On the convergence of the HMC algorithm and NUTS sampler.

Samuel Gruffaz

Introduction to the recent paper :
« On the convergence of dynamic implementations of Hamiltonian Monte Carlo and No U-Turn Samplers »,
Alain Durmus, Samuel Gruffaz, Miika Kailas, Eero Saksman, Matti Vihola, July- 2023

18/09

Introduction

1. Motivations and contributions.
2. Hamiltonian Monte Carlo (HMC) and the NUTS intuition.
3. Dynamic HMC algorithms.

Introduction

Bayesian Computational goals :

Compute $\int f \, \mathrm{d}\pi$, denoting by f a test function and π a target distribution.

Monte Carlo (MC) :

Markov Chain Monte Carlo (MCMC) :

Metropolis Hasting algorithm (MH) :

Hamiltonian Monte Carlo (HMC) :
[Duane and al, 1987]

State of the art

No U-Turn Sampler (NUTS) :
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Hamiltonian Monte Carlo (HMC) : [Duane and al, 1987]

Given the the target **potential** $U = -\log \pi$ and its gradient ∇U,
a *stepsize* h and a *number of steps* T,
define $\tilde{\mathrm{K}}_{h,T}$ by integrating a system of
Hamiltonian equations using the **leapfrog** integrator.

State of the art

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State of the art
No U-Turn Sampler (NUTS) :
[Hoffman and al, 2011]

Given $(U, \nabla U)$ and a stepsize h, define $\mathrm{K}_h^{\mathrm{U}}$ the NUTS kernel .

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NUTS is used in **PyMC3**, **Stan** and **Turing**, widely used software for Bayesian computational statistics.

Other libraries use Gibbs sampling for its flexibility. (BUGS, JAGS)

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OK, in practice, everyone use **NUTS** when it is possible, but why does it work well ?

Litterature on the qualitative properties of HMC and NUTS.

Qualitative property	π-invariance $\int K(x,.)d\pi = \pi$	Ergodicity $\lim_{n\to\infty} \|\|K^n(x,\cdot) - \pi\|\|_{TV} = 0,$	Geometric ergodicity $\|\|K^n(x,\cdot) - \pi\|\|_{\mathscr{V}} = O(\rho^n), \quad \rho < 1$
HMC T is fixed	✓ [Duane and al, 1987]	✓ [Durmus and al, 2017]	✓ [Durmus and al, 2017]
NUTS T varies	✓ ↻ Appendix of [Betancourt, 2017] Not reviewed	?	?

Our contributions on the qualitative properties of HMC and NUTS.

Qualitative property	π-invariance $\int \mathrm{K}(x,.)\mathrm{d}\pi = \pi$	Ergodicity $\lim_{n\to\infty} \|\|\mathrm{K}^n(x,\cdot) - \pi\|\|_{TV} = 0,$	Geometric ergodicity $\|\|\mathrm{K}^n(x,\cdot) - \pi\|\|_{\mathscr{V}} = O(\rho^n), \quad \rho < 1$
HMC T is fixed	✓ [Duane and al, 1987]	NEW ! ✓ **Without bounding the stepsize** [Durmus and al, 2023]	✓ [Durmus and al, 2017]
NUTS T varies	✓ Appendix of [Betancourt, 2017] Not reviewed NEW ! + **give a proof with a general formalism** [Durmus and al, 2023]	NEW ! ✓ **By bounding the stepsize h and the HMC's assumptions on U, or without bounding the stepsize with more stringent regularity conditions on U.** [Durmus and al, 2023]	NEW ! ✓ **Conditions of the ergodicity + Conditions of HMC geometric ergodicity** [Durmus and al, 2023]

Why this paper was not done before ?

1

The study of NUTS is highly technical.
We introduce a general formalism and explicit expressions.

2

NUTS relies on a stopping time $(q_0, p_0) \in (\mathbb{R}^d)^2 \mapsto S(a, q_0, p_0)$.
Its regularity is hard to analyze.

3

Theoretical properties are not very attractive.
We try to stick to the practical situation framework.

