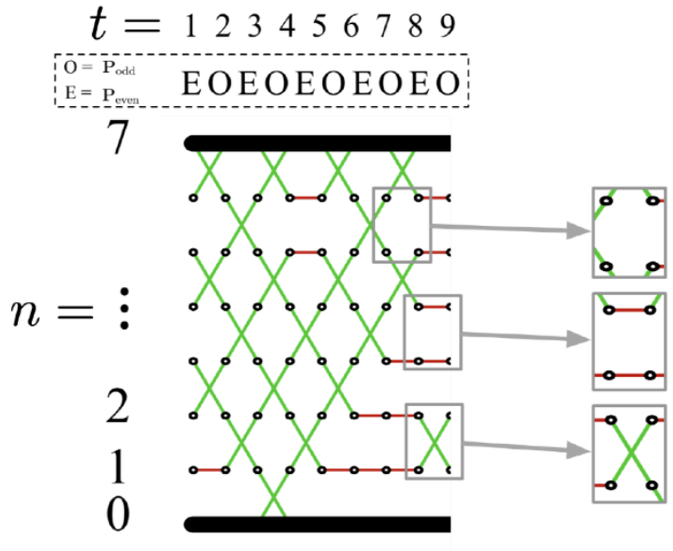

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$$\mathbf{Y}_t = (Y_t^0, \ldots, Y_t^N)$$

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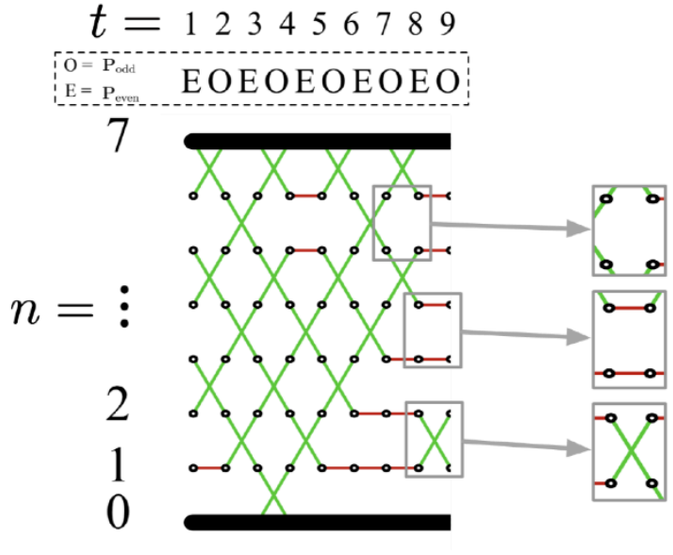

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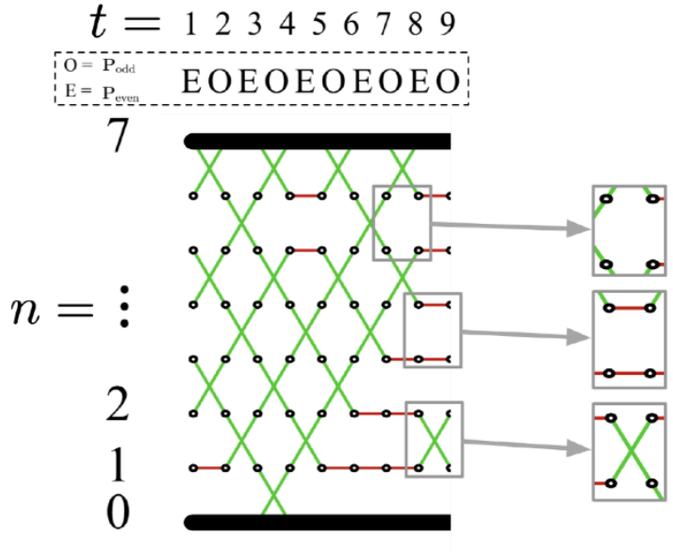
- X_t^n is commonly referred to as n-th **chain** and Y_t^m the m-th **replica**



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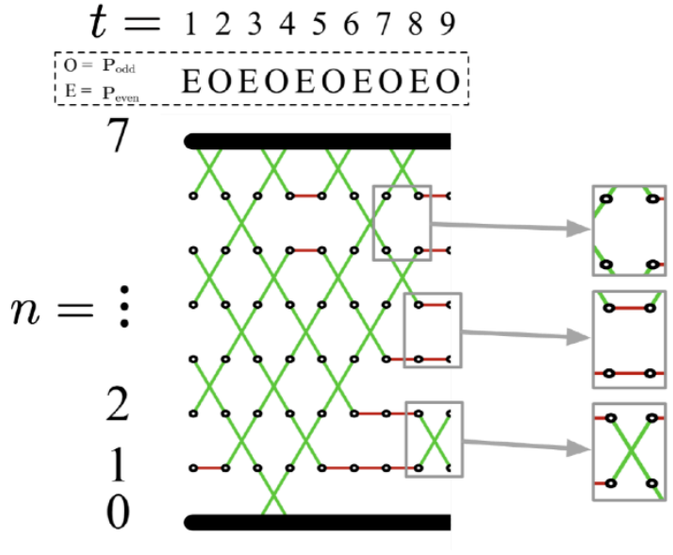
- X_t^n is commonly referred to as n-th **chain** and Y_t^m the m-th **replica**
- We note that $\mathbf{Y}_t$ is $\mathbf{X}_t$ shuffled according to permutation $\mathbf{I}_t$



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$$Y_0^m = X_0^m, \qquad I_0^m = m, \qquad \epsilon_0^m = (-1)^m$$

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$$Y_{t+1}^m \sim K_{\beta_t^m}(Y_t^m, \mathrm{d}y)$$

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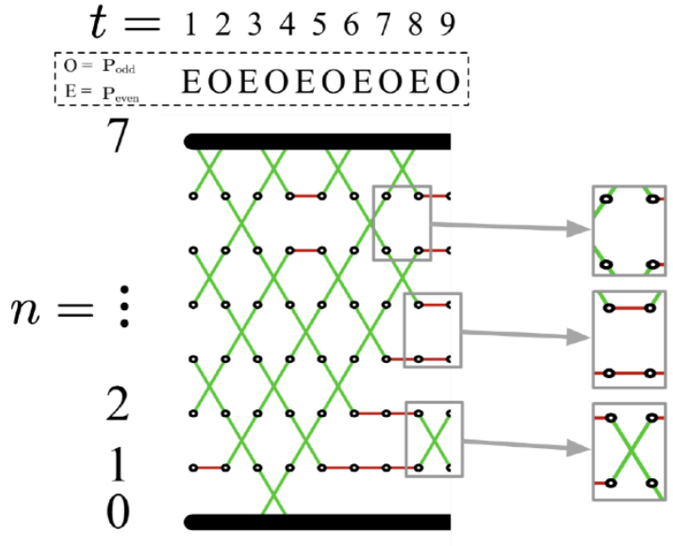

