Probabilistic Path Hamiltonian Monte Carlo

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Motivation

If the probabilistic model contains both continuous and structural discrete parameters, how can we sample from the posterior efficiently?

- Simple MCMCs are not efficient at sampling continuous parameters
- Advanced MCMCs, e.g. Hamiltonian Monte Carlo, can not handle discrete parameters

BL on Orthant Complexes

An *orthant complex* is a geometric object $\mathcal{X}$ obtained by gluing orthants of the same dimension

$$\mathcal{X} = \{(\tau, q) : \tau \in \Gamma,\ q \in \mathbb{R}^n_{\geq 0}\}$$

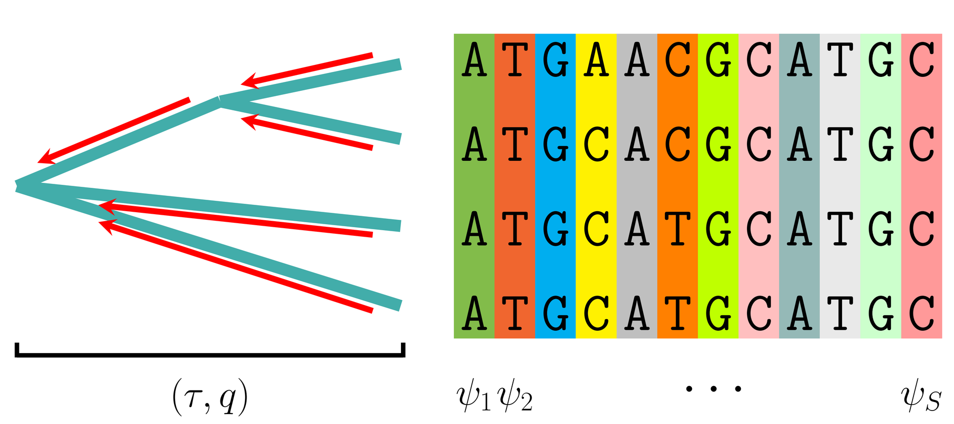
where Γ is a countable set. Given observations D and proper priors $\pi_0(\tau, q)$, the posterior

$$P(\tau, q|D) \propto L(D|\tau, q)\pi_0(\tau, q)$$

- $(\tau, q_\tau) = (\tau', q_{\tau'}) \Rightarrow q_\tau = q_{\tau'},\ \tau' \in \mathcal{N}(\tau, q_\tau)$
- The adjacency graph of $\mathcal{X}$ has finite diameter k.
- $U(\tau, q) = -\log P(\tau, q)$ is continuous and smooth up to the boundary.

A Challenging Example

Let (τ, q) be a phylogenetic tree and $\psi = \{\psi_i\}_{i=1}^S$ be the observed sequences over the leaves.



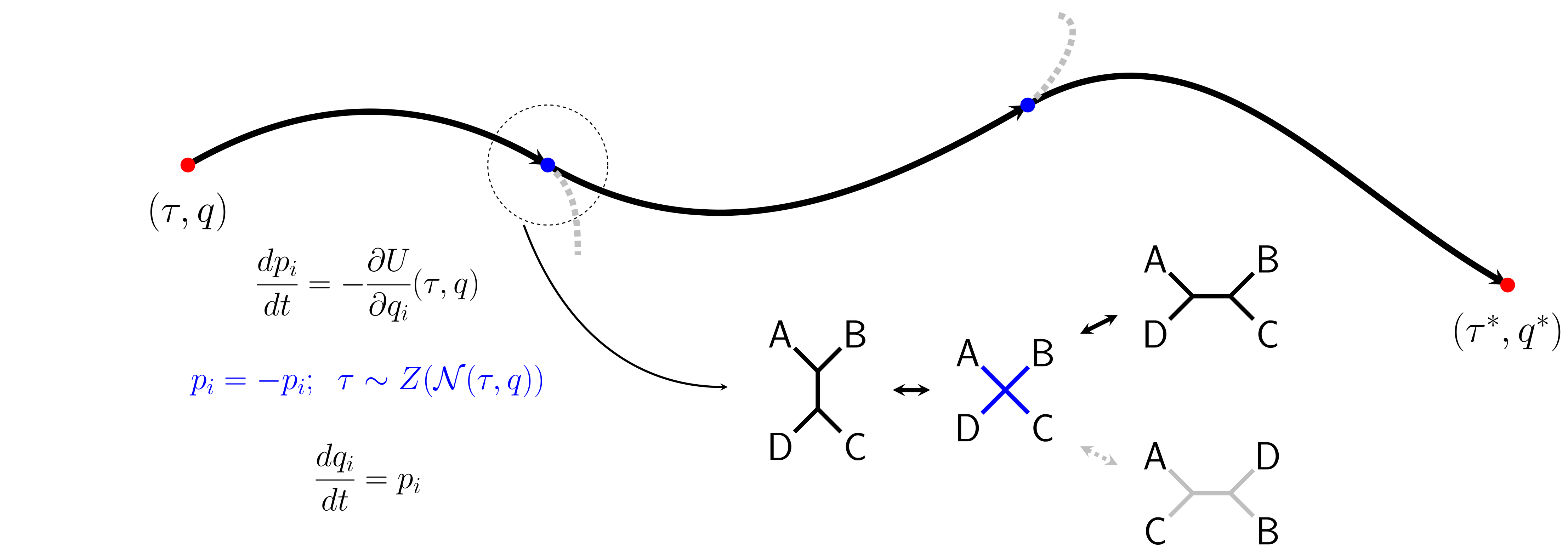
A continuous-time Markov chain is usually used to model the evolution history

$$L(\psi|\tau, q) = \prod_{s=1}^{S} \sum_{a^s} \eta(a^s_\rho) \prod_{(u,v)\in E(\tau,q)} P^{uv}_{a^s_u a^s_v}(q_{uv})$$

- Efficient computation via Felsenstein's pruning algorithm [1].
- Orthant Complexes: **NNI neighbors**.
- # possible topologies: $T(n)$, # leaves: n

$$T(n) = \frac{(2n-5)!}{(n-3)!\,2^{n-3}} = e^{\mathcal{O}(n \log n)}$$

Hamiltonian: $H(\tau, q, p) = U(\tau, q) + K(p),\quad U(\tau, q) = -\log P(\tau, q),\quad K(p) = \frac{1}{2}\|p\|^2$



Theoretical Properties

Augmented state: $s = (\tau, q, p)$. Let A, B be a pair of measurable sets in the augmented state space. We assume the following condition

$$P(\tau'|\tau, q) = P(\tau|\tau', q),\ \tau' \in \mathcal{N}(\tau, q)$$

which is true with *uniform* topology proposal Z.

1. **Probabilistic Reversibility.**

$$P((\tau, q, p), (\tau^*, q^*, p^*)) = P((\tau^*, q^*, -p^*), (\tau, q, -p))$$

2. **Stochastic Volume Presevation.**

$$\int_A \int_B P(s, s')ds'\,ds = \int_B \int_A P(s', s)ds\,ds'$$

3. **k-accessibility.** Any two states in $\mathcal{X}$ can be connected by k iterations of probabilistic path HMC.

Theorem. *Probabilistic Path HMC preserves the posterior and is ergodic.*

Surrogate Smoothing

∂U is usually non-differentiable on the boundary which lead to $\mathcal{O}(C\epsilon + T\epsilon^3)$ global numerical error, where C is the number of reflection/refraction events. We found a recipe by using a surrogate smoothing strategy and refraction in the leap-frog steps.

$$\tilde{U}(\tau, q) = U(\tau, G(q))$$

$$G(q) = (g_\delta(q_1), g_\delta(q_2), \ldots, g_\delta(q_{2n-3}))$$

and

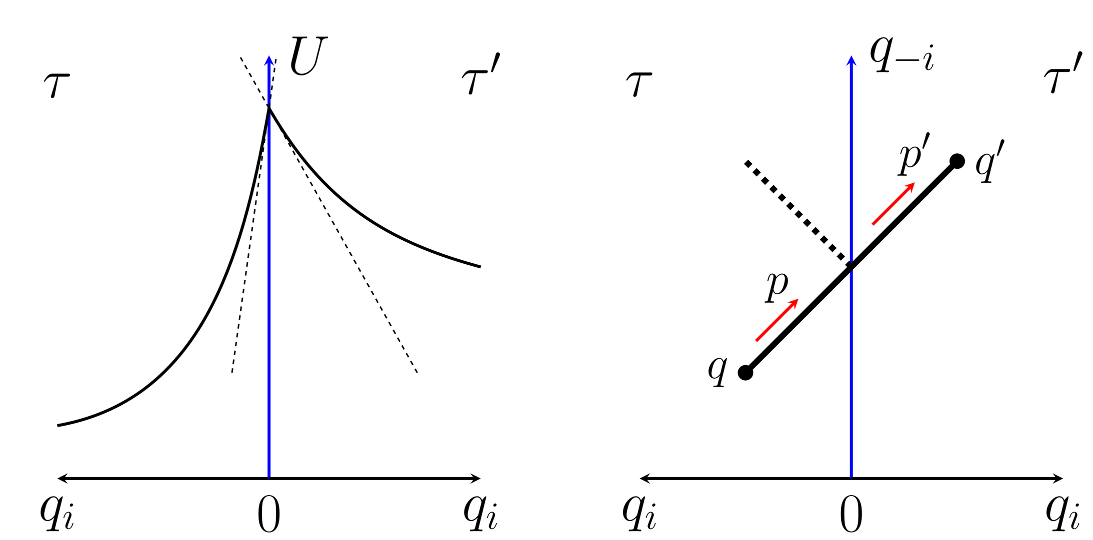
$$g_\delta(x) = \begin{cases} x, & x \geq \delta \\ \frac{1}{2\delta}(x^2 + \delta^2), & 0 \leq x < \delta \end{cases}$$

Reflection and Refraction

To maintain the desired properties of Hamiltonian dynamics, we adopted the *reflection* and *refraction* technique [2] when jumping between topologies.

- Reflection. $U(\tau, q)$ is continuous across boundary

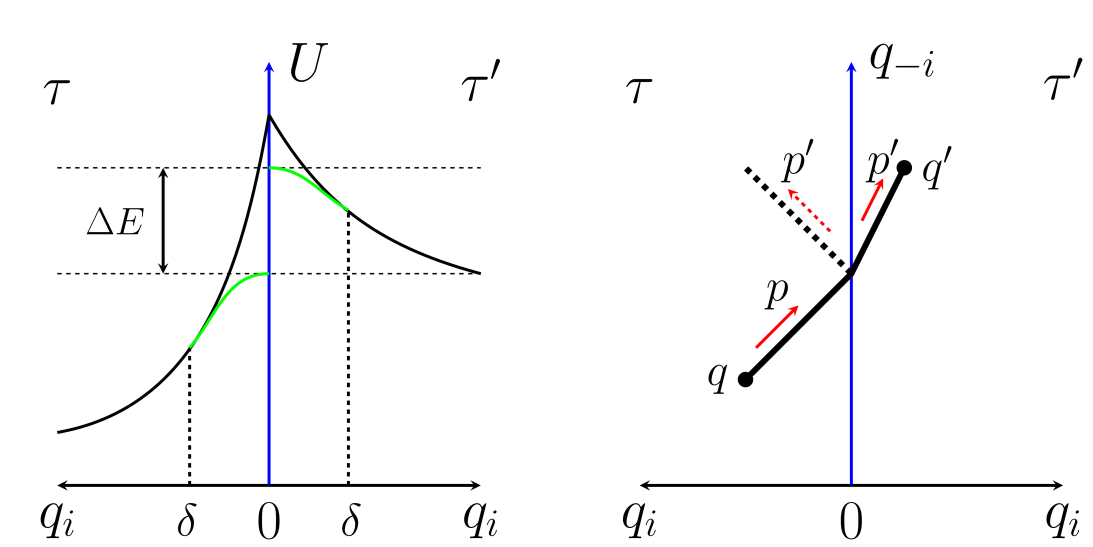
$$\Delta E = U(\tau', q) - U(\tau, q) = 0,\quad q_i = 0$$



Momentum & topology update:

$$p_i = -p_i, \quad \tau = \tau'$$

- Refraction. Surrogate evens the gradients while creating controllable energy gaps $\Delta E \neq 0$



Momentum & topology update:

$$(\tau, p_i) = \begin{cases} (\tau', \sqrt{\|p_i\|^2 - 2\Delta E}) & \|p_i\|^2 > 2\Delta E \\ (\tau, -p_i) & \text{otherwise} \end{cases}$$

Results

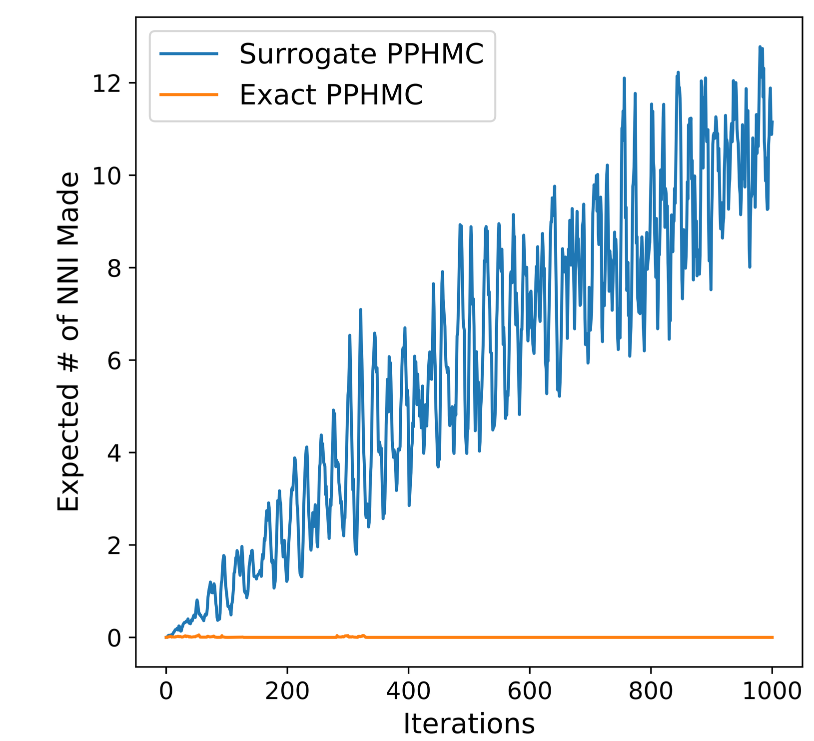


Figure 1: Expected number of NNI moves on a real data set.

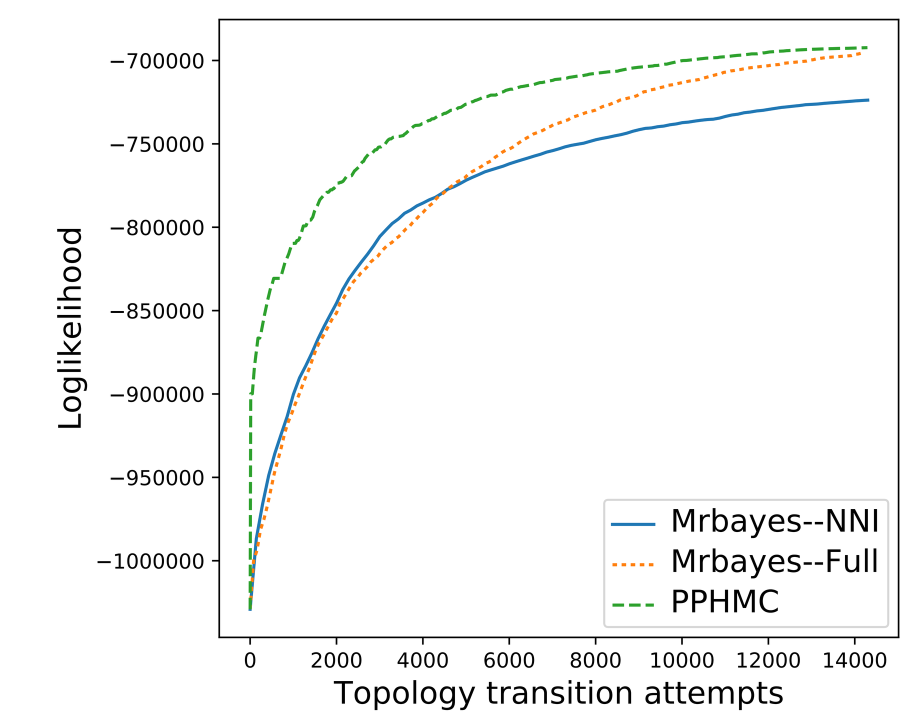


Figure 2: Loglikelihood vs topology transitions on a 1000 taxa simulated data set.

Contributions

- Extended HMC towards sampling both continuous and structural discrete parameters.
- Developed a smoothing surrogate function that enables long HMC paths with potential non-differentiable boundary transitions.

References

[1] J. Felsenstein, J. Mol. Evol., **17**(6) (1981), 368-376

[2] H. M. Afshar, J. Domke, NIPS (2015), 2989-2997

Acknowledgements