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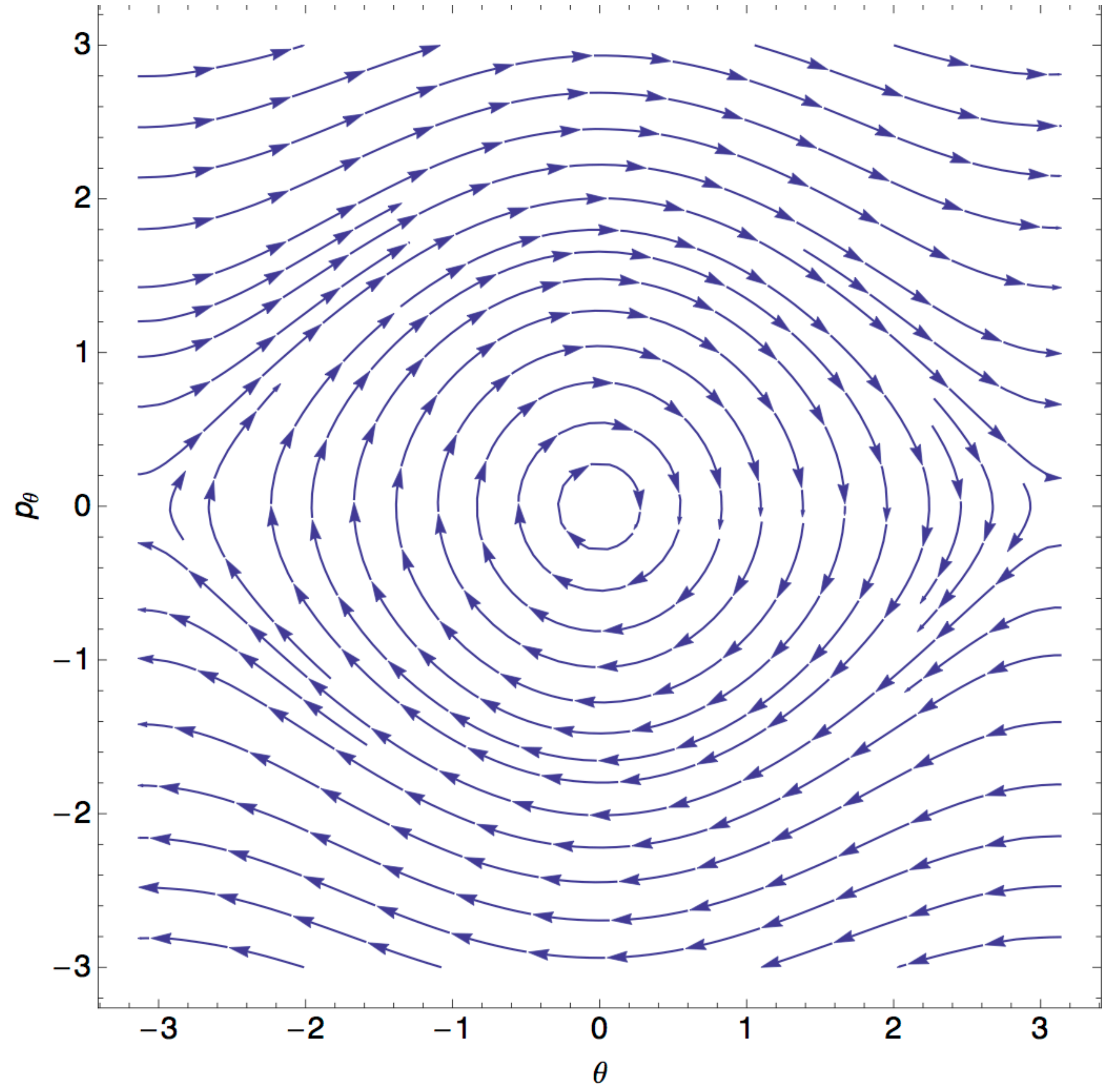
Hamiltonian Monte Carlo

Define **potential energy** $U(q) = -\log(\pi(q))$ and **Hamiltonian** $H(q,p) = U(q) + p^\top p/2$ for any $(q,p) \in (\mathbb{R}^d)^2$.

Hamiltonian dynamics $(q(t), p(t)) \in (\mathbb{R}^d)^2$, for any $t \geq 0$.

$$\frac{dq(t)}{dt} = \nabla_p H(q(t), p(t)) = p(t)$$

$$\frac{dp(t)}{dt} = -\nabla_q H(q(t), p(t)) = -\nabla U(q(t))$$



Hamiltonian dynamics related to a pendulum.

HMC algorithm (h, T)

At iteration t, Markov chain at state X_t :

1. Sample $P_0 \sim \mathcal{N}(0_d, I_d)$ and set $\big(q(0), p(0)\big) = \big(X_t, P_0\big)$
2. Solve dynamics over time lengths T with the **leapfrog integrator using** (h, T) to get $\Phi_h^{(T)}(X_t, P_0) = \big(q_T, p_T\big)$.

(MH) 3. Sample $U^* \sim \mathcal{U}([0,1])$. If $U^* \leq \min\left\{1, \exp\left[H(q_0, p_0) - H(q_T, p_T)\right]\right\}$, set $X_{t+1} = q_T$, otherwise set $X_{t+1} = X_t$.

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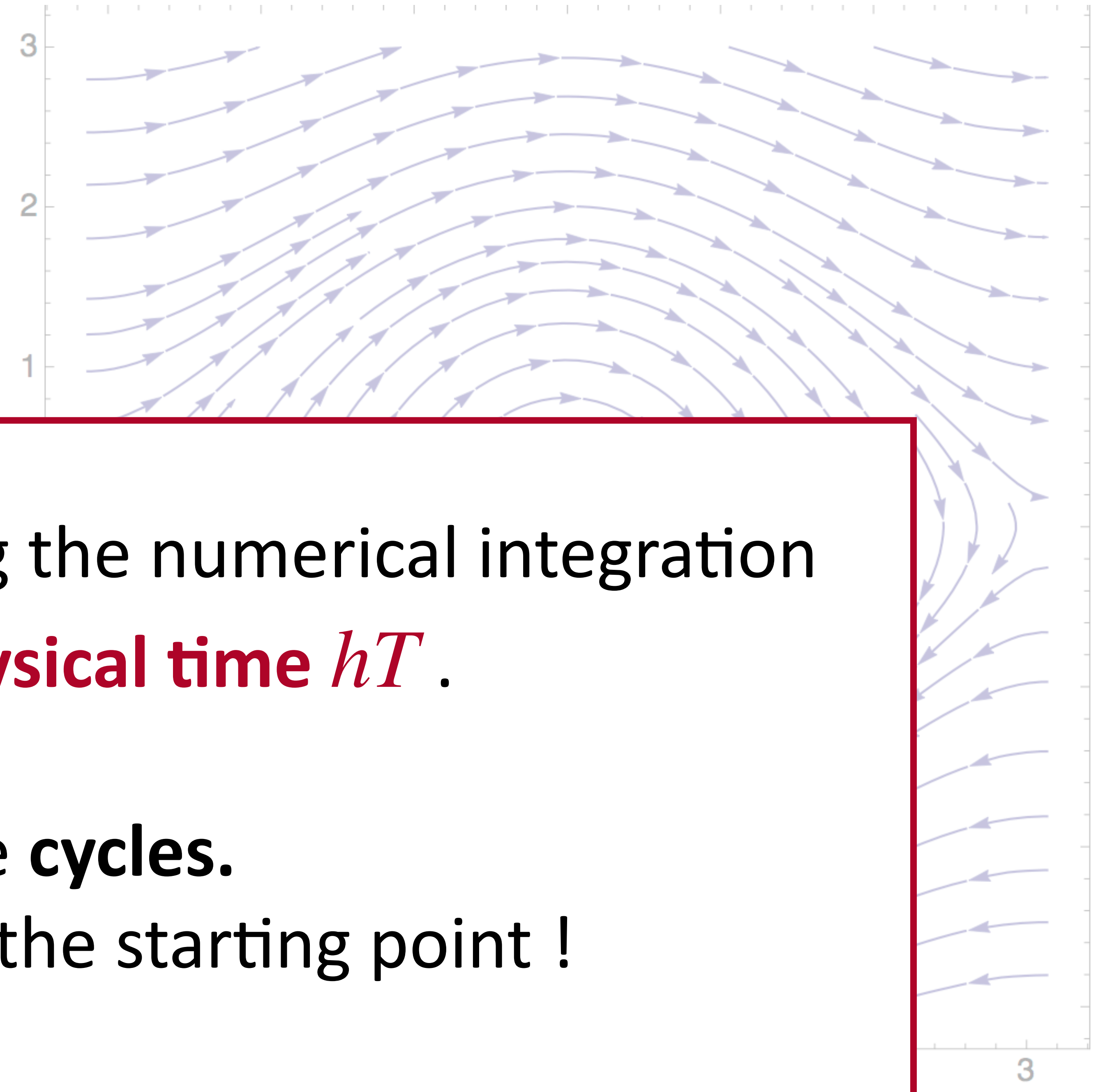