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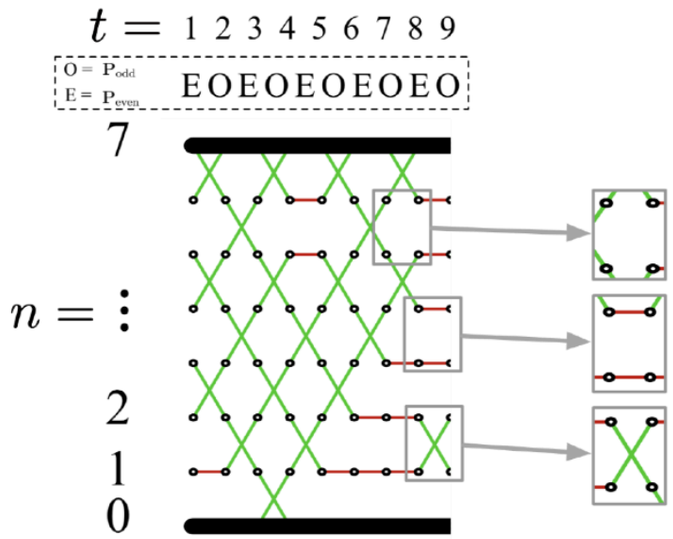
  - If proposed swap is accepted:

$$I_{t+1}^m = I_t^m + \epsilon_t^m, \qquad S_t^{(I_t^m, I_t^m + \epsilon_t^m)} = 1$$



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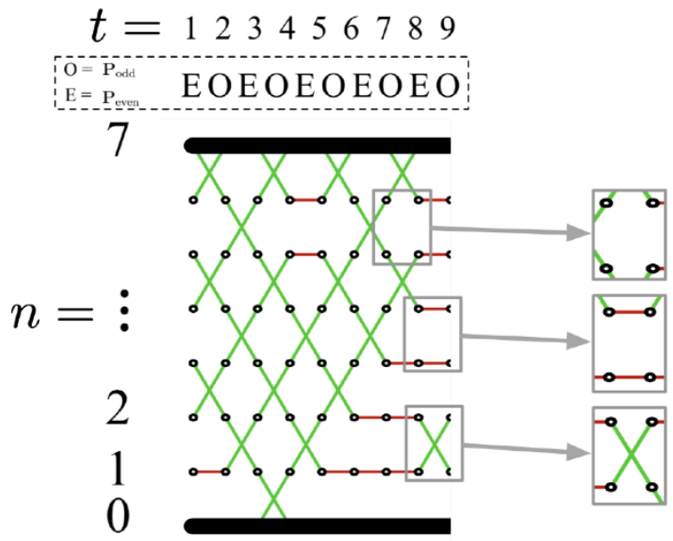
$$I_{t+1}^m = I_t^m + \epsilon_t^m, \qquad S_t^{(I_t^m, I_t^m + \epsilon_t^m)} = 1$$

  - Otherwise

$$I_{t+1}^m = I_t^m$$



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DISTRIBUTED PT

- **Intialise:**

$$Y_0^m = X_0^m, \qquad I_0^m = m, \qquad \epsilon_0^m = (-1)^m$$

- **Local exploration:** For each m update Y_t^m with the local move $K_{\beta_t^m}$ targeting $\pi_{\beta_t^m}$

$$Y_{t+1}^m \sim K_{\beta_t^m}(Y_t^m, \mathrm{d}y)$$

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  - If the next scheduled proposal is an increase

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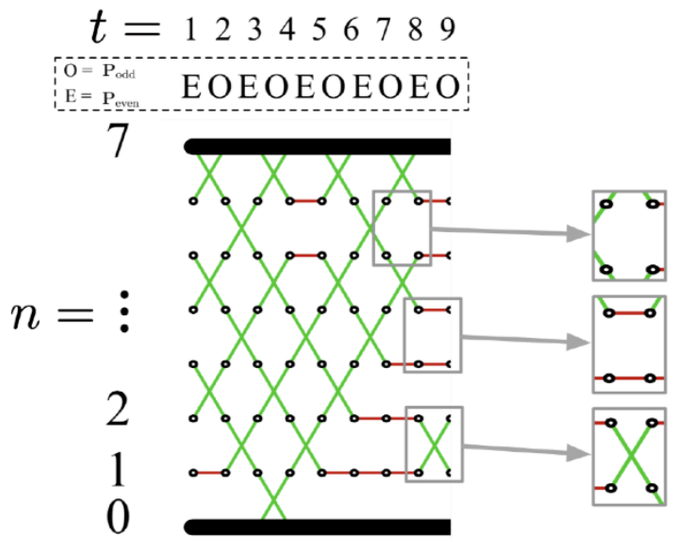

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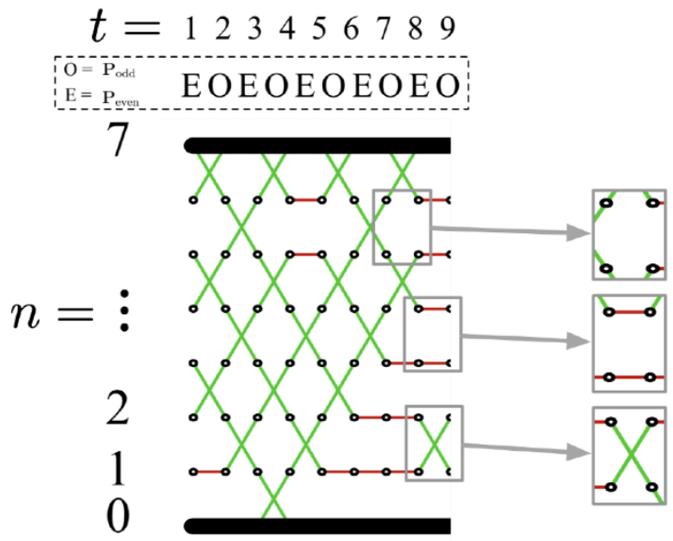

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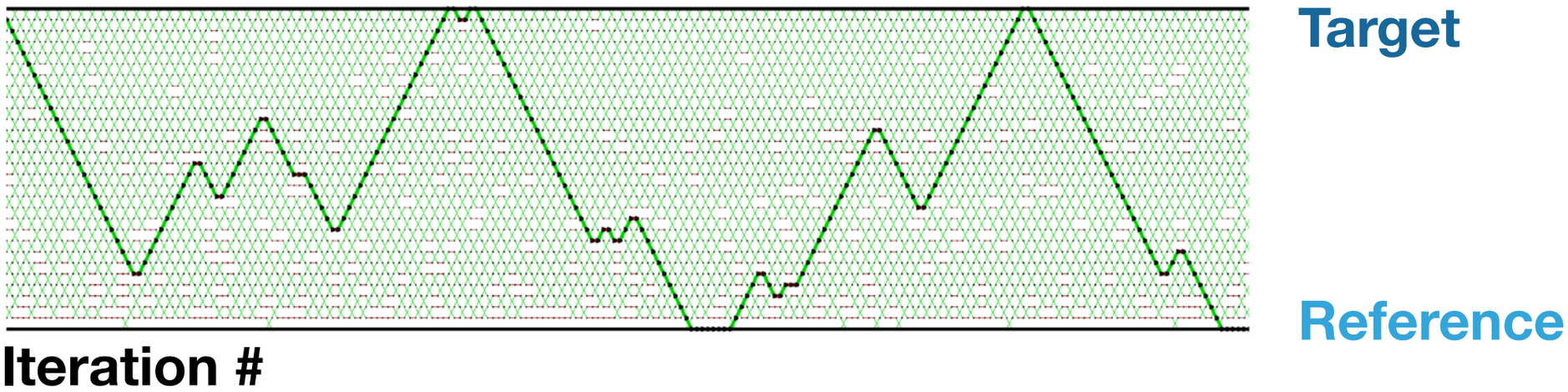

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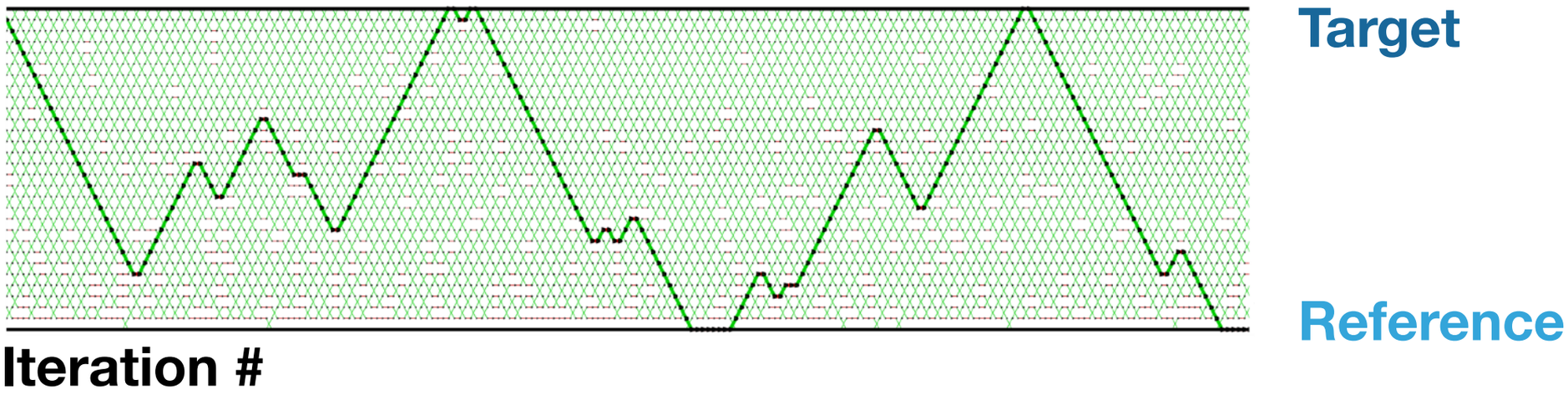

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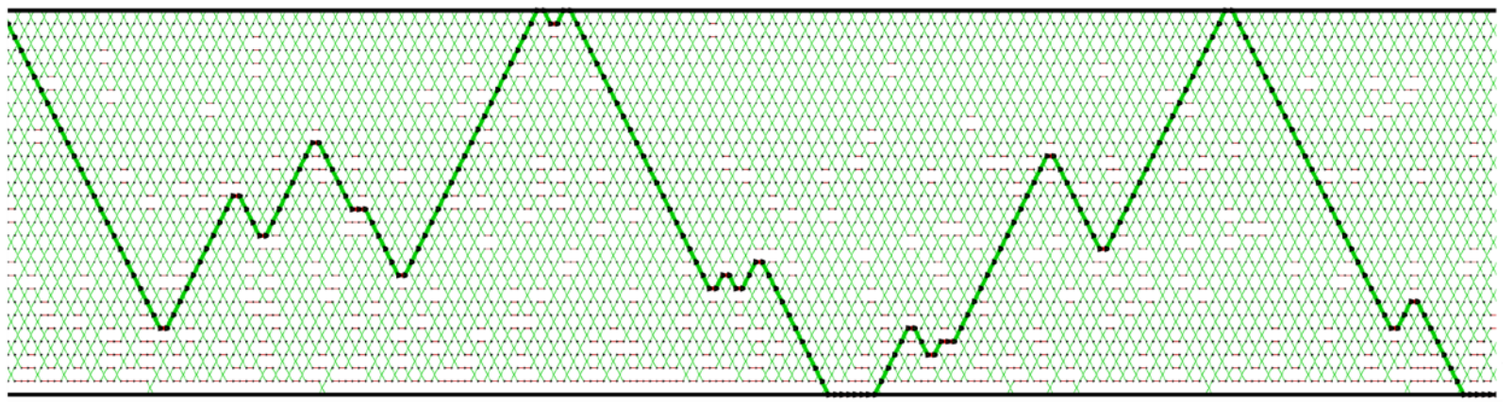

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- **Round trip rate** % of iterations with round trip

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

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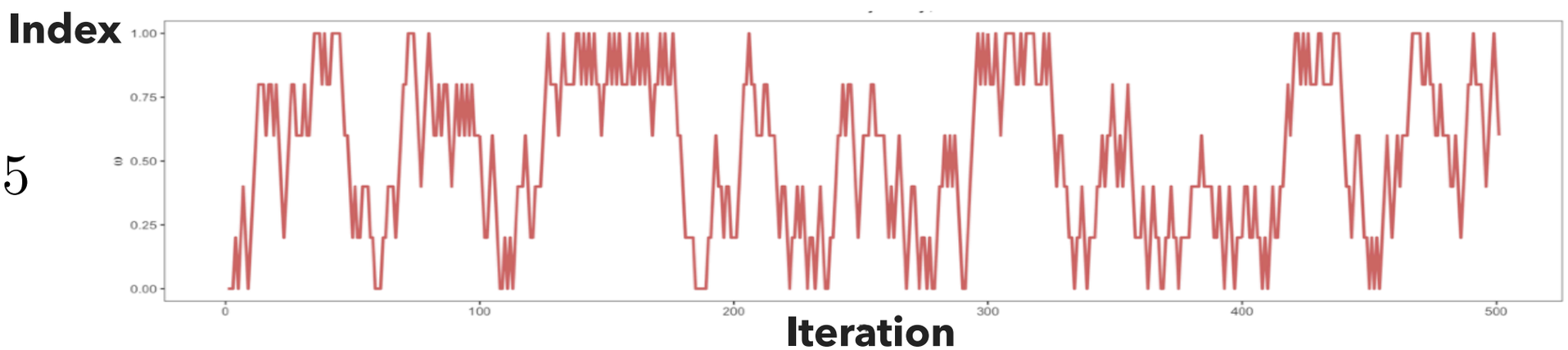

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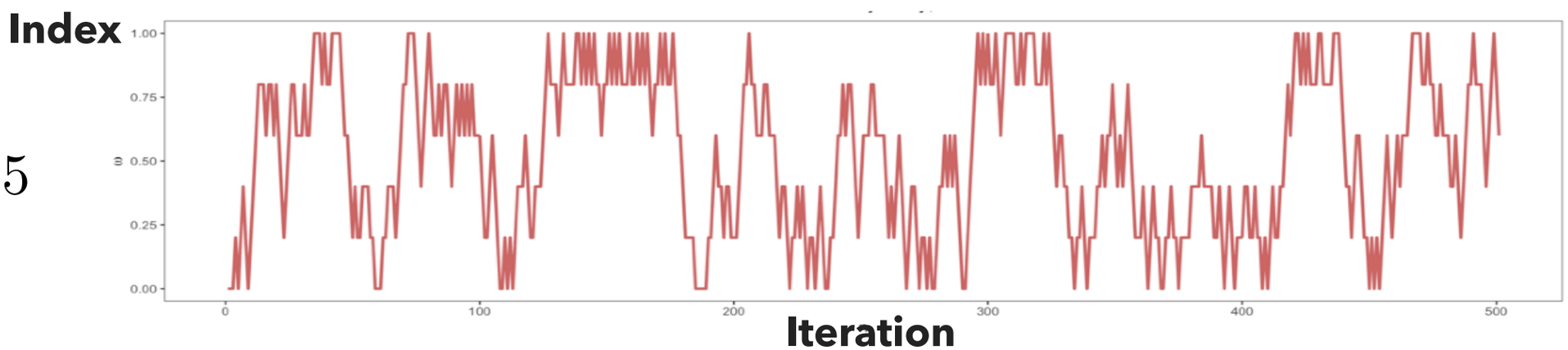

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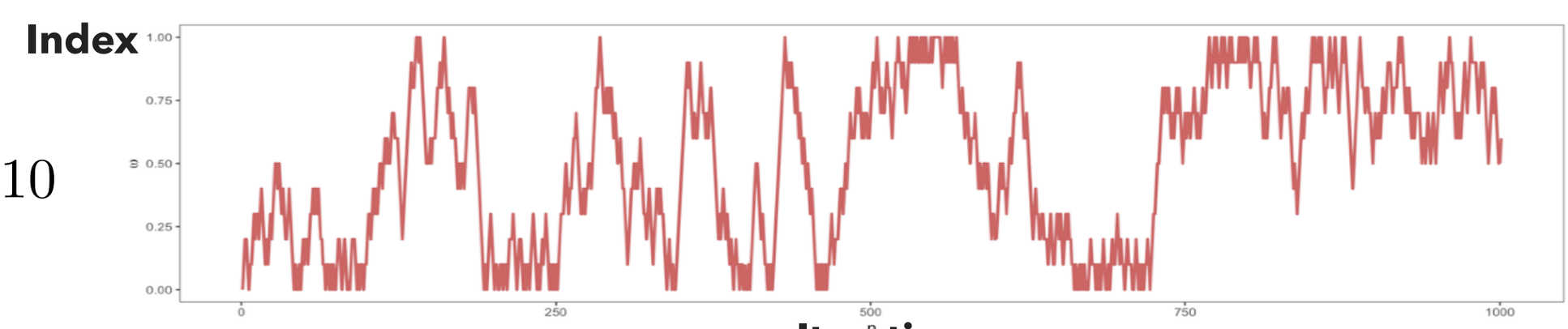

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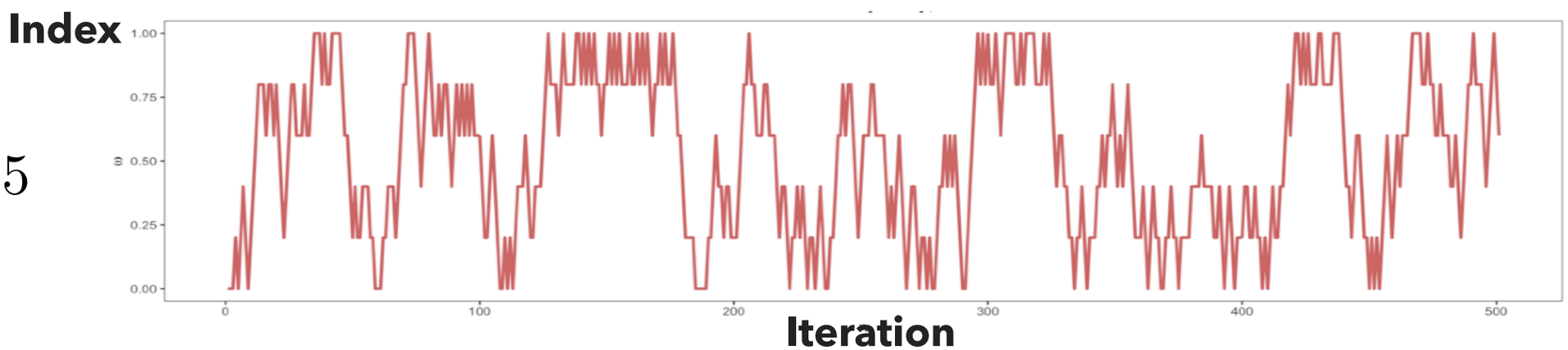

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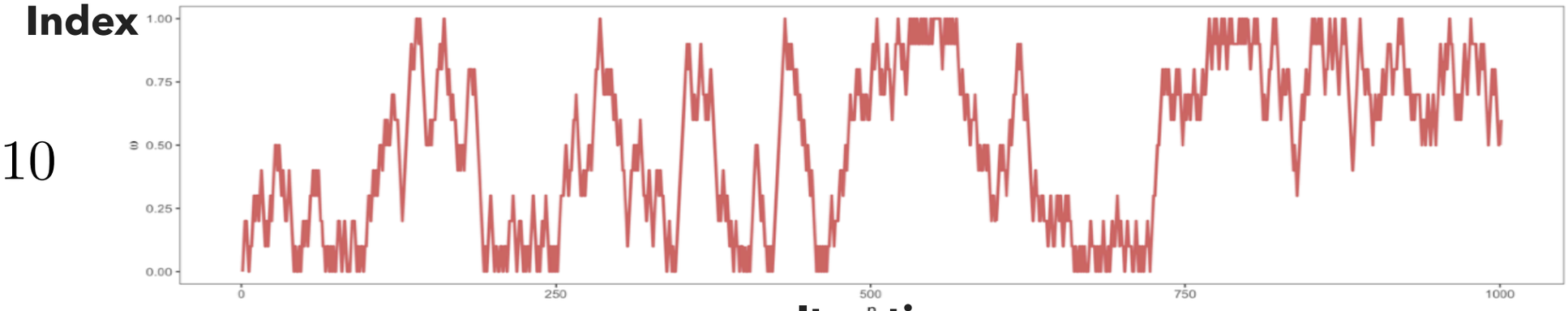
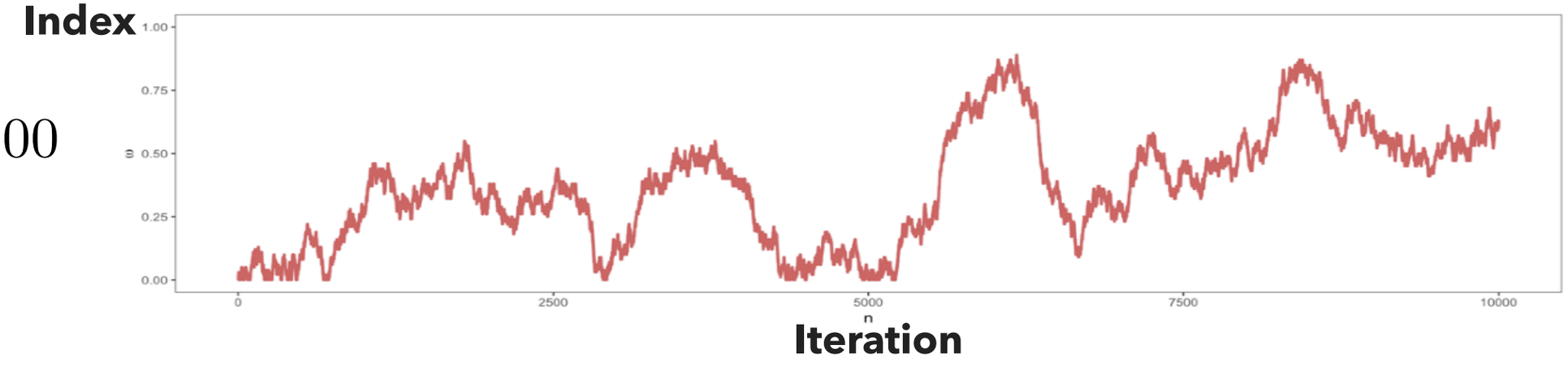


$N = 100$



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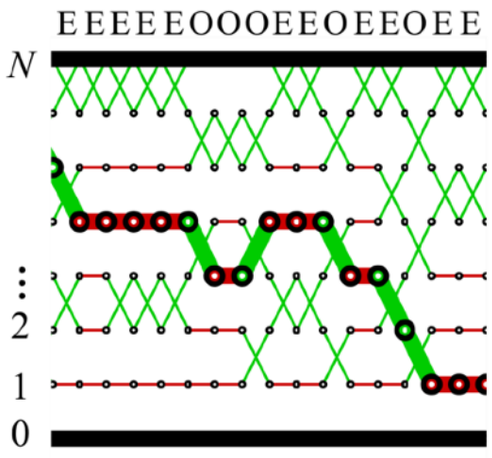

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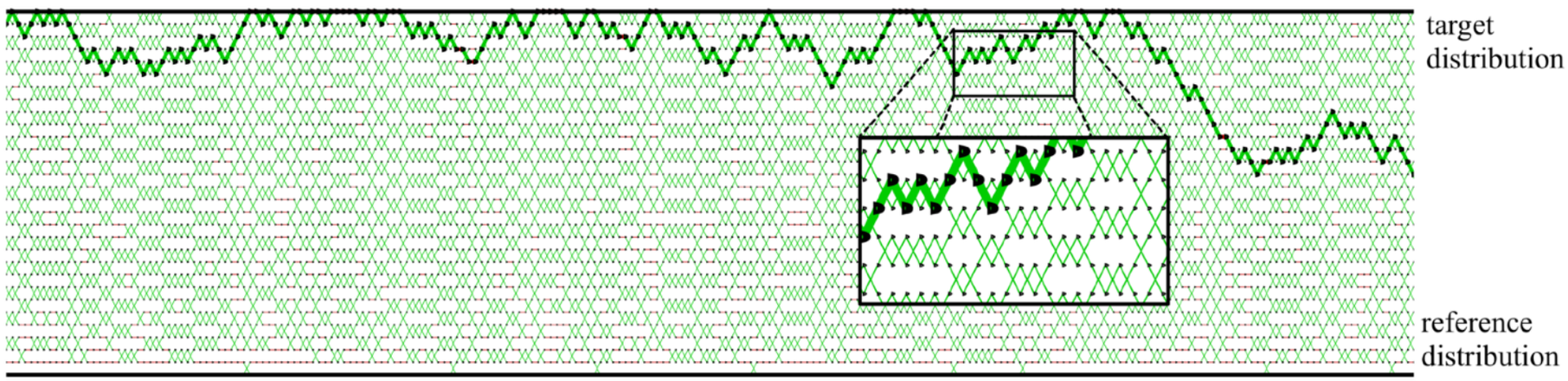

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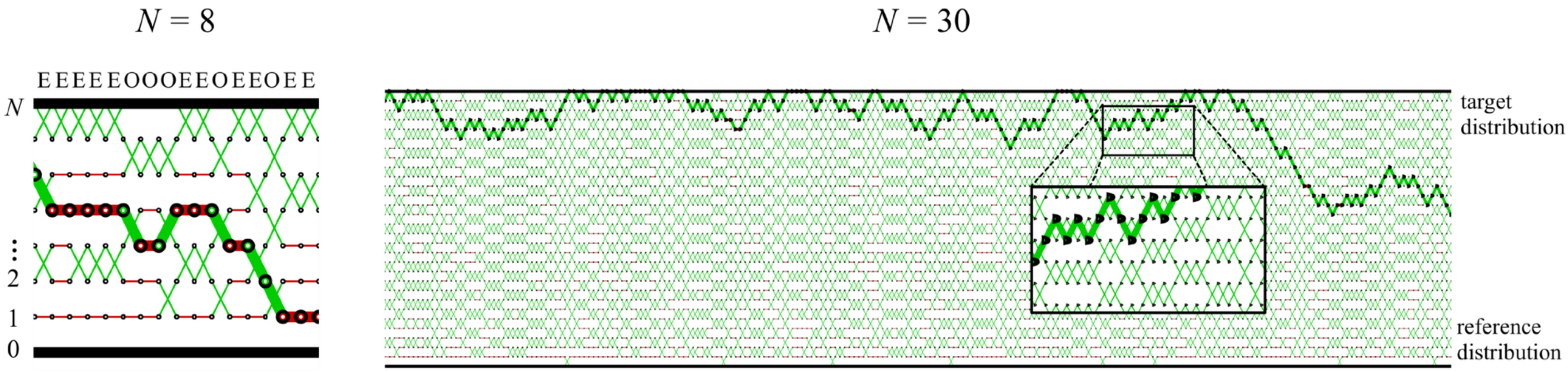
- The index process behaves like a lazy random walk!



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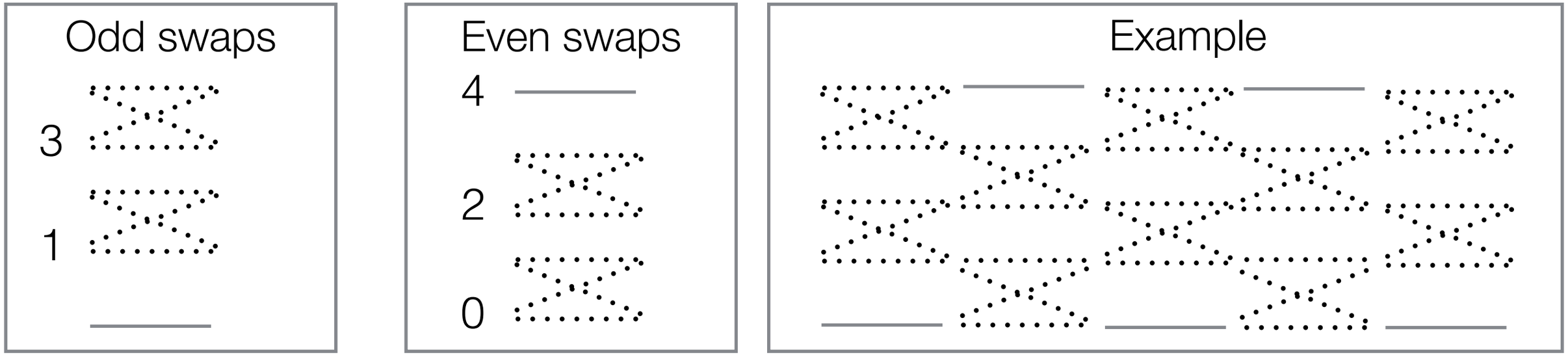

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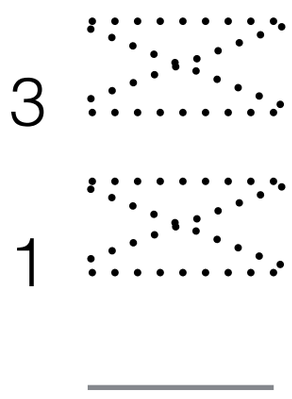
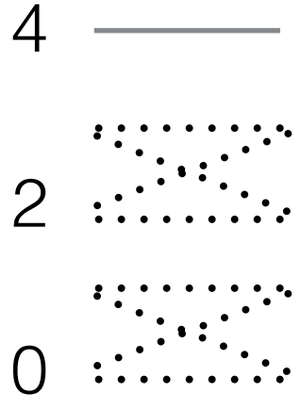
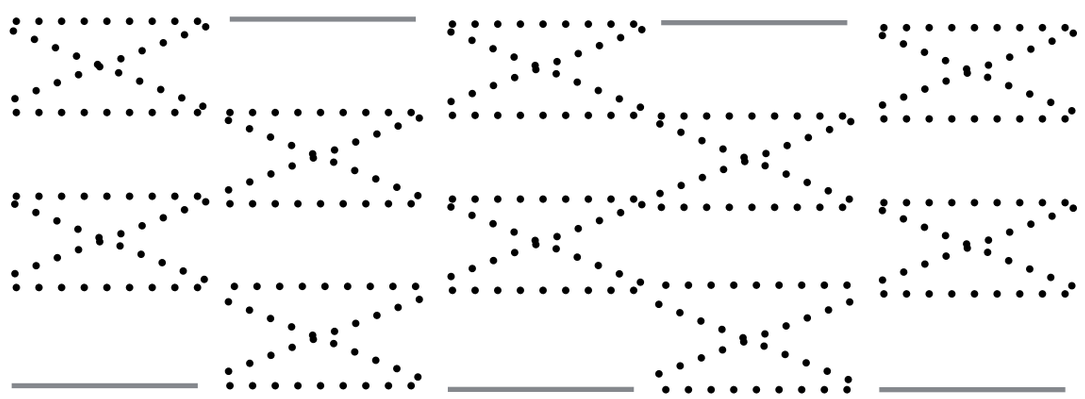


Even swaps



Example



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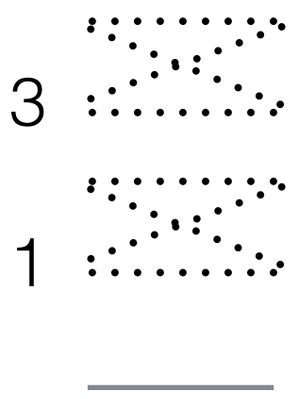

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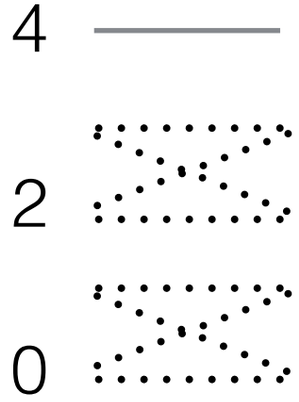

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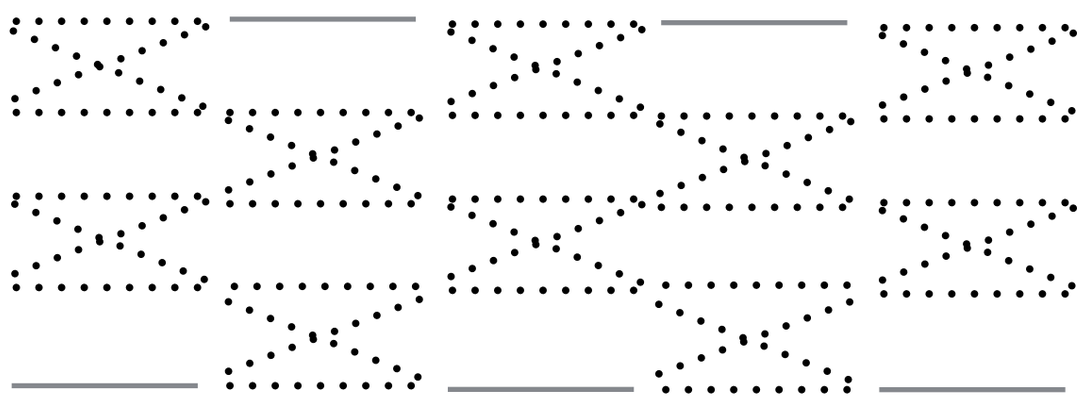

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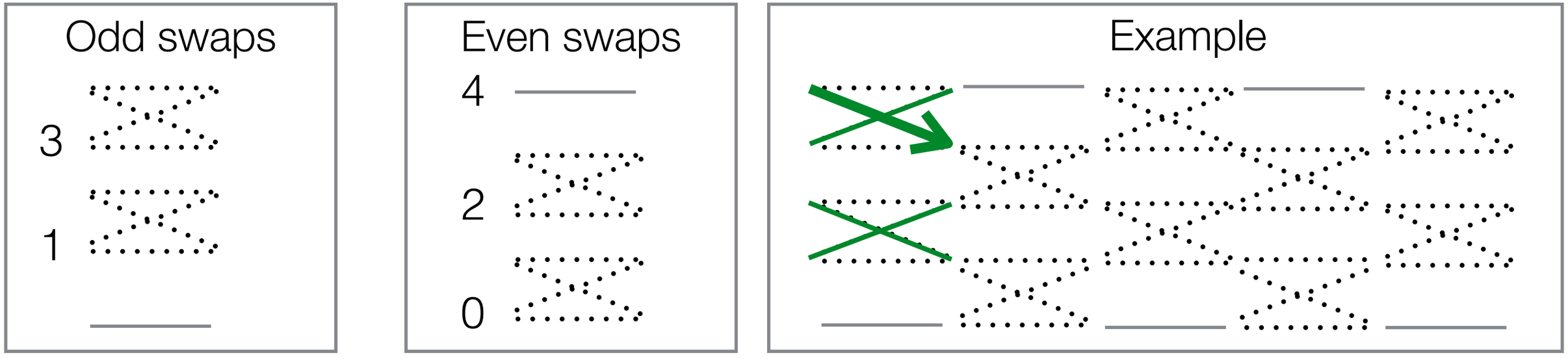

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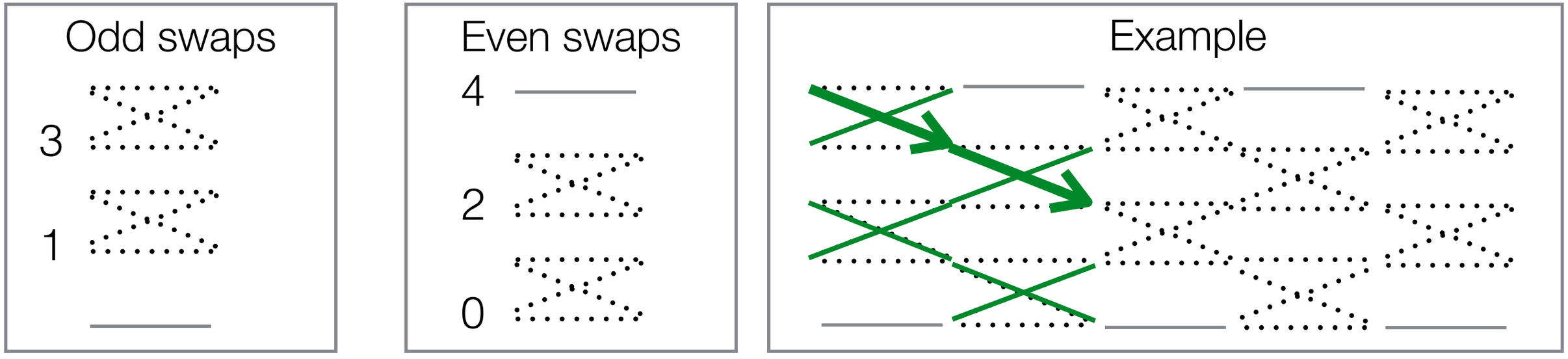

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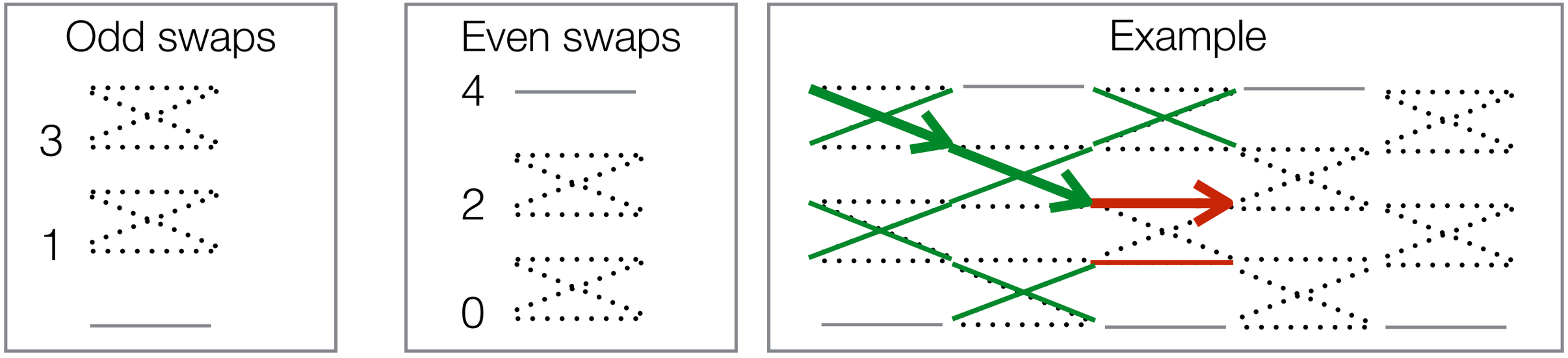

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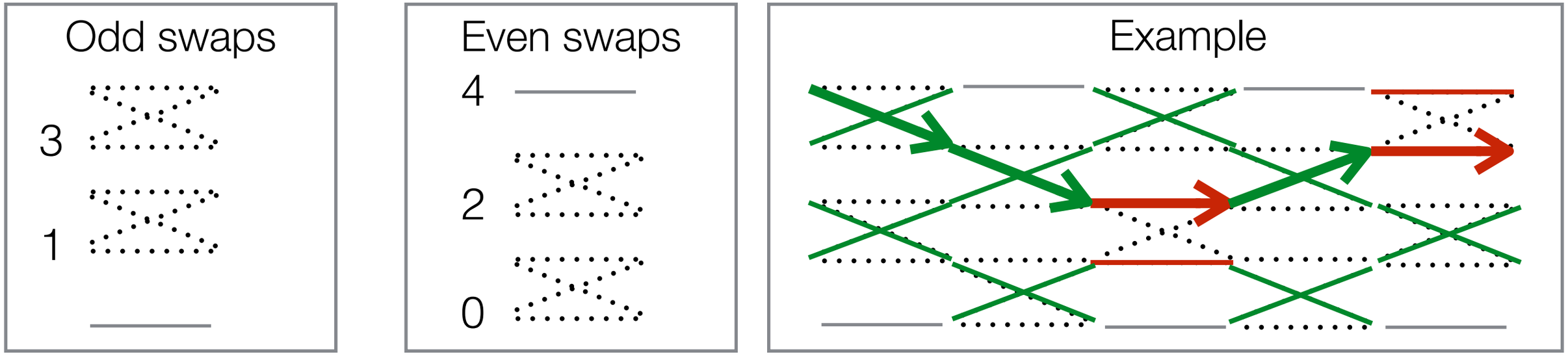

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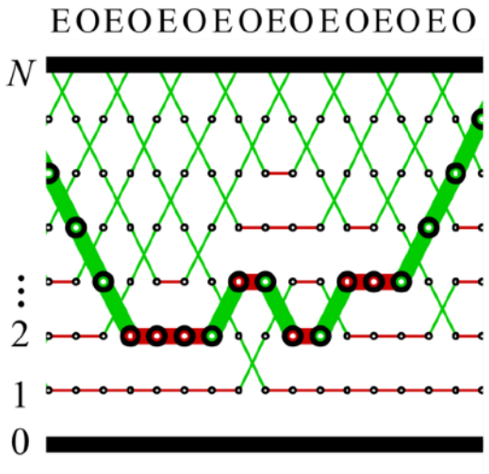

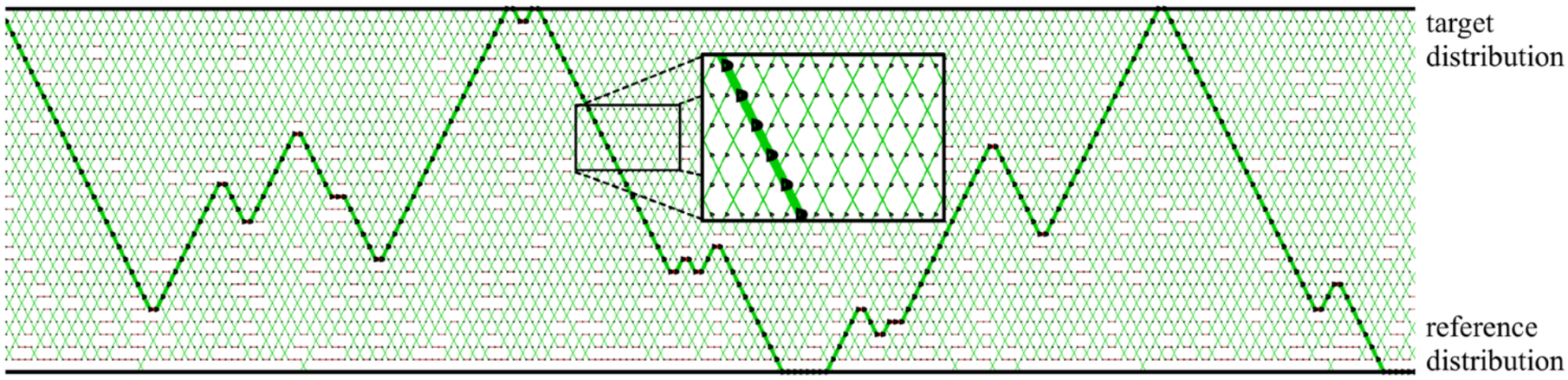

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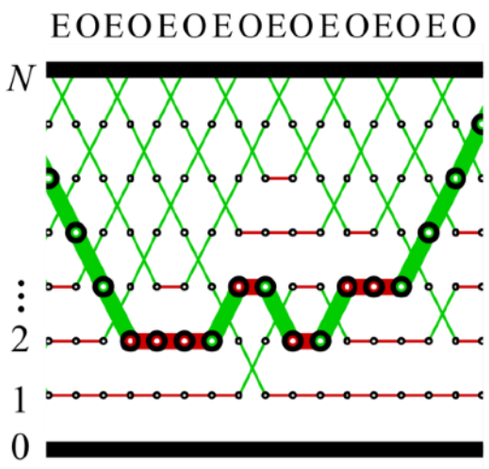

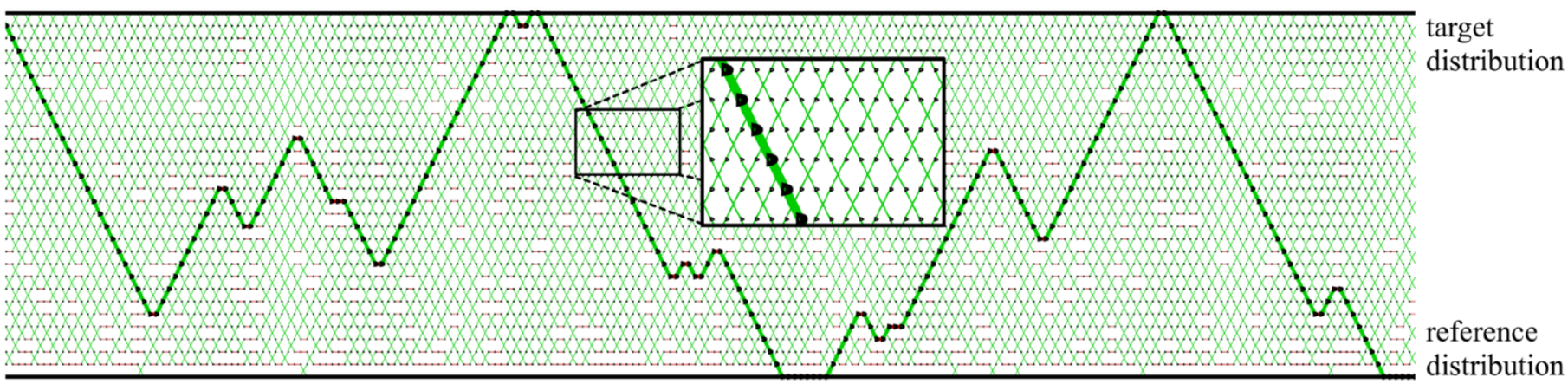

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