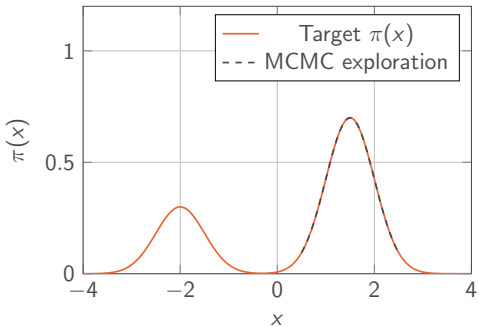
The Challenge: Multimodal Distributions

Standard MCMC Problems:

- Gets trapped in local modes
- Exponentially slow mixing times
- Poor exploration of state space
- Fails to discover all modes

Common in:

- Mixture models
- Bayesian model selection
- Phase transitions in physics
- Protein folding simulations



The Temperature Mechanism

Key Idea: Tempered Distributions

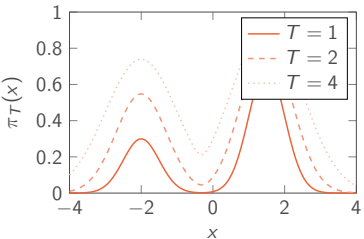
Define a family of distributions indexed by inverse temperature $0 < \gamma_1 < \gamma_2 < \ldots < \gamma_N = 1$:

$$\pi_{\gamma_n}(x) \propto \pi(x)^{\gamma_n}$$

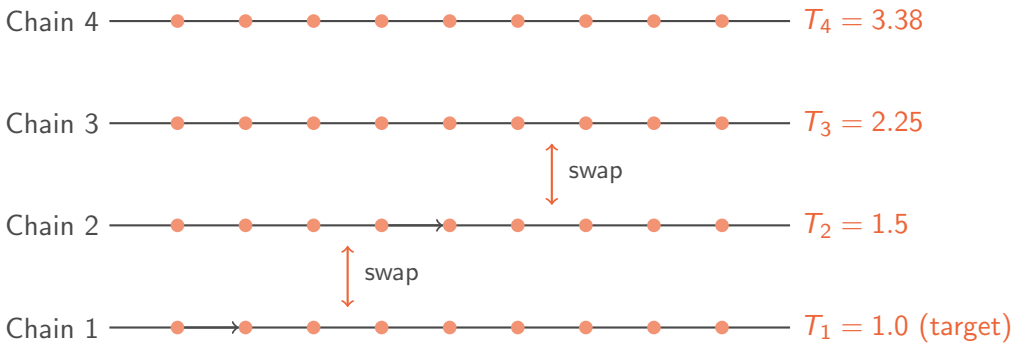
where $n = 1, \ldots, N$ and $\pi(x)$ is our target distribution.

Properties:

- $T = 1$: Original target distribution
- $T > 1$: "Heated" - flatter distribution
- $T \to \infty$: Approaches uniform
- $T < 1$: "Cooled" - more peaked



Parallel Chains Architecture



Two Types of Moves

1. **Within-chain updates**: Standard MCMC at each temperature
2. **Between-chain swaps**: Exchange states between adjacent temperatures

Parallel Tempering Algorithm Prerquisites

- **Target Distribution**: $\pi(x)$
- **Proposal Distribution**: $q(x'|x)$ - could potentially depend on temperature
- **Initialization**: $x_n^{(0)}$ for $n = 1, \ldots, N$
- **Standard MCMC Step**: Any MCMC kernel (e.g., RWM, MALA)
- **Number of Chains**: N
- **Number of Samples per Chain**: T
- **Swapping Interval**: s
- **Temperature Schedule**: $\{\gamma_n\}_{n=1}^N$ with $\gamma_N = 1$

Parallel Tempering Algorithm

Algorithm 1 Parallel Tempering MCMC

for $t = 1$ **to** T **do**
  for all $n \in \{1, \ldots, N\}$ **in parallel do**
    Sample $x_n^{(t)}$ using a standard MCMC step targeting π^{γ_n}
  end for
  if $t \bmod s = 0$ **then**
    $k \sim \text{Uniform}\{1, \ldots, N-1\}$
    $$\alpha_{\text{swap}} = \min\left\{1, \left(\frac{\pi(x_{k+1}^{(t)})}{\pi(x_k^{(t)})}\right)^{\gamma_k - \gamma_{k+1}}\right\}$$
    Swap $(x_k^{(t)}, x_{k+1}^{(t)})$ with probability α_{swap}
  end if
end for
return $\{x_N^{(t)}\}_{t=1}^{T}$

Parallel Tempering: Swap Move Acceptance

Setup

- **Joint target:** $\pi^{\gamma_1} \otimes \pi^{\gamma_2} \otimes \cdots \otimes \pi^{\gamma_N}$ where $\gamma_i = 1/T_i$ (inverse temperature)
- Chain i at state x_i with temperature T_i (cold: $T_N = 1$, hot: $T_1 > 1$)

Metropolis-Hastings Derivation

Propose swap: Exchange states $x_{k_1} \leftrightarrow x_{k_2}$ between chains k_1 and k_2
MH acceptance ratio:

$$\alpha = \frac{\text{Probability of proposed state}}{\text{Probability of current state}} = \frac{\pi^{\gamma_{k_1}}(x_{k_2})\pi^{\gamma_{k_2}}(x_{k_1})}{\pi^{\gamma_{k_1}}(x_{k_1})\pi^{\gamma_{k_2}}(x_{k_2})}$$

Accept with probability: $\min(1, \alpha)$
This ensures detailed balance w.r.t. the joint distribution!

Swap Acceptance Ratio Derivation

Detailed Balance Requirement

For the extended state space with joint distribution $\pi(x_1, \ldots, x_K) = \prod_{i=1}^{K} \pi_i(x_i)$

Consider swapping states between chains i and j:

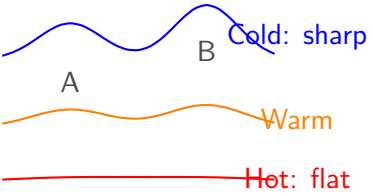
$$
\begin{aligned}
\alpha_{\text{swap}} &= \min\left\{1, \frac{\pi^{\gamma_{k_1}}(x_{k_2}) \cdot \pi^{\gamma_{k_2}}(x_{k_1})}{\pi^{\gamma_{k_1}}(x_{k_1}) \cdot \pi^{\gamma_{k_2}}(x_{k_2})}\right\} \\
&= \min\left\{1, \frac{[\pi(x_{k_2})]^{\gamma_{k_1}}}{[\pi(x_{k_2})]^{\gamma_{k_2}}} \cdot \frac{[\pi(x_{k_1})]^{\gamma_{k_2}}}{[\pi(x_{k_1})]^{\gamma_{k_1}}}\right\} \\
&= \min\left\{1, [\pi(x_{k_2})]^{\gamma_{k_1}-\gamma_{k_2}} \cdot [\pi(x_{k_1})]^{\gamma_{k_2}-\gamma_{k_1}}\right\} \\
&= \min\left\{1, \frac{[\pi(x_{k_2})]^{\gamma_{k_1}-\gamma_{k_2}}}{[\pi(x_{k_1})]^{\gamma_{k_1}-\gamma_{k_2}}}\right\} = \min\left\{1, \left(\frac{\pi(x_{k_2})}{\pi(x_{k_1})}\right)^{\gamma_{k_1}-\gamma_{k_2}}\right\}
\end{aligned}
$$

Note: Normalizing constants cancel out!

The Problem and Solution

The Problem:

- Standard MCMC gets stuck in local modes
- Can't explore separated peaks
- Dilemma: small steps (stuck) vs. large steps (rejected)



The Solution: Temperature Ladder

- Run N chains targeting π^{γ_n}
- $0 < \gamma_1 < \cdots < \gamma_N = 1$
- Hot ($\gamma \approx 0$): Explores freely
- Cold ($\gamma = 1$): Exploits peaks

Key Insight

Different temperatures see the same distribution differently - hot chains explore, cold

Parallel Tempering MCMC: Normalization Requirements

Target Distribution

NOT required to be normalized

Tempered Distributions

Also NOT normalized

Why It Works: Acceptance Ratios

Within-chain moves:

$$\alpha = \min\left(1, \frac{\pi_i(\mathbf{x}')}{\pi_i(\mathbf{x})}\right)$$

Normalizing constants cancel!

Between-chain swaps:

$$\alpha = \min\left(1, \frac{\pi_i(\mathbf{x}_j)\pi_j(\mathbf{x}_i)}{\pi_i(\mathbf{x}_i)\pi_j(\mathbf{x}_j)}\right)$$

Constants cancel again!

Practical Advantage

Why Swapping Works

The Relay Race Mechanism:

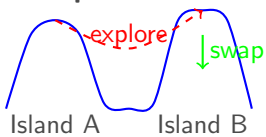
1. Hot chain randomly discovers new mode
2. Swap propagates discovery downward
3. Cold chain thoroughly explores it
4. Information flows both ways

Swap Acceptance (adjacent chains):

$$\alpha = \min\left\{1, \left(\frac{\pi(x_{k+1})}{\pi(x_k)}\right)^{\gamma_k - \gamma_{k+1}}\right\}$$

- Favors moving high-prob states to cold
- Favors moving low-prob states to hot
- Adjacent swaps $\rightarrow$ high acceptance

Example: Two Islands



Without PT: Stuck on Island A forever
With PT: Both islands sampled!

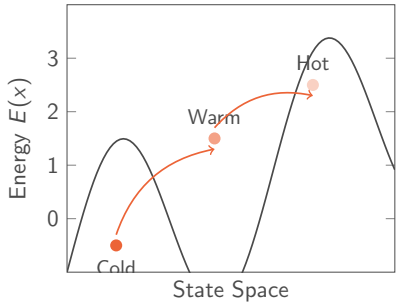
Intuition: Why Swaps Work

Energy Landscape Analogy:

- Low energy = high probability
- High temperature = less selective
- Low temperature = more selective

Swap Success Scenarios:

- Good state to cold chain
- Bad state to hot chain
- Bad state to cold chain
- Good state to hot chain



Hot chains explore broadly
Cold chains exploit locally

Choosing Temperatures: The Critical Decision

The Temperature Selection Problem

- Too few temperatures $\Rightarrow$ poor communication between chains
- Too many temperatures $\Rightarrow$ computational waste
- Poor spacing $\Rightarrow$ inefficient mixing

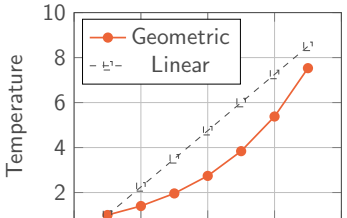
Common Strategies:

1. **Geometric spacing:**

$$T_i = T_1 \cdot \rho^{i-1}$$

2. **Optimal for Gaussians:**

$$T_{i+1}/T_i \approx 1 + \sqrt{\frac{2\alpha}{n}}$$



Optimal Number of Temperatures

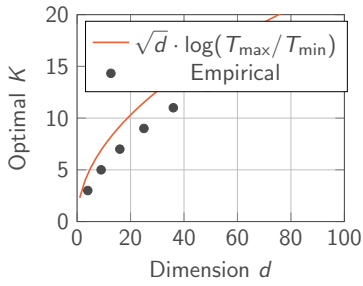
Theorem (Atchadé et al., 2011)

For a d-dimensional problem, the optimal number of temperatures scales as:

$$K_{opt} \propto \sqrt{d} \cdot \log\left(\frac{T_{\max}}{T_{\min}}\right)$$

Exchange Acceptance Rate:

- Target: 20-40% (problem-dependent)
- Kone & Kofke (2005): 23.4% optimal
- Monitor during runtime



Adaptive Algorithm:

$$\log T_i^{(n+1)} = \log T_i^{(n)} + \gamma_n(\alpha_{i,i+1} - \alpha^*)$$

Detailed Balance and Ergodicity

Proposition (Detailed Balance)

The parallel tempering algorithm satisfies detailed balance with respect to the joint distribution:

$$\pi(x_1, \ldots, x_K) = \prod_{i=1}^{K} \frac{1}{Z_i} \pi(x_i)^{1/T_i}$$

Proof Sketch:

1. Within-chain moves: Standard MCMC detailed balance
2. Swap moves: Show $\pi(\mathbf{x})P(\mathbf{x} \to \mathbf{x}') = \pi(\mathbf{x}')P(\mathbf{x}' \to \mathbf{x})$
3. Symmetry of proposal + Metropolis ratio ensures balance

Ergodicity Conditions

- Each chain must be irreducible
- Temperature set must include $T_i = 1$

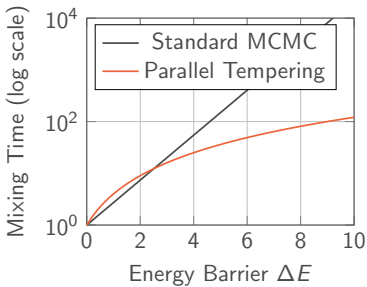
Mixing Time Improvements

Theorem (Woodard et al., 2009)

For certain multimodal distributions, parallel tempering reduces mixing time from exponential to polynomial in problem size.

Example: Double-well potential

- Standard MCMC: $\tau_{\text{mix}} \sim e^{\beta \Delta E}$
- Parallel Tempering: $\tau_{\text{mix}} \sim K^2$
- Where K = number of temperatures



Exponential → Polynomial speedup!

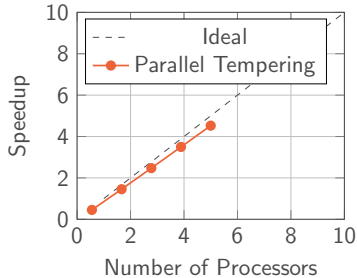
Implementation Considerations

Computational Aspects:

- **Parallelization:** Natural parallelism across chains
- **Communication:** Minimal (only for swaps)
- **Memory:** Linear in number of chains
- **Scaling:** Near-linear with processors

Software Packages:

- `emcee` (Python) - adaptive PT
- `PyMC3` - Bayesian modeling
- `PLUMED` - molecular dynamics
- `MCMCpack` (R) - general purpose

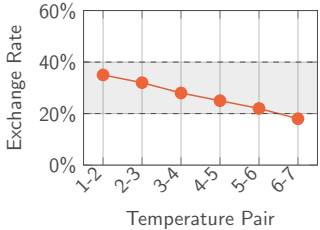


Communication Pattern:

Diagnostics and Convergence

Key Diagnostics:

1. **Exchange acceptance rates**
   - Monitor between all pairs
   - Target: 20-40%
2. **Round-trip times**
   - Time for state to visit all temperatures
   - Should be finite and reasonable
3. **Temperature diffusion**
   - States should visit all temperatures
   - Check histogram of visits



Convergence Criteria:

- Standard $\hat{R}$ statistic
- Effective sample size (ESS)
- KL divergence between chains

Modern Extensions

1. Non-reversible PT

- Syed et al. (2022)
- Persistent direction of swaps
- Further reduces mixing time

2. Infinite Swapping

- Plattner et al. (2011)
- Continuous-time limit
- Optimal temperature schedules

3. PT with Normalizing Flows

- Learn optimal proposal distributions
- Adaptive temperature mappings
- Neural network augmentation

4. Simulated Tempering vs PT

Aspect	PT	ST
Chains	Multiple	Single
Memory	$O(K)$	$O(1)$
Parallel	Yes	No
Tuning	Easier	Harder

5. PT-based Model Selection

- Thermodynamic integration
- Model evidence estimation
- Bayes factor computation

Limitations and When Not to Use PT

Limitations:

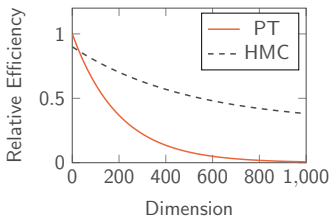
- Computational cost scales with K
- Memory requirements $\propto K \times d$
- Temperature tuning can be difficult
- Less effective in very high dimensions

When PT Struggles:

- Modes separated by vast low-probability regions
- Dimension $d > 1000$
- When modes have very different scales
- Real-time applications

Alternatives to Consider:

- **SMC:** For sequential problems
- **HMC:** For smooth, high-dim targets
- **Variational Inference:** When approximate is OK
- **Annealed Importance Sampling:** For evidence estimation



Key Takeaways

Strengths:

- Excellent for multimodal distributions
- Naturally parallel
- Theoretically rigorous
- Automatic diagnostics via exchange rates
- Wide applicability

Key Design Choices:

- Number of temperatures: $O(\sqrt{d})$
- Spacing: Geometric or adaptive
- Target exchange rate: 20-40%

Remember:

- Temperature = "exploration parameter"
- Hot chains explore, cold chains exploit
- Swaps enable global communication
- Detailed balance is preserved

The PT Philosophy

"Heat to explore, cool to exploit, swap to communicate"

Active Research Areas:

- Optimal temperature schedules

References

- **Foundational:**
  - Geyer (1991). "Markov chain Monte Carlo maximum likelihood"
  - Hukushima & Nemoto (1996). "Exchange Monte Carlo method"
- **Reviews:**
  - Earl & Deem (2005). "Parallel tempering: Theory, applications, and new perspectives"
  - Swendsen & Wang (2016). "Replica Monte Carlo simulation (revisited)"
- **Theory:**
  - Atchadé et al. (2011). "Towards optimal scaling of Metropolis-coupled Markov chain Monte Carlo"
  - Woodard et al. (2009). "Conditions for rapid mixing of parallel and simulated tempering"
- **Recent Advances:**
  - Syed et al. (2022). "Non-reversible parallel tempering: A scalable highly parallel MCMC scheme"
  - Vousden et al. (2016). "Dynamic temperature selection for parallel tempering"

Questions?

Thank you!