Hamiltonian dy

$\frac{dq(t)}{dt} =$

$\frac{dp(t)}{dt} =$

The **sampler efficiency** related to **the energy loss** during the numerical integration $\left[H(q_0,p_0) - H(q_T,p_T)\right]$ depends on the **physical time** hT .

The Hamiltonian dynamics can create **cycles.**
If T is **too large**, the proposition can be close to the starting point !

How to select h, T ?

HMC algorithm

pendulum.

At iteration t,

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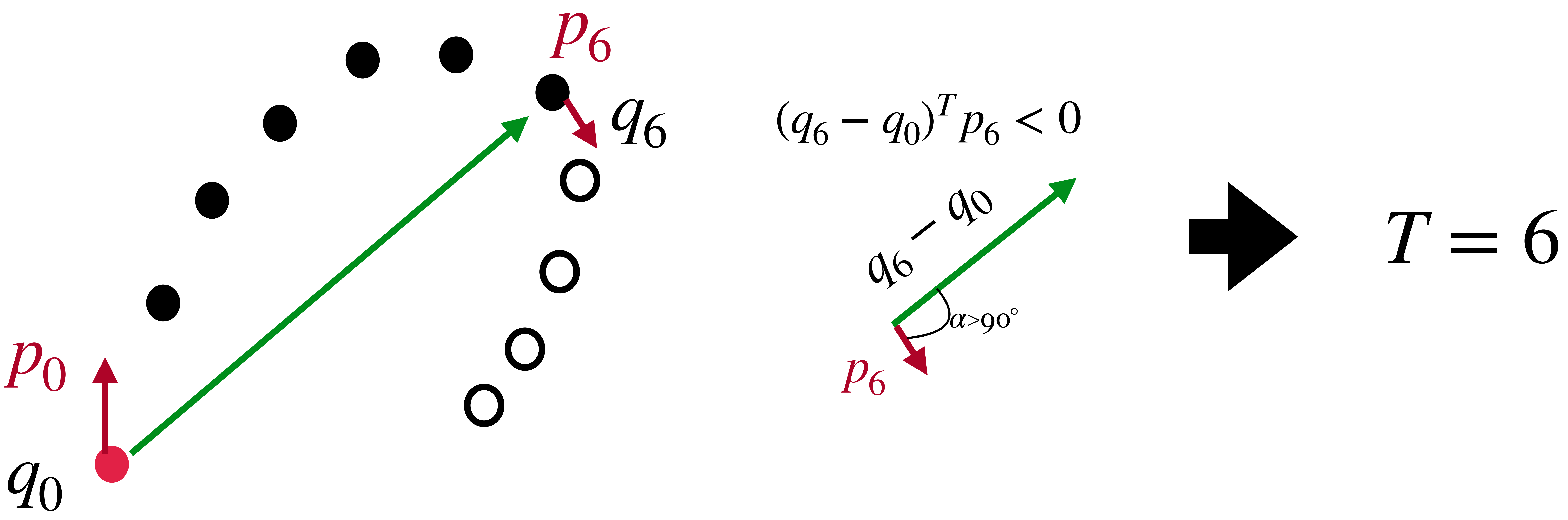
The intuition behind the No U-Turn Sampler.

No U-turn criteria between T_1 and T_2, by denoting $\Phi_h^{(j)}(q_0, p_0) = (q_j, p_j)$ for any $(q_0, p_0) \in (\mathbb{R}^d)^2$,

$F_{q_0}^{T_1,T_2}(p_0) = (q_{T_2} - q_{T_1})^\top p_{T_1} < 0$ or $(q_{T_2} - q_{T_1})^\top p_{T_2} < 0$.



We can not just take the last point p_6 before the U-turn to have the target invariance !

The intuition behind the No U-Turn Sampler.

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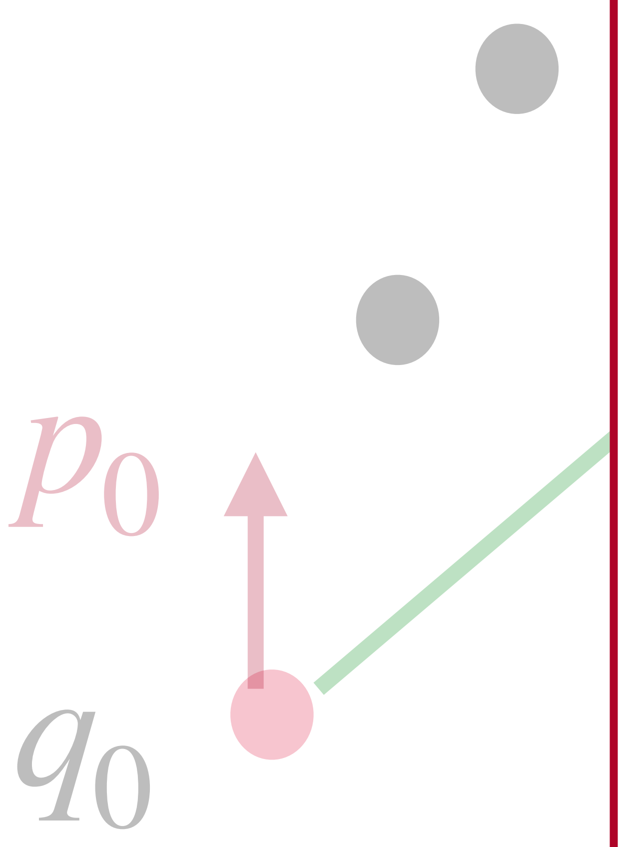

We can not just tak

Stopping time regularity condition :

For any $q \in \mathbb{R}^d$ the following set is dense,

$$\mathsf{F}_{q,-0} = \{p \in \mathbb{R}^d : F_q^{T_1,T_2}(p) \neq 0, T_1, T_2 \in [-2^{K_m} + 1 : 2^{K_m} - 1]^2, T_1 \neq T_2\}$$

A more « human » condition to satisfy the previous one :

∇U is L-lypschitz and the stepsize is bounded by $C/(L2^{K_m})$ with $C > 0$.

or

π is gaussian and the stepsize is in $\mathbb{R}_+^* \backslash \mathscr{H}$ with $\mathscr{H}$ countable.

or

U is real-analytic and $\lim_{|q| \to \infty} |\nabla^2 U(q)| = 0$

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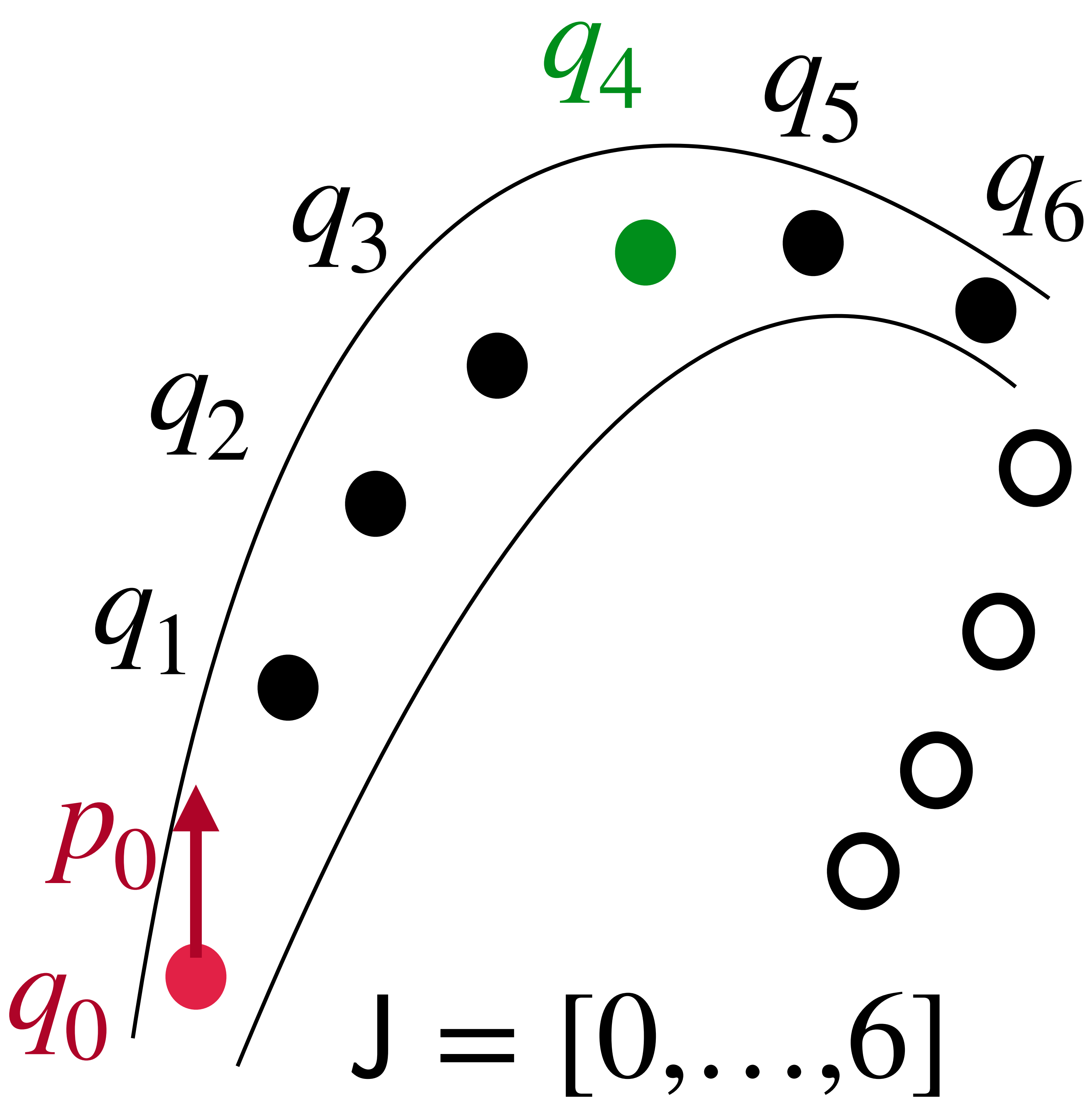
Introduction of Dynamic HMC kernels

1. Let $h > 0$, $K_m \in \mathbb{N}$ and let an **orbit selection** kernel be a family of probability distributions on $\mathscr{P}([-2^{K_m}, \ldots, 2^{K_m}])$

$$\{\mathrm{P}_h(\cdot \mid q_0, p_0) : (q_0, p_0) \in (\mathbb{R}^d)^2\}$$

2. Let an **index selection** kernel be a family of probability distributions on $[-2^{K_m}, \ldots, 2^{K_m}]$

$$\{\mathrm{Q}_h(\cdot \mid \mathrm{J}, q_0, p_0) : \mathrm{J} \subset [-2^{K_m}, 2^{K_m}], (q_0, p_0) \in (\mathbb{R}^d)^2\}$$



Dynamic HMC algorithm

Define the Dynamic HMC $(\mathrm{P}_h, \mathrm{Q}_h)$ *as the Markov chain* $(Q_k)_{k\in\mathbb{N}}$ *defined by the following steps that define* Q_{k+1} *given* Q_k *:*

1. *Sample* $P_{k+1} \sim \mathcal{N}(0_d, I_d)$
2. *Sample* $\mathtt{I}_{k+1}$ *with distribution* $\mathrm{P}_h(\,\cdot\,|\,Q_k, P_{k+1})$
3. *Sample* J_{k+1} *with distribution* $\mathrm{Q}_h(\,\cdot\,|\,\mathtt{I}_{k+1}, Q_k, P_{k+1})$
4. *Set* $Q_{k+1} = \mathrm{proj}_1\left\{\Phi_h^{J_{k+1}}(Q_k, P_{k+1})\right\}$, *where*

$\mathrm{proj}_1 : (x, y) \in (\mathbb{R}^d)^2 \mapsto x \in \mathbb{R}^d$

HMC case :

$$\mathrm{P}_h^{\mathrm{HMC}}(\{0,T\} \mid q_0, p_0) = 1$$

$$\mathrm{Q}_h^{\mathrm{HMC}}(\,\cdot\,|\,\{0,T\}, q_0, p_0) = \left(1 \wedge \frac{\tilde{\pi}(\Phi_h^{(T)}(q_0, p_0))}{\tilde{\pi}(q_0, p_0)}\right)\delta_T(\,\cdot\,) + \left(1 - 1 \wedge \frac{\tilde{\pi}(\Phi_h^{(T)}(q_0, p_0))}{\tilde{\pi}(q_0, p_0)}\right)\delta_0(\,\cdot\,)$$

where we denote by $\tilde{\pi}(q, p) \propto \exp(-H(q, p)) = \pi(q) \times \exp(-p^\top p/2)$

Dynamic HMC properties

General expression of the Dynamic HMC kernel for any $\mathsf{A} \in \mathscr{B}(\mathbb{R}^d)$:

$$\mathrm{K}_h(q_0, \mathsf{A}) = \int \mathcal{N}(p; 0_d, I_d)(p_0)\tilde{\mathrm{K}}_h((q_0, p_0), \mathsf{A})\mathrm{d}\, p_0$$

$$\tilde{\mathrm{K}}_h((q_0, p_0), \mathsf{A}) = \sum_{\mathsf{J}\subset\mathbb{Z}} \sum_{j\in\mathsf{J}} \mathrm{P}_h(\mathsf{J}\,|\,q_0, p_0)\mathrm{Q}_h(j\,|\,\mathsf{J}, q_0, p_0)\delta_{\mathrm{proj}_1(\Phi_h^{(j)}(q_0,p_0))}(\mathsf{A})$$

It is **not** a trivial extension of the HMC case $\mathrm{K}_h(q_0, \mathsf{A}) \neq \sum_{j\in\mathbb{Z}} \omega_j(q_0)\, \mathrm{K}_{h,j}^{\mathrm{HMC}}(q_0, \mathsf{A})$

Proposition :

Assume that $(\mathrm{P}_h, \mathrm{Q}_h)$ satisfy the **following equation** for any $(q_0, p_0) \in (\mathbb{R}^d)^2, \mathsf{J} \subset \mathbb{Z}$:

$$\tilde{\pi}(q_0, p_0)\mathrm{P}_h\left(\mathsf{J}\,|\,q_0, p_0\right) = \sum_{j\in\mathbb{Z}} 1_{\mathsf{J}}(0)\tilde{\pi}\left(\Phi_h^{(-j)}(q_0, p_0)\right)\mathrm{P}_h\left(\mathsf{J}+j\,|\,\Phi_h^{(-j)}(q_0, p_0)\right)\mathrm{Q}_h\left(j\,|\,\mathsf{J}+j, \Phi_h^{(-j)}(q_0, p_0)\right)$$

Then, K_h leaves the target measure π invariant

Dynamic HMC properties

General expression of the Dynamic HMC kernel for any $A \in \mathscr{B}(\mathbb{R}^d)$:

Assume,

For any $(q_0, p_0) \in (\mathbb{R}^d)^2$, $\mathsf{J} \subset \mathbb{Z}$ and $-j \in \mathsf{J}$, $\mathrm{P}_h\left(\mathsf{J} + j \,|\, \Phi_h^{(-j)}(q_0, p_0)\right) = \mathrm{P}_h\left(\mathsf{J} \,|\, q_0, p_0\right)$,

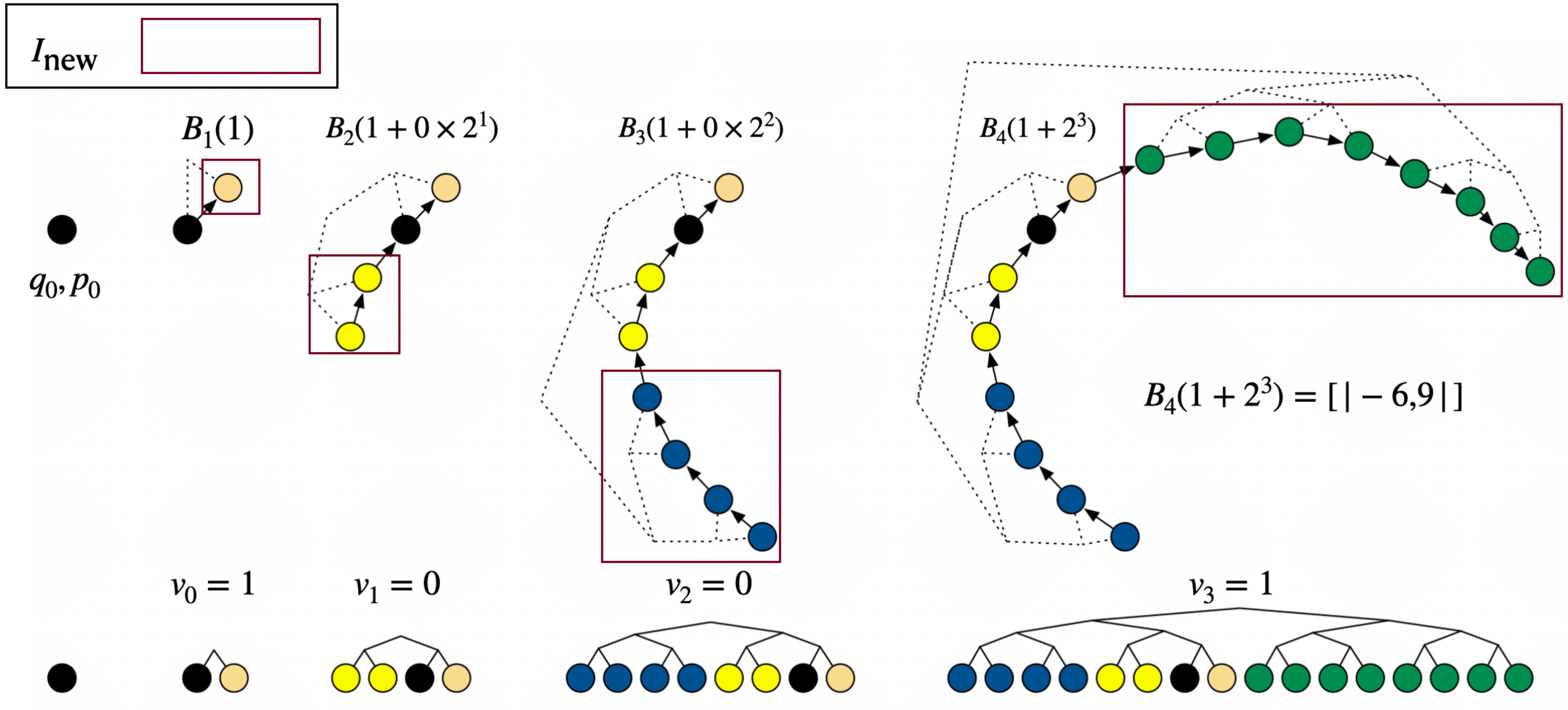
Then, the invariant condition reduces to

$$\tilde{\pi}(q_0, p_0) = \sum_{j \in \mathbb{Z}} 1_{\mathsf{J}}(0) \tilde{\pi}\left(\Phi_h^{(-j)}(q_0, p_0)\right) \mathrm{Q}_h\left(j \,|\, \mathsf{J} + j, \Phi_h^{(-j)}(q_0, p_0)\right)$$

$$\tilde{\pi}(q_0, p_0)\mathrm{P}_h\left(\mathsf{J} \,|\, q_0, p_0\right) = \sum_{j \in \mathbb{Z}} 1_{\mathsf{J}}(0) \tilde{\pi}\left(\Phi_h^{(-j)}(q_0, p_0)\right) \mathrm{P}_h\left(\mathsf{J} + j \,|\, \Phi_h^{(-j)}(q_0, p_0)\right) \mathrm{Q}_h\left(j \,|\, \mathsf{J} + j, \Phi_h^{(-j)}(q_0, p_0)\right)$$

Then, K_h leaves the target measure π invariant

NUTS' orbit selection kernel p_h



Binary tree enable fast practical recursive implementation.

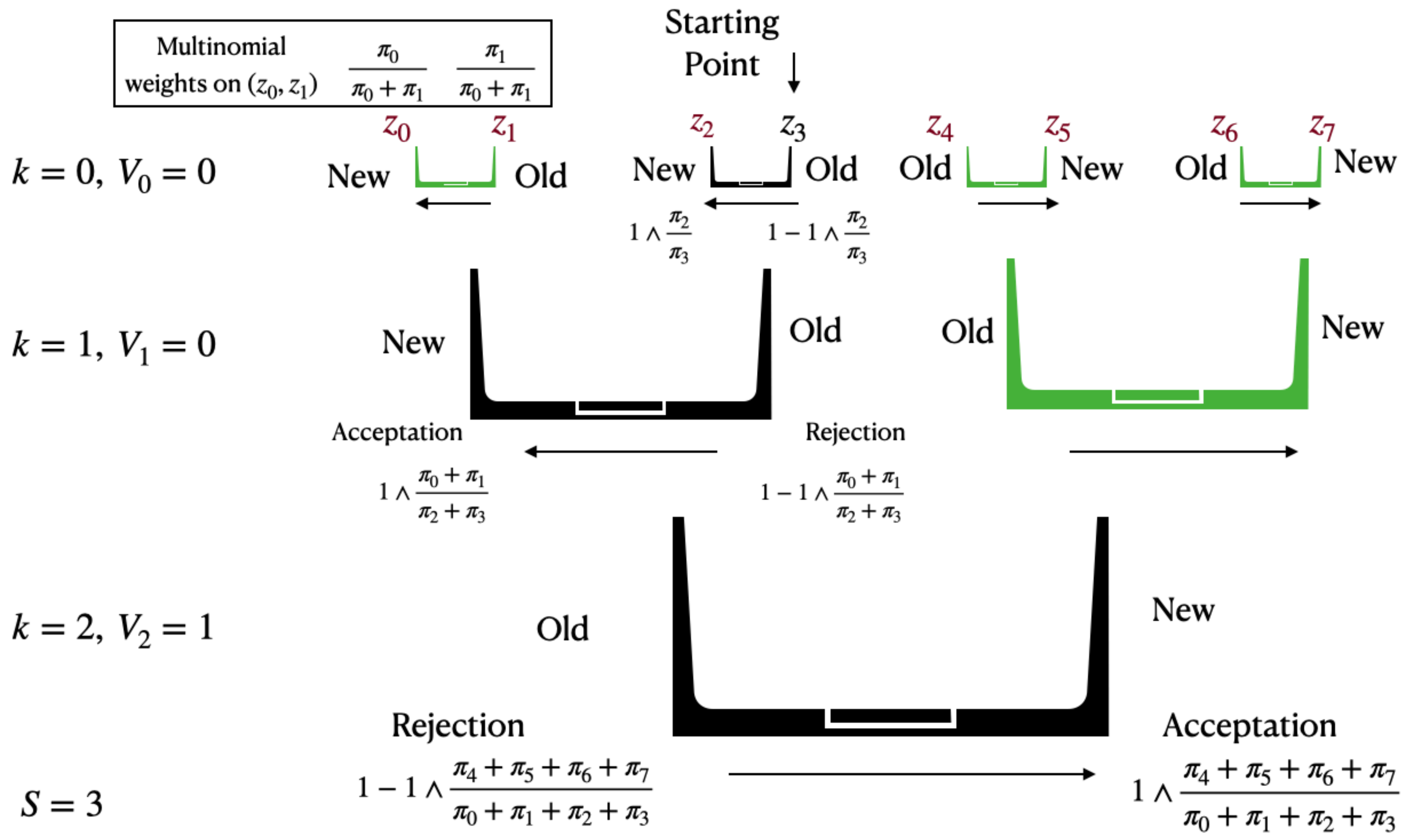
Scheme of the construction of the index set I_f in the Algorithm 1 presented in [Durmus and al, 2023].

Symmetry property : For any $(q_0, p_0) \in (\mathbb{R}^d)^2$, $\mathsf{J} \subset \mathbb{Z}$ and $-j \in \mathsf{J}$, $\mathrm{P}_h\left(\mathsf{J} + j \,|\, \Phi_h^{(-j)}(q_0, p_0)\right) = \mathrm{P}_h\left(\mathsf{J} \,|\, q_0, p_0\right)$

Explicit expression of p_h in the paper.

Thank you again !

NUTS selection kernel q_h .



$$\mathrm{I} = [|0, 2^3-1|] \quad z_0 = q_0, p_0\ ,\ z_i = \Phi_h^i(z_0), i \in \mathrm{I},\ \mathcal{O}_{\mathrm{I}}(z_3) = \{z_0, \ldots, z_7\},\ \pi_i = \tilde{\pi}(z_i)$$

$$\bar{q}_h(3,0\,|\,\mathrm{I}, z_0) = \left(1-1 \wedge \frac{\pi_4+\pi_5+\pi_6+\pi_7}{\pi_0+\pi_1+\pi_2+\pi_3}\right)\left(1 \wedge \frac{\pi_0+\pi_1}{\pi_2+\pi_3}\right)\frac{\pi_0}{\pi_0+\pi_1} \qquad \bar{q}_h(3,3\,|\,\mathrm{I}, z_0) = \left(1-1 \wedge \frac{\pi_4+\pi_5+\pi_6+\pi_7}{\pi_0+\pi_1+\pi_2+\pi_3}\right)\left(1-1 \wedge \frac{\pi_0+\pi_1}{\pi_2+\pi_3}\right)\left(1-1 \wedge \frac{\pi_2}{\pi_3}\right)$$

Litterature on the qualitative properties of HMC and NUTS.

Qualitative property	π-invariance $\int \mathrm{K}(x,.)\mathrm{d}\pi = \pi$	Ergodicity $\lim_{n\to\infty} \|\|\mathrm{K}^n(x,\cdot) - \pi\|\|_{TV} = 0,$	Geometric ergodicity $\|\|\mathrm{K}^n(x,\cdot) - \pi\|\|_{\mathscr{V}} = O(\rho^n), \quad \rho < 1$
HMC	By construction, with the MH mechanism. [Duane and al, 1987]	By assuming U continuously differentiable , ∇U lipschitz and by bounding the stepsize h. [Durmus and al, 2017]	By assuming U to be a gaussian perturbed outside of a compact and by bounding the stepsize h. [Durmus and al, 2017]
NUTS	Less trivial to check, performed in the Appendix of [Betancourt, 2017] Not reviewed	?	?

Our contributions on the qualitative properties of HMC and NUTS.

Qualitative property	π-invariance $\int K(x,.)d\pi = \pi$	Ergodicity $\lim_{n\to\infty} \|\|K^n(x,\cdot) - \pi\|\|_{TV} = 0,$	Geometric ergodicity $\|\|K^n(x,\cdot) - \pi\|\|_{\mathscr{V}} = O(\rho^n), \quad \rho < 1$
HMC	By construction, with the MH mechanism. [Duane and al, 1987]	NEW ! **Without bounding the stepsize, by assuming U to be a gaussian perturbated outside of a compact.** [Durmus and al, 2023]	By assuming U to be a gaussian perturbed outside of a compact and by bounding the stepsize h. [Durmus and al, 2017]
NUTS	Less trivial to check, performed in the Appendix of [Betancourt, 2017] Not reviewed NEW ! + **rewrite a proof with a general formalism** [Durmus and al, 2023]	NEW ! **By bounding the stepsize h and the HMC's assumptions on U, or without bounding the stepsize with more stringent regularity conditions on U.** [Durmus and al, 2023]	NEW ! **Conditions of the ergodicity + Conditions of HMC geometric ergodicity** [Durmus and al, 2023]

Hamiltonian Monte Carlo

HMC algorithm (h, T)

At iteration t, Markov chain at state X_t :

1. Sample $p_0 \sim \mathcal{N}(0_d, I_d)$ and set $q_0 = X_t$
2. **Leapfrog integrator**: define for any $l = 0,\ldots, T-1$,

   $$\Phi_h^{(1)} = (\Psi_{h/2}^{(1)} \circ \Psi_h^{(2)} \circ \Psi_{h/2}^{(1)}), \quad \Phi_h^{(l+1)} = \Phi_h^{(1)} \circ \Phi_h^{(l)},$$

   $$\Psi_t^{(1)}(q,p) = (q, p - t\nabla U(q)),$$

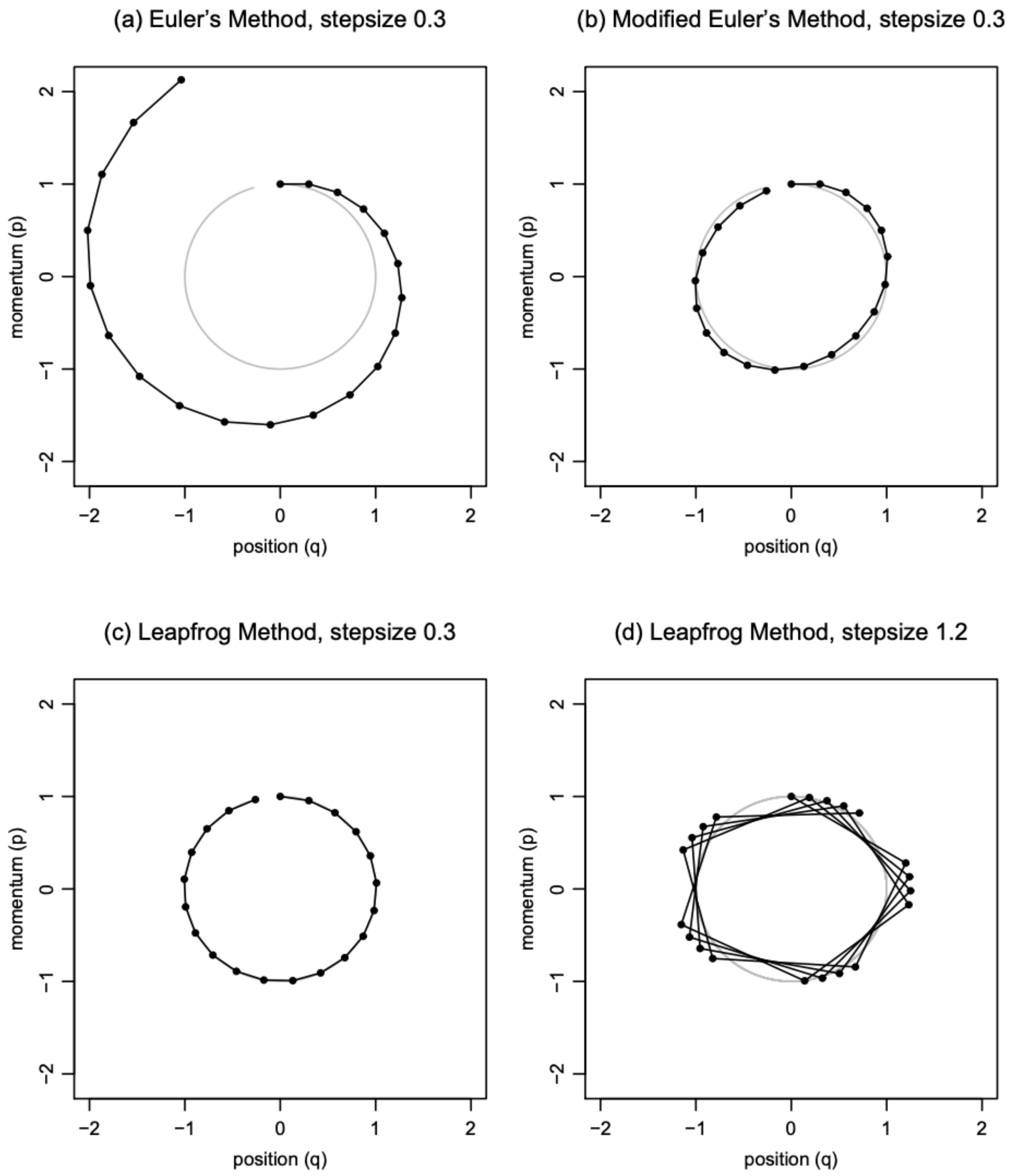
   $$\Psi_t^{(2)}(q,p) = (q + tp, p),$$

   for any $(q,p) \in (\mathbb{R}^d)^2$ and $t \geq 0$.

   Then, set $(q_T, p_T) = \Phi_h^{(T)}(q_0, p_0)$.
3. Sample $U^* \sim \mathcal{U}([0,1])$

   If $U^* \leq \min\left\{1, \exp\left[H(q_0, p_0) - H(q_T, p_T)\right]\right\}$

   Set $X_{t+1} = q_T$, otherwise set $X_{t+1} = X_t$.



Comparison of the Euler types and Leapfrog methods on the Gaussian